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# Sensitivity analysis with external stochastic forcings : application to a water and pesticide transfer model

Katarina Radišić<sup>1,2</sup>

Claire Lauvernet<sup>1</sup>, Arthur Vidard<sup>2</sup>

<sup>1</sup>INRAE, RiverLy, Lyon-Villeurbanne

<sup>2</sup>Univ. Grenoble-Alpes, Inria, CNRS, Grenoble-INP, LJK

## Context: PESHMELBA

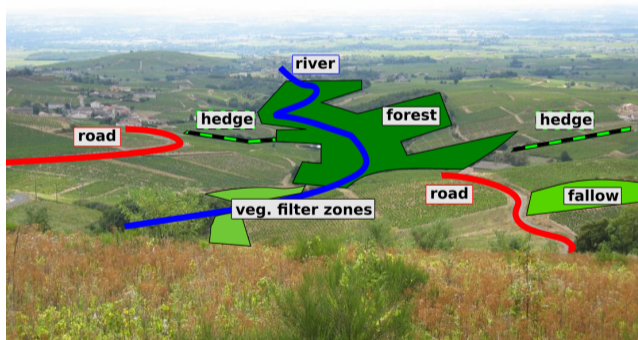
Landscape features speed up or slow down pesticide transfer from the plots to the river.



⇒ The configuration of the catchment can influence the water quality.

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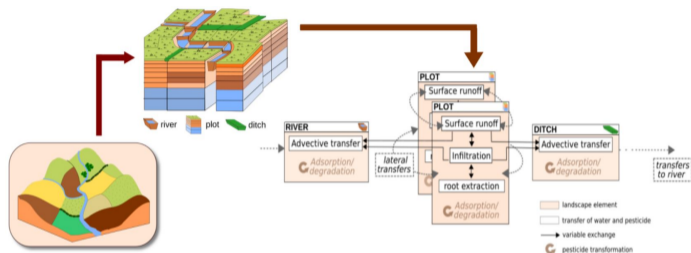
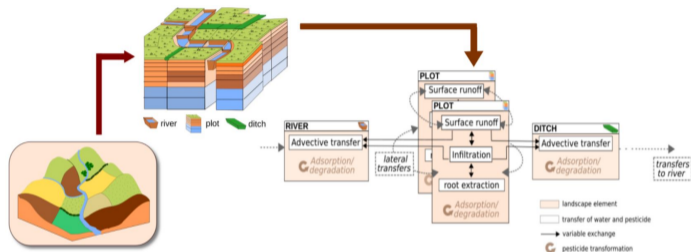


Figure: PESHMELBA<sup>a</sup>, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

<sup>a</sup>Emilie Rouzies et al. (June 2019). “From agricultural catchment to management scenarios: A modular tool to assess effects of landscape features on water and pesticide behavior”. en. In: *Science of The Total Environment* 671, pp. 1144–1160. DOI: 10.1016/j.scitotenv.2019.03.060.

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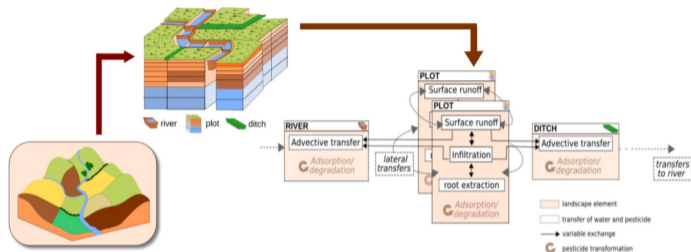


- Not all model parameters can be measured directly

Figure: PESHMELBA<sup>a</sup>, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

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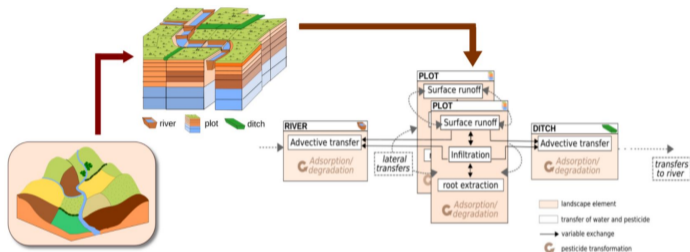


**Figure:** PESHMELBA<sup>a</sup>, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

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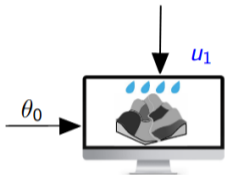
- Impact of external uncertainties on the calibration results



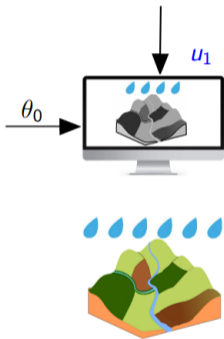


# Context: model calibration

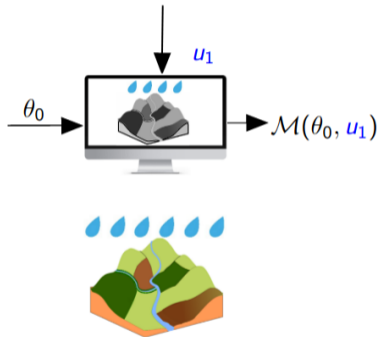
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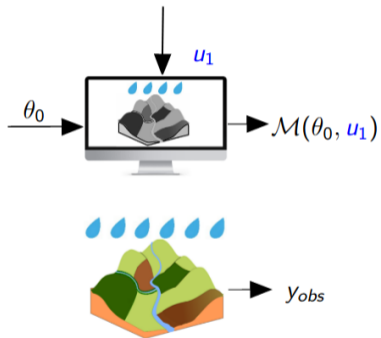
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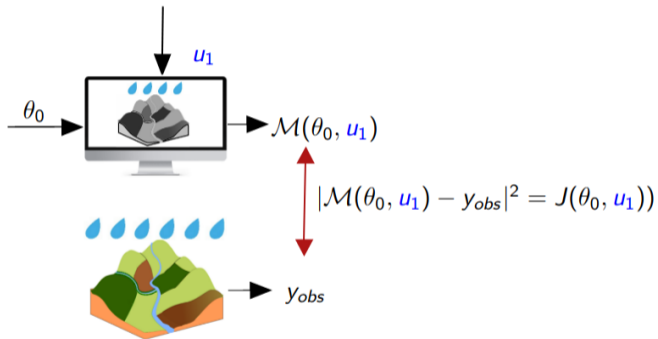
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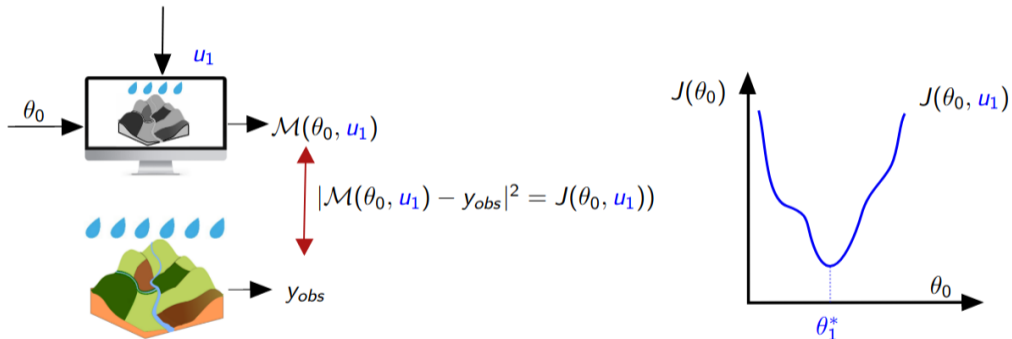
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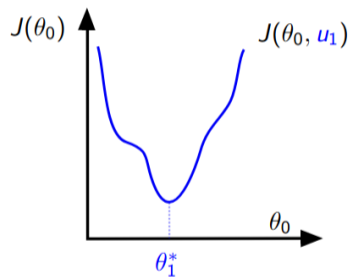
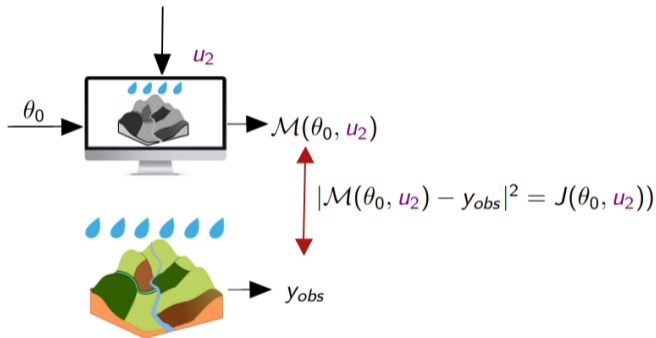
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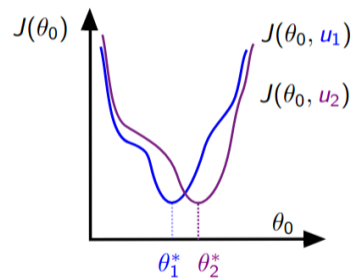
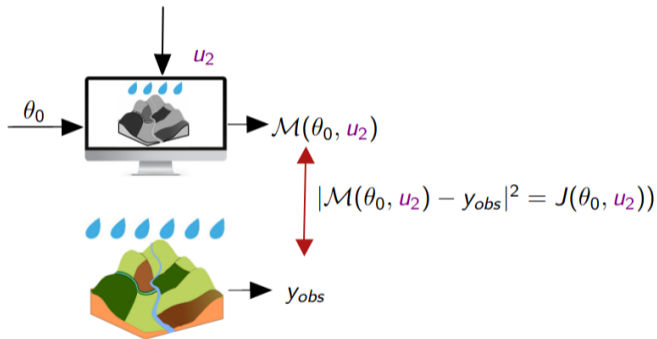


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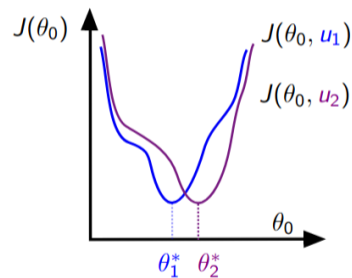
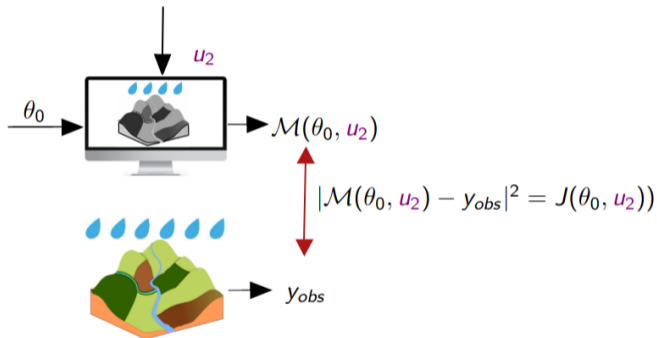




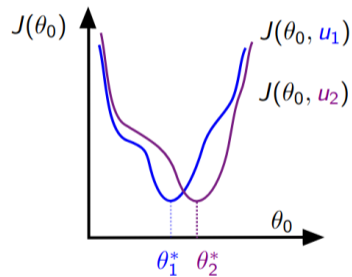
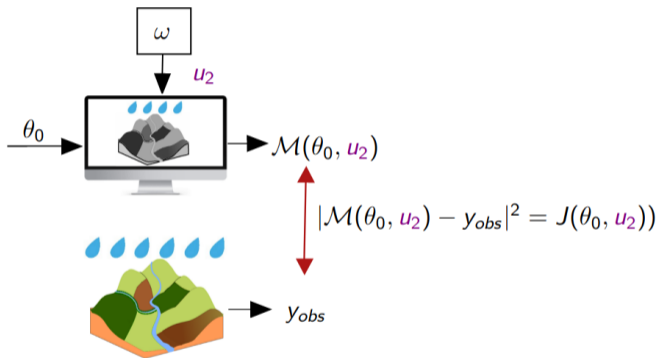
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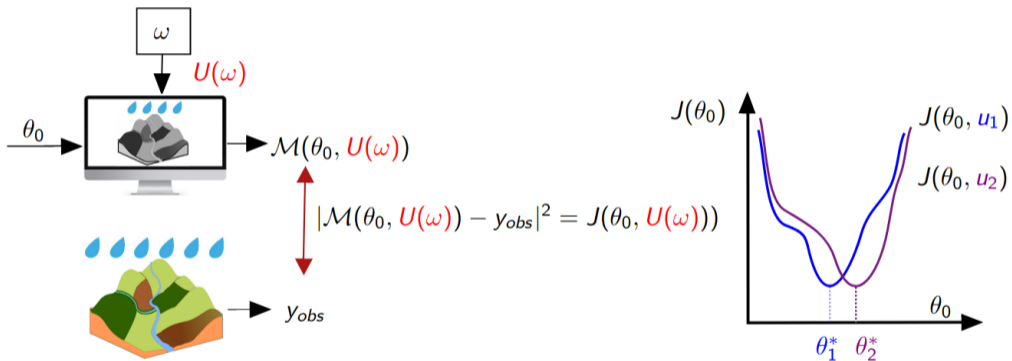
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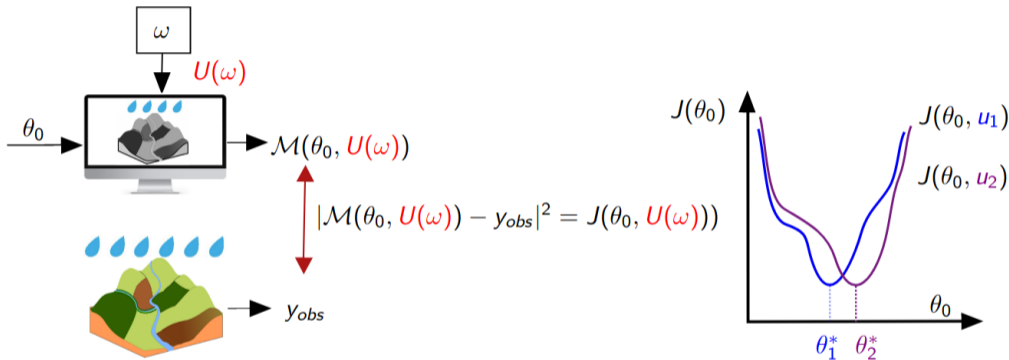
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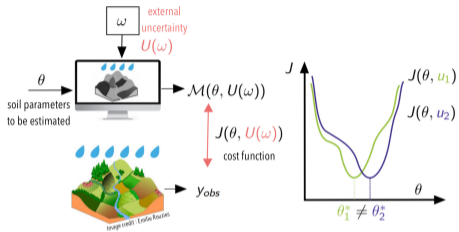


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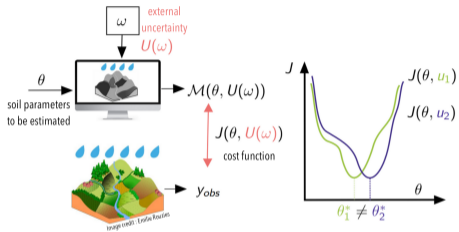
Before passing to calibration: a **sensitivity analysis on the cost function** can provide the information on the **identifiability** of the parameters, (Mai 2023).

# 1. Introduction: Sensitivity analysis



The variability in  $J$  comes from two types of inputs :

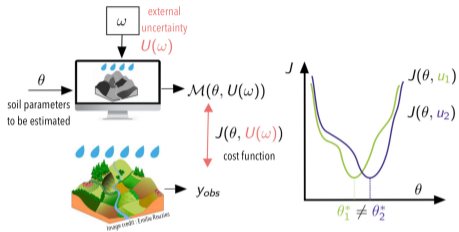
# 1. Introduction: Sensitivity analysis



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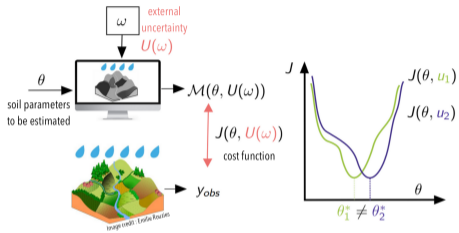


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2. *stochastic* ( $U(\omega)$ ) : external forcing (rain)



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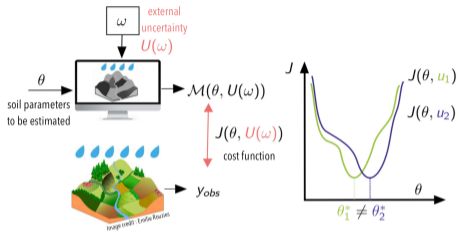


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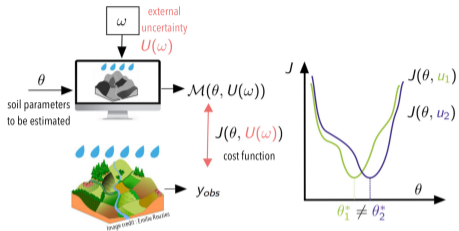
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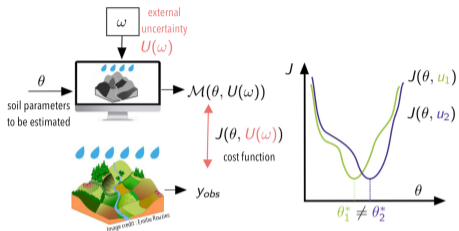
*What is the sensitivity of the output to the parameters, given the uncertainty about the stochastic inputs? (Dell'Oca 2023)*

## 2. Methodology: Sobol' indices as random variables



$$J : \mathcal{D} \times \Omega \rightarrow \mathbb{R},$$
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$$S_i(\omega) = \frac{\text{Var}_{\theta_i} [\mathbb{E}[Y | \theta_i, \omega]]}{\text{Var}[Y | \omega]}$$

Sobol' indices as random variables,<sup>a</sup>.

<sup>a</sup>Hart, Alexanderian, and Gremaud 2017; Jimenez, Le Maître, and Knio 2017; Zhu and Sudret 2021.

Estimation of Sobol' indices with polynomial chaos expansion,<sup>a</sup>:

$$J(\theta) = \sum_{\alpha \in \mathcal{N}^K} c_\alpha \psi_\alpha(\theta) \approx \sum_{\alpha \in \mathcal{A}} c_\alpha \psi_\alpha(\theta)$$

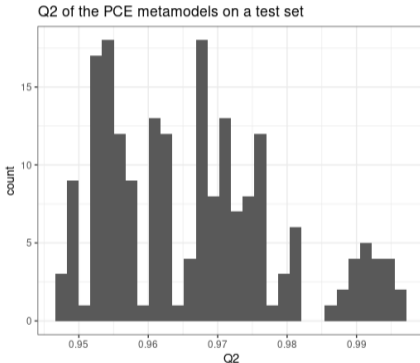
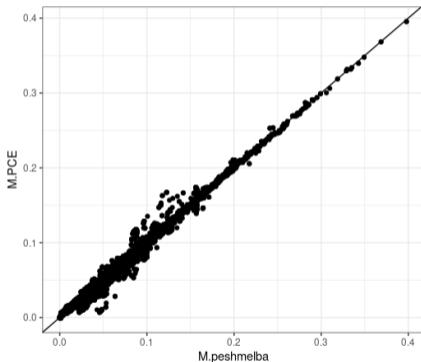
$$\hat{S}_i = \sum_{\substack{\alpha \in \mathcal{A}: \\ \alpha_i > 0, \\ \alpha_{j \neq i} = 0}} c_\alpha^2 / D,$$

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

<sup>a</sup>Sudret 2008; Marelli and Sudret 2014.

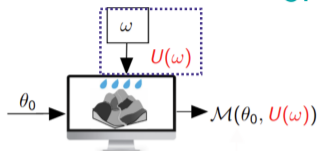
## 2. Methodology: metamodel validation

The  $Q^2$  of the PCE metamodels are calculated on an independent test set for each rain:

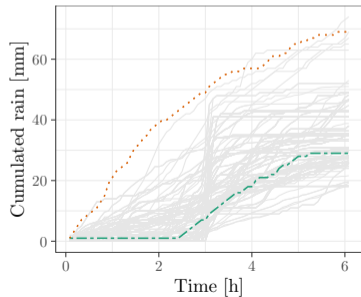


We deem the metamodels a correct approximation of the original and proceed to Sobol' indices calculation.

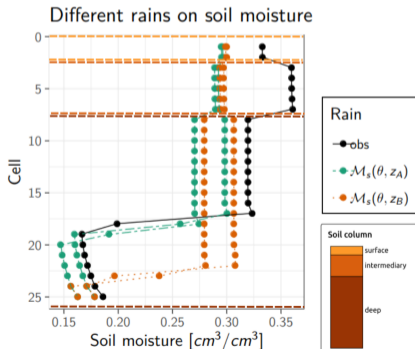
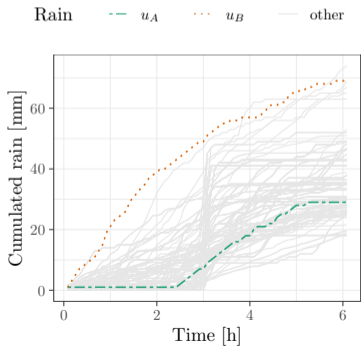
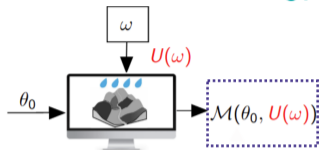
### 3. Case study: moisture profiles



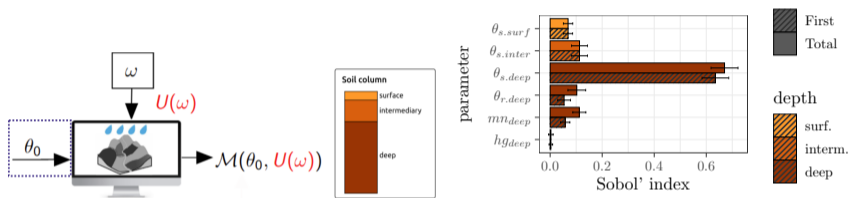
Rain —  $u_A$  —  $u_B$  — other



### 3. Case study: moisture profiles



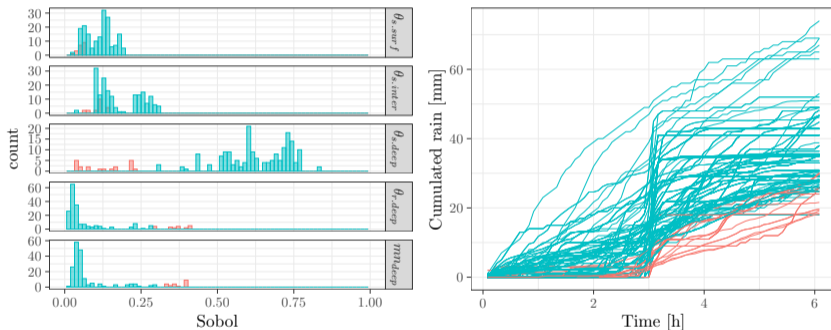
### 3. Case study: Sobol' indices under one rain realization



Name	Definition	Unit	Distribution
$\theta_{s,surf}$	water content at saturation (surface)	$[L^3 L^{-3}]$	$\mathcal{N}(0.3375, 0.0338^2)$
$\theta_{s,inter}$	water content at saturation (intermediary)	$[L^3 L^{-3}]$	$\mathcal{N}(0.3322, 0.0332^2)$
$\theta_{s,deep}$	water content at saturation (deep)	$[L^3 L^{-3}]$	$\mathcal{N}(0.316, 0.0316^2)$
$\theta_{r,deep}$	residual water content (deep)	$[L^3 L^{-3}]$	$\mathcal{N}(0.0612, 0.0153^2)$
$mn_{deep}$	Van Genuchten retention curve parameter (deep)	$[-]$	$\mathcal{N}(0.1791, 0.0179^2)$
$hg_{deep}$	Van Genuchten retention curve parameter (deep)	$[-]$	$\mathcal{N}(-9.69, 0.969^2)$

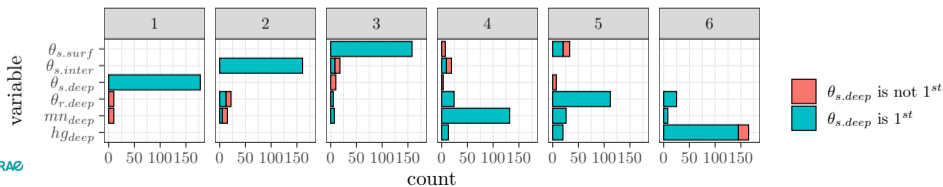
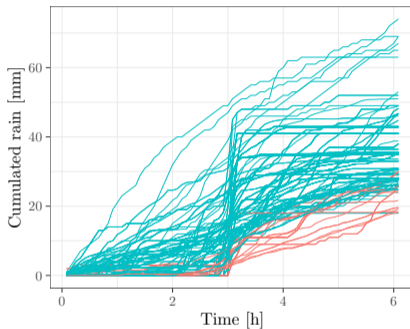
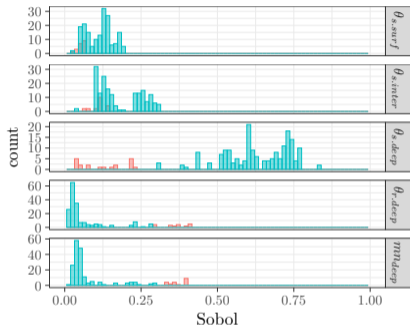


## 4. Results: Sobol' indices depending on rain



Parameter	$\theta_{s.surf}$	$\theta_{s.inter}$	$\theta_{s.deep}$	$mn_{deep}$	$\theta_{r.deep}$	$hg_{deep}$
$\hat{\mu}(S_i^T)$	0.11	0.17	0.58	0.09	0.10	< 0.01
$\hat{\sigma}(S_i^T)$	0.04	0.07	0.19	0.11	0.11	< 0.01

## 4. Results: Sobol' indices depending on rain







## 5. Conclusion:

1. Sobol' indices were obtained for 6 input parameters in 200 different rain realizations.
2. the sensitivity analysis disentangles the variability in the parameters  $\theta$  from the one in the stochastic forcing  $\omega$ .
3. the parameter  $hg$  was found non-identifiable in all rain realizations.
4. the ranking of the input parameters varies depending on  $\omega$





What's next? :

1. other ways of synthesizing information of  $S(\omega)$  ?
2. based on the sensitivity analysis results, implement a robust calibration method
3. study different model outputs, such as transferred pesticide mass.
4. study different stochastic inputs, such as pesticide application dates.

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