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

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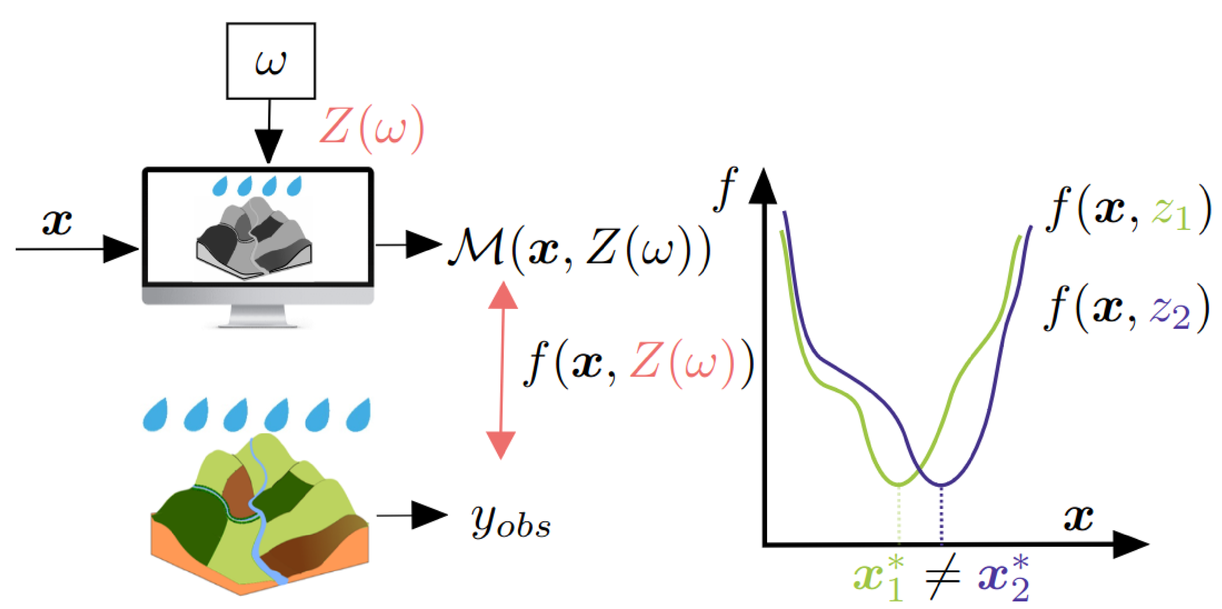
Uncertainty quantification in decision support for water quality

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)

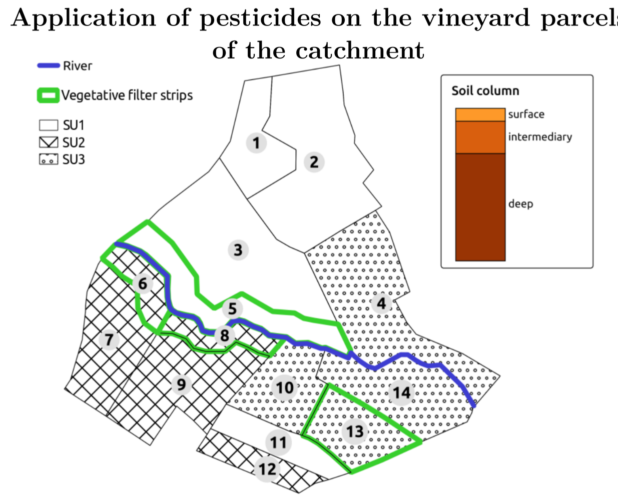


Uncertainty in forcings is propagated to:

- 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

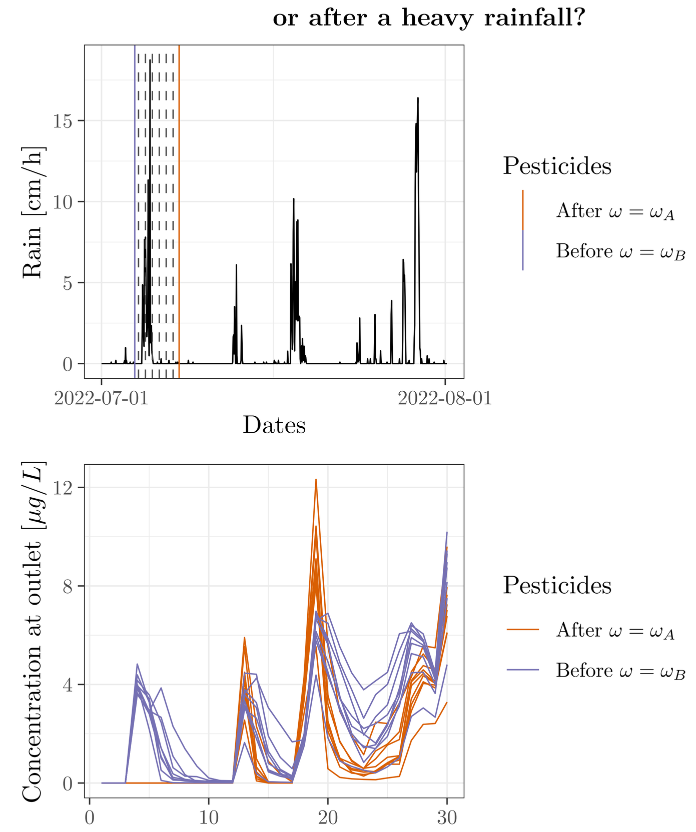
Application of pesticides on the vineyard parcels of the catchment



- ✓ 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]

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

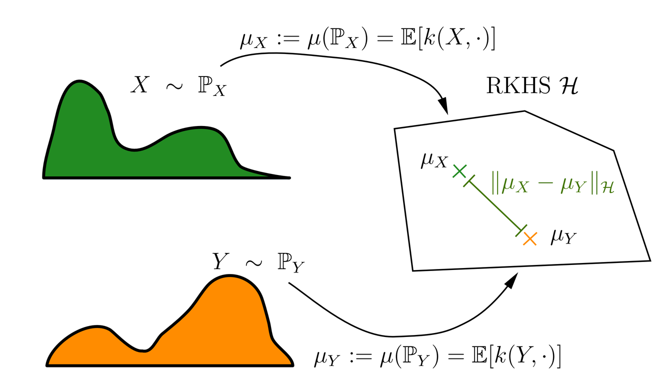


2-steps GSA

❶ Screening with HSIC independence test

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

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

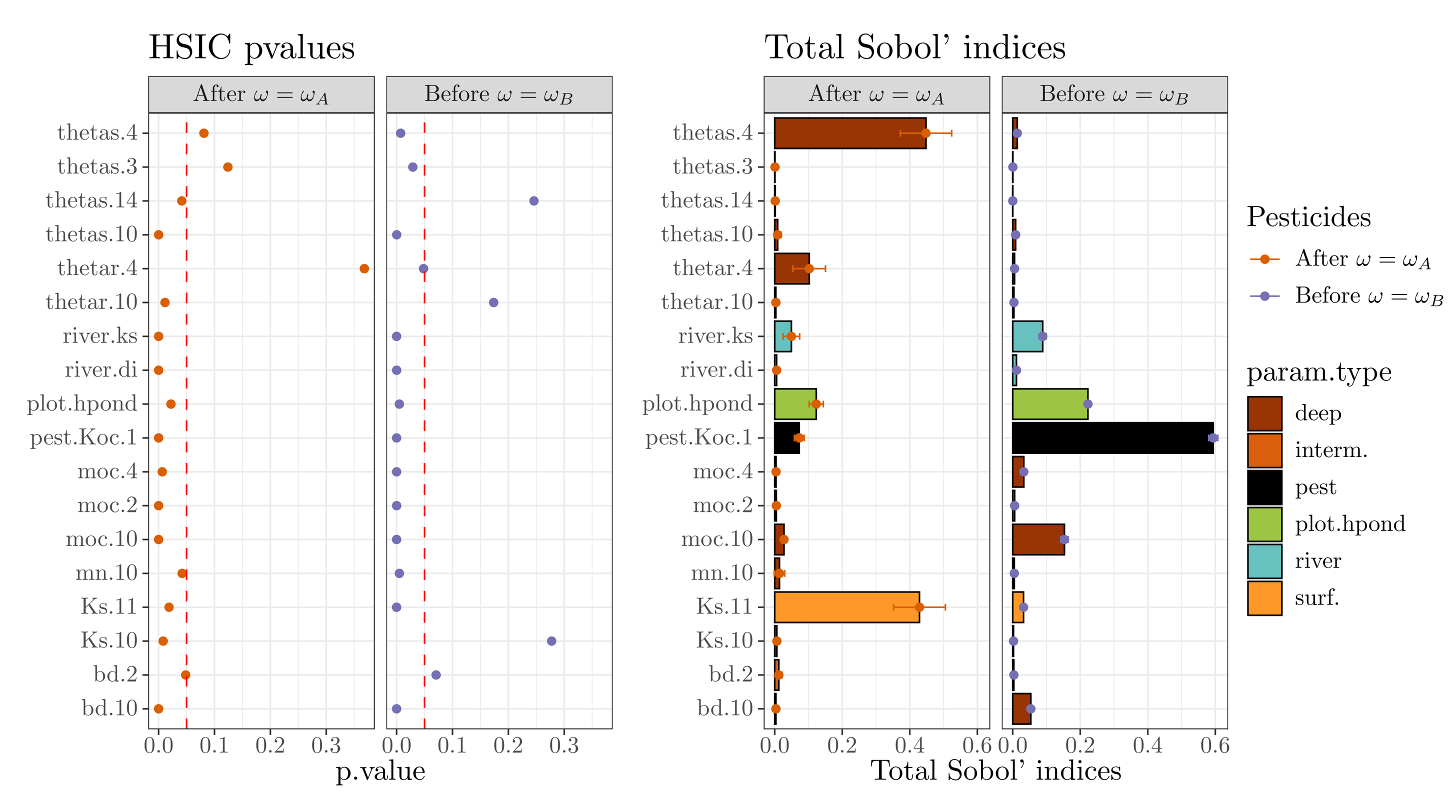


HSIC indices, ©Guerlain Lambert

❷ Sobol' indices with Polynomial Chaos Exp.

$$\begin{aligned} Y &= f_d(\boldsymbol{X}) \approx f_{PCE}(\boldsymbol{X}) = \sum_{\alpha\in\mathcal{A}} c_{\alpha}\psi_{\alpha}(\boldsymbol{X}), \\ \hat{S}_i &= \sum_{\alpha\in\mathcal{A}_i} c_{\alpha}^2/\hat{D}, \quad \mathcal{A}_i = \{\alpha \in \mathcal{A} : \alpha_i > 0, \alpha_{j\neq i} = 0\}, \\ \hat{S}_{T_i} &= \sum_{\alpha\in\mathcal{A}_{T_i}} c_{\alpha}^2/\hat{D}, \quad \mathcal{A}_{T_i} = \{\alpha \in \mathcal{A} : \alpha_i > 0\}, \\ \hat{D} &= \text{Var}\Big[\sum_{\alpha\in\mathcal{A}} c_{\alpha}\psi_{\alpha}(\boldsymbol{X})\Big] = \sum_{\substack{\alpha\in\mathcal{A} \\ \alpha\neq\{0\}}} c_{\alpha}^2 \end{aligned} \tag{2}$$

Sensitivity in two contrasting scenarios



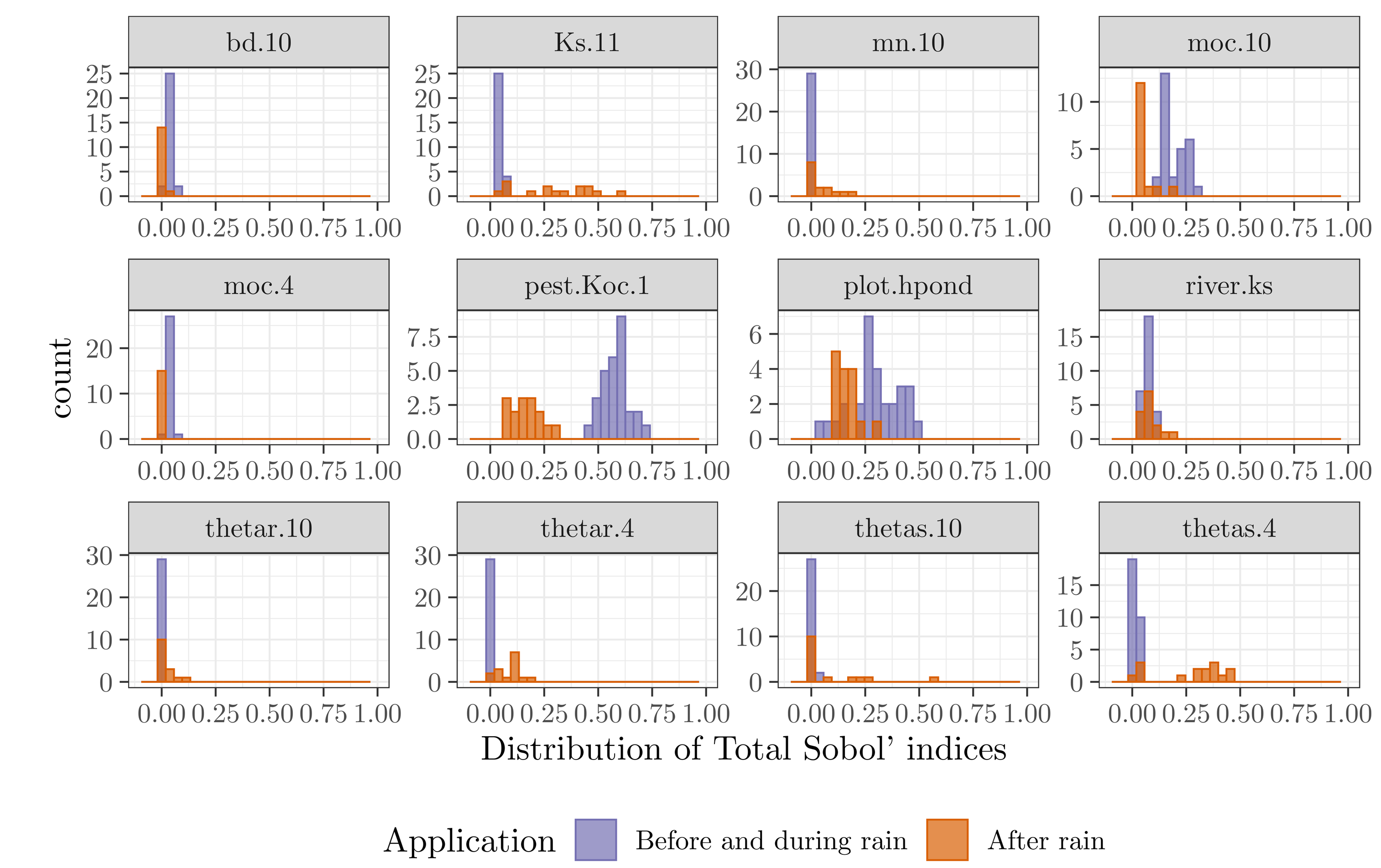
- The HSIC identifies 28 influential parameters on 150
- The Sobol' indices for the 28 parameters are calculated
- **GSA results are different in the two cases**

⇝ 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.ress.2007.04.002 [5] Gretton et al., 2005 10.5555/1046920.1194914 [6] Lüthen et al., 2023 10.1016/j.cma.2022.115875

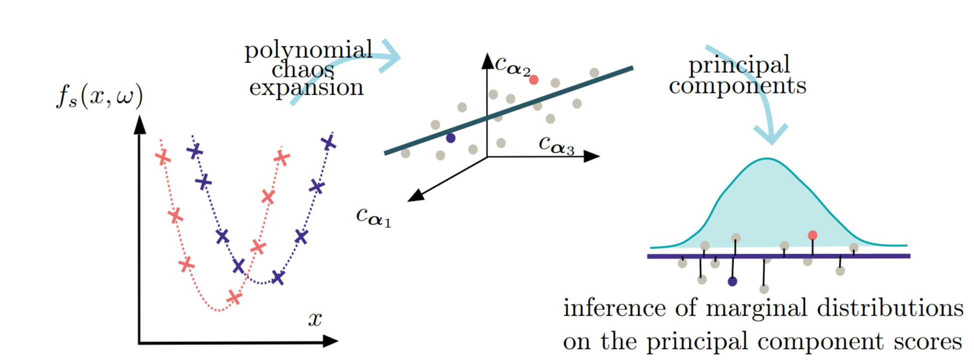
A more global approach: Sobol' indices as random variables



- ✓ 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 infering distrib.of the coeff. such as KDE, GMM, Principal Curve Analysis in 3D on the PCs