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

Katarina Radišić, Claire Lauvernet, Arthur Vidard

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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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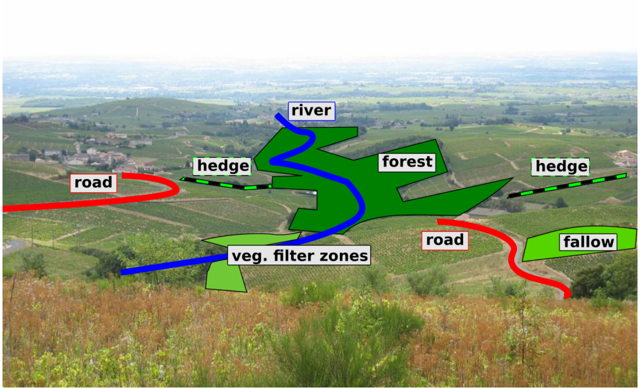

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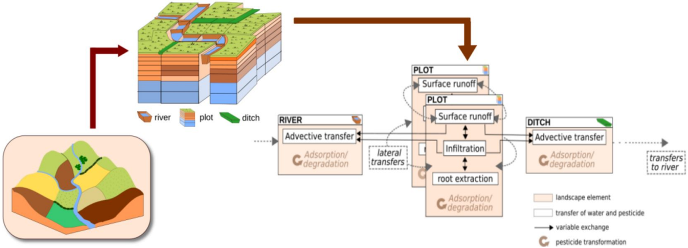

Figure: PESHMELBA[a], a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

[a] 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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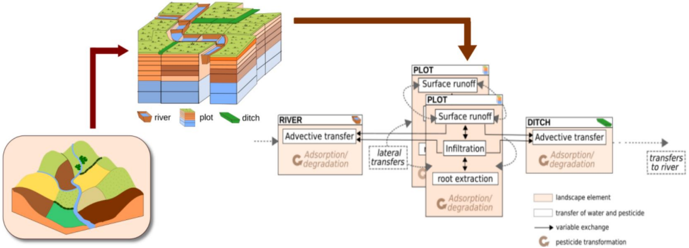

Figure: PESHMELBA[a], a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

- Not all model parameters can be measured directly

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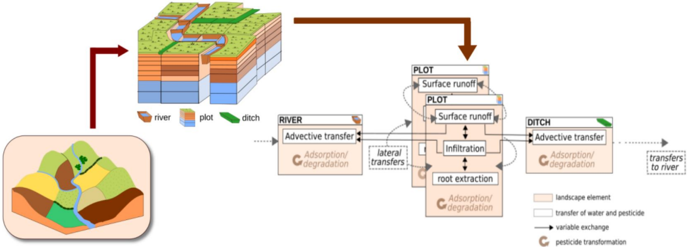

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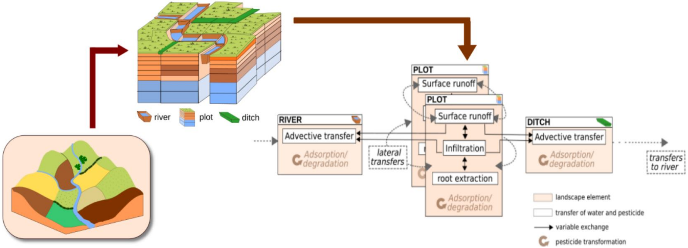

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- Impact of external uncertainties on the calibration results

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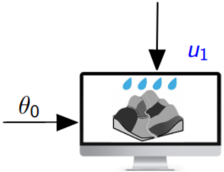

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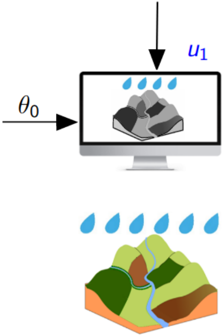

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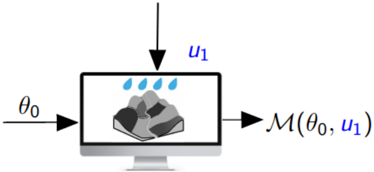

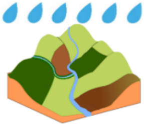

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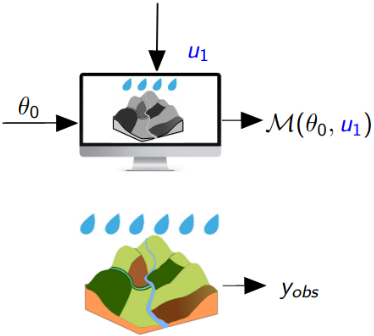

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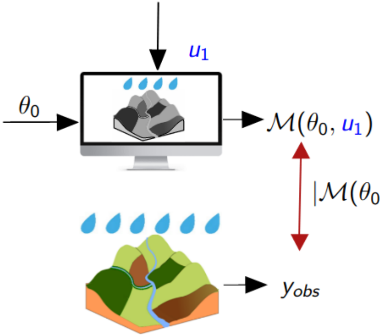

$$|\mathcal{M}(\theta_0, u_1) - y_{obs}|^2 = J(\theta_0, u_1))$$

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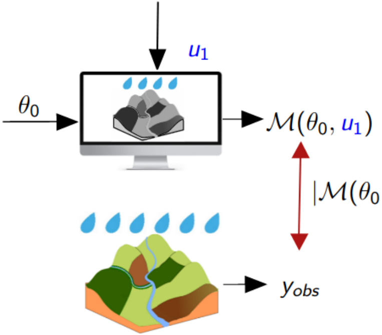

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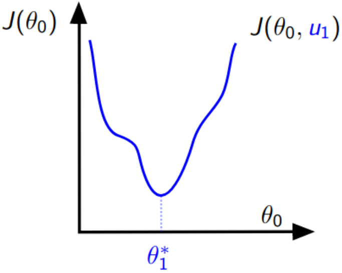

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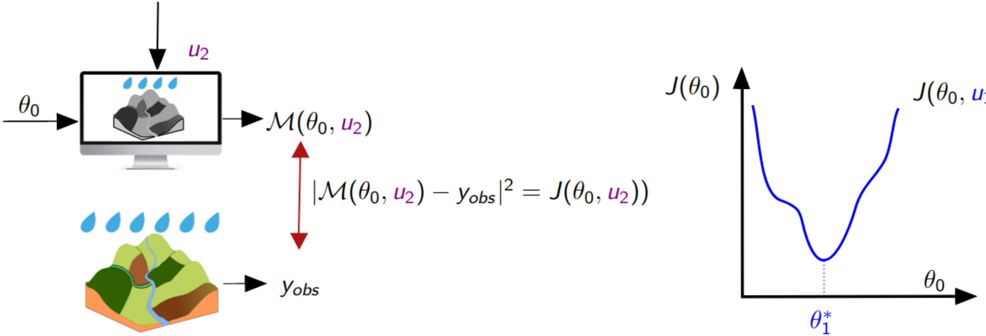

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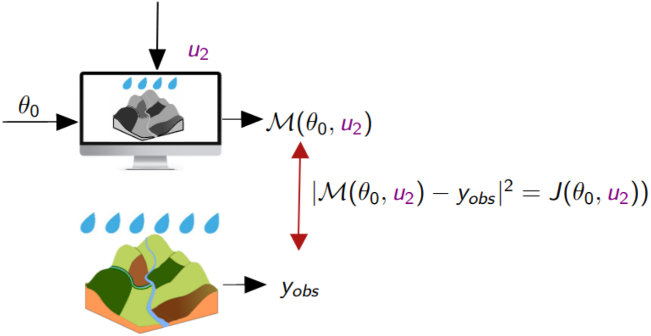

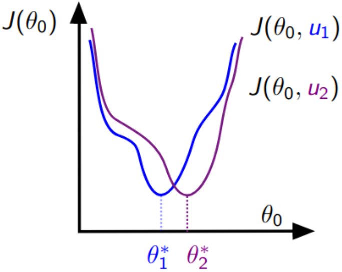

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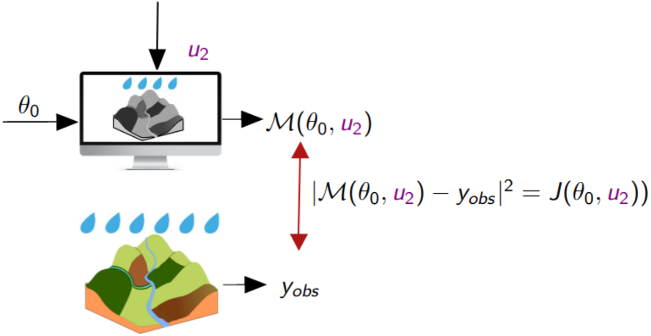

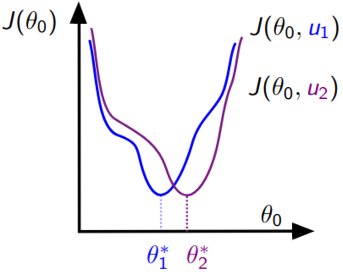

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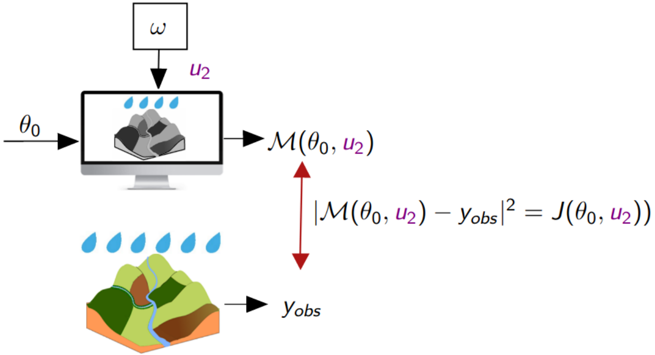

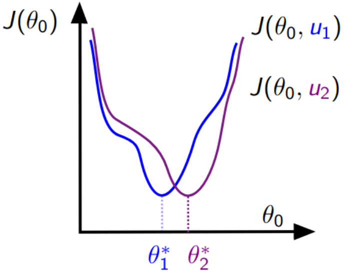

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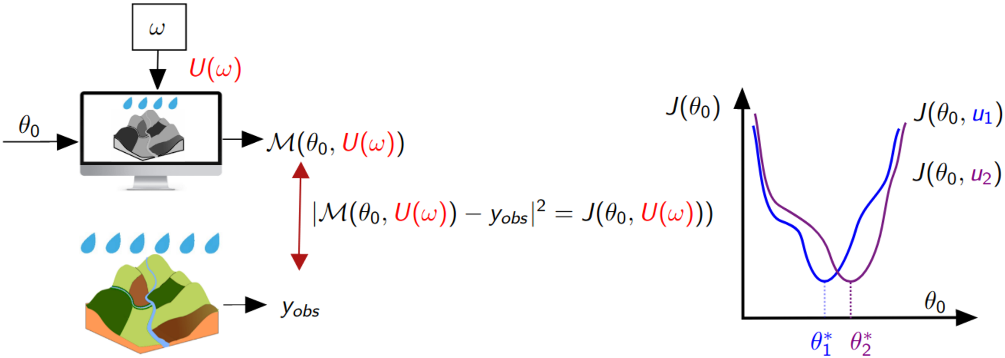

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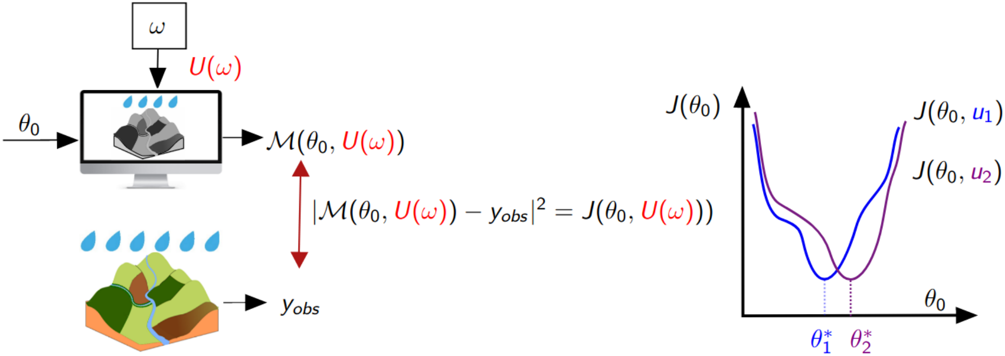
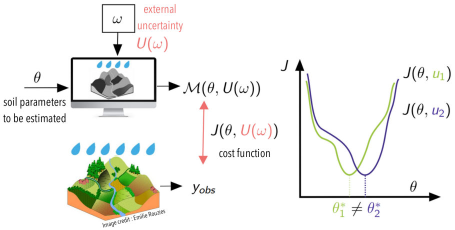


Before passing to calibration: a **sensitivity analysis on the cost function** can provide the information on the **identifiability** of the parameters, (Mai 2023).

1. Introduction: Sensitivity analysis



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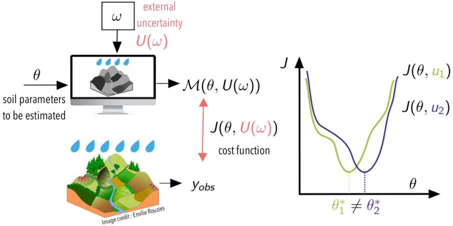

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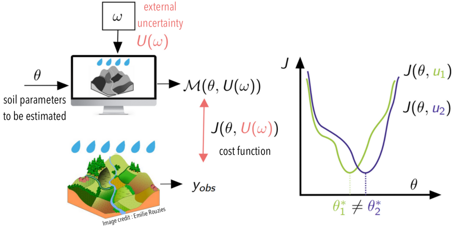

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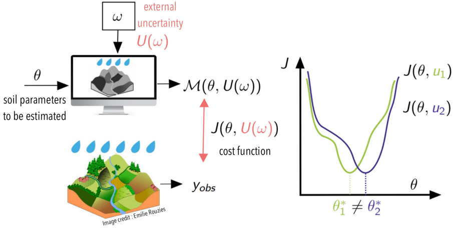

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Only the parameters can be controlled by the modeler.

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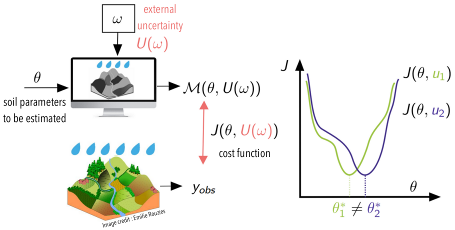

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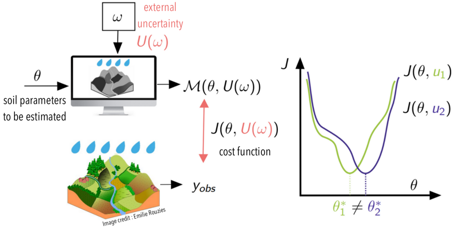
What is the sensitivity of the output to the parameters, given the uncertainty about the stochastic inputs? (Dell'Oca 2023)

2. Methodology: Sobol' indices as random variables



$$
\begin{aligned}
J : \mathcal{D} \times \Omega &\to \mathbb{R}, \\
(\boldsymbol{\theta}, \omega) &\mapsto J(\boldsymbol{\theta}, \boldsymbol{U}(\omega)),
\end{aligned}
$$

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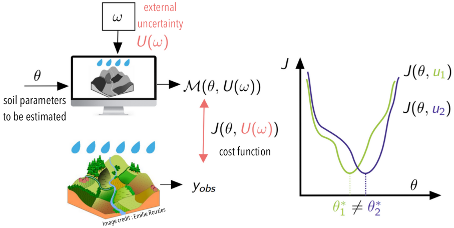


$$J : \mathcal{D} \times \Omega \to \mathbb{R},$$
$$(\boldsymbol{\theta}, \omega) \mapsto J(\boldsymbol{\theta}, \boldsymbol{U}(\omega)),$$

$$S_i(\omega) = \frac{\mathrm{Var}_{\theta_i}\left[\mathbb{E}\left[Y \mid \boldsymbol{\theta}_i, \omega\right]\right]}{\mathrm{Var}[Y|\omega]}$$

Sobol' indices as random variables,[a].

[a]Hart, Alexanderian, and Gremaud 2017; Jimenez, Le Maître, and Knio 2017; Zhu and Sudret 2021.

Estimation of Sobol' indices with polynomial chaos expansion,[a]:

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

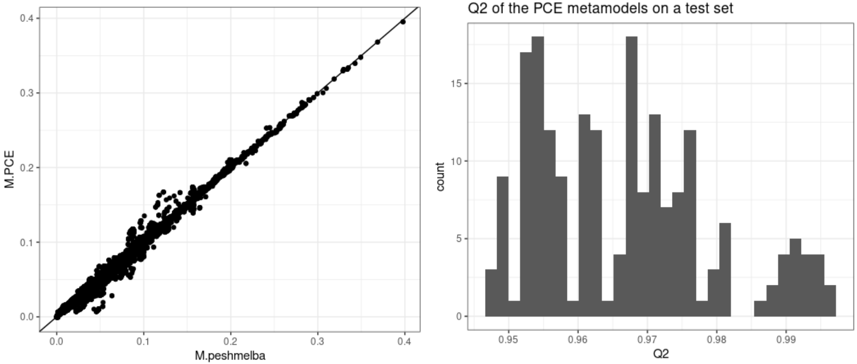
$$\hat{S}_i = \sum_{\substack{\alpha \in \mathcal{A}: \\ \alpha_i > 0, \\ \alpha_{j \neq i} = 0}} {c_\alpha}^2 / D,$$

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

[a]Sudret 2008; Marelli and Sudret 2014.

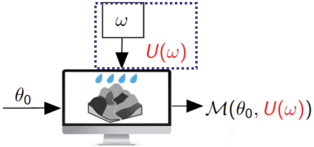
2. Methodology: metamodel validation

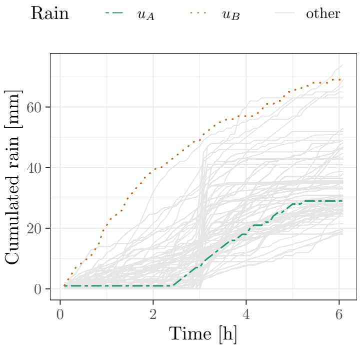
The Q^2 of the PCE metamodels are calculated on an independent test set for each rain:



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

3. Case study: moisture profiles





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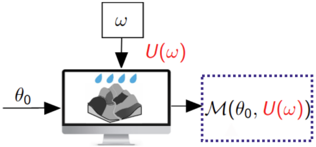
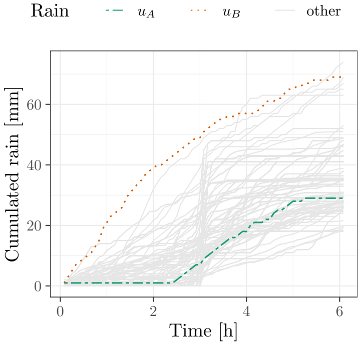
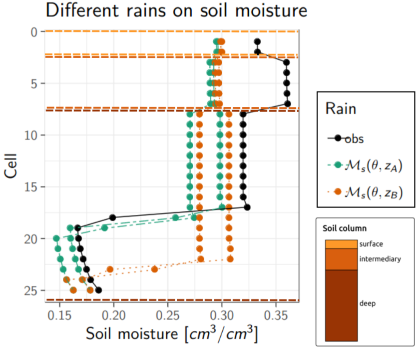
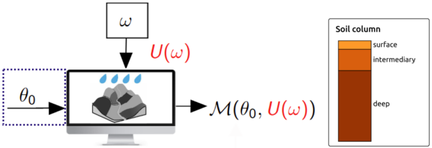
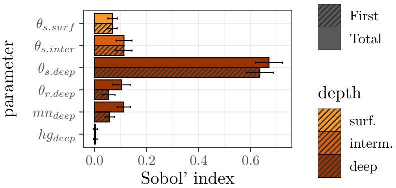






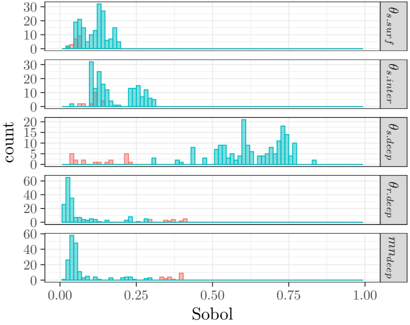
3. Case study: Sobol' indices under one rain realization

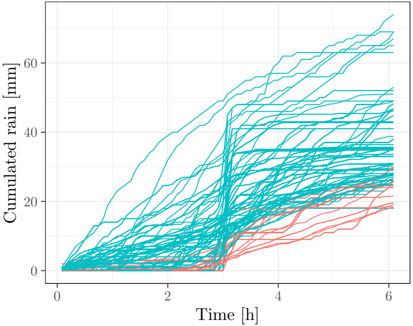




Name	Definition	Unit	Distribution
$\theta_{s.surf.}$	water content at saturation (surface)	$[L^3 L^{-3}]$	$\mathcal{N}(0.3375, 0.0338^2)$
$\theta_{s.inter.}$	water content at saturation (intermediary)	$[L^3 L^{-3}]$	$\mathcal{N}(0.3322, 0.0332^2)$
$\theta_{s.deep}$	water content at saturation (deep)	$[L^3 L^{-3}]$	$\mathcal{N}(0.316, 0.0316^2)$
$\theta_{r.deep}$	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

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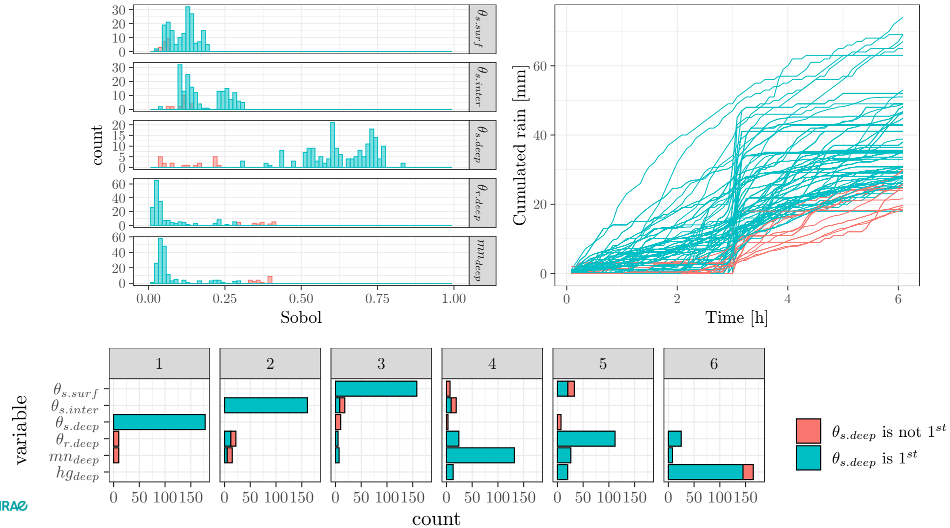

5. Conclusion:

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

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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