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# Sensitivity analysis of a spatio-temporal hydrological model for water and pesticide transfers

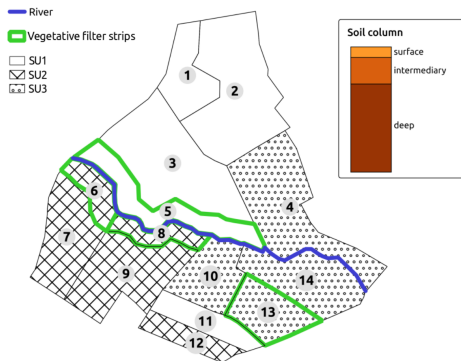
Katarina Radišić  
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10th International Conference on Sensitivity Analysis of Model Output  
(SAMO) March 14-16, 2022

# Introduction

## PESHMELBA model

### The PESHMELBA model Rouzies et al.<sup>1,2</sup>



Landscape units and soil horizons, illustration from Rouzies et al.<sup>2</sup>

- simulates water and pesticide transfers at a catchment scale
- heterogeneous soil types
- 14 landscape units
- heterogeneous layers : soil horizons
- infiltration, surface runoff and lateral subsurface exchanges
- heterogeneous vegetation types
- large number of input parameters ( $K = 145$ )
- input parameters are independent
- expensive, process based, hydrologic model

1. ROUZIES, LAUVERNET, BARACHET et al., "From agricultural catchment to management scenarios", 2019.

2. ROUZIES, LAUVERNET, SUDRET et al., [How to perform global sensitivity analysis of a catchment-scale, distributed pesticide transfer model?](#), 2021.

## 1 Case study

## 2 Methodology

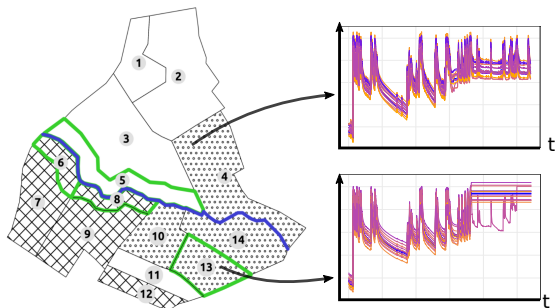
- Sobol' indices and PCE metamodels
- Functional principal components

## 3 Results

- Interpretation of principal components
- Validation of metamodels
- Sobol' indices

# 1. Case study

Sensitivity analysis on : **surface moisture outputs.**



$$\begin{bmatrix} Y^{(1)}(t) \\ Y^{(2)}(t) \\ \vdots \\ Y^{(14)}(t) \end{bmatrix} = \mathcal{M}(\mathbf{X}, t)$$

- time dependent outputs
- spatialized outputs
- large number of input parameters ( $K = 52$  after screening)

Two types of behaviour :

$$\underbrace{\text{flat}}_{\text{plateau}} \mathcal{G}_{\text{plateau}}$$

$$\underbrace{\text{wavy}}_{\text{no-plateau}} \mathcal{G}_{\text{no-plateau}}$$

## 1 Case study

## 2 Methodology

- Sobol' indices and PCE metamodels
- Functional principal components

## 3 Results

- Interpretation of principal components
- Validation of metamodels
- Sobol' indices

## 2. Methodology

### 2.1. Sobol' indices and PCE metamodels

Polynomial Chaos Expansion (PCE), metamodel for analytical Sobol' indices calculation<sup>3</sup>, calculations were done in the UQLab<sup>4</sup> Matlab environment.

$$\begin{aligned} Y &= \mathcal{M}(\mathbf{X}) \\ &= \sum_{\alpha \in \mathbb{N}^K} y_{\alpha} \Psi_{\alpha}(\mathbf{X}) \end{aligned}$$

$$D = \text{Var}(Y)$$

$$S_i = \sum_{\substack{\alpha \in \mathbb{N}^K: \\ \alpha_i > 0, \alpha_{j \neq i} = 0}} y_{\alpha}^2 / D$$

$$\begin{aligned} Y &\approx \mathcal{M}_{PCE}(\mathbf{X}) \\ &= \sum_{\alpha \in \mathcal{A}_q^{K,p}} y_{\alpha} \Psi_{\alpha}(\mathbf{X}) \end{aligned}$$

$$\hat{D} = \text{Var}(\mathcal{M}_{PCE}(\mathbf{X}))$$

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

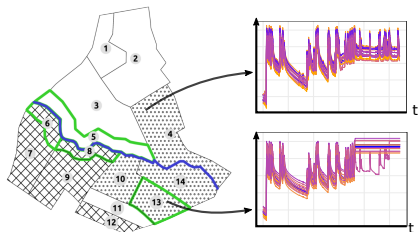
- Useful for models with large input spaces, needs little model simulations
- Scalar outputs  $\rightarrow$  application to principal components (PC)

3. SUDRET, "Global sensitivity analysis using polynomial chaos expansions", 2008.

4. MARELLI et SUDRET, "UQLab", 2014.

## 2. Methodology

### 2.2. Functional principal components



$$\begin{bmatrix} Y^{(1)}(t) \\ Y^{(2)}(t) \\ \vdots \\ Y^{(14)}(t) \end{bmatrix} = \mathcal{M}(\mathbf{X}, t), \quad t \in \mathcal{T}$$

$$Y^{(m)}(t) = \mu^{(m)}(t) + \sum_{j=1}^{\infty} H_j^{(m)} \mathbf{v}_j^{(m)}(t)$$

$$Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)} \mathbf{v}_1^{(m)}(t) + H_2^{(m)} \mathbf{v}_2^{(m)}(t)$$

$$H_1^{(m)} = \mathcal{M}_{PC1}^{(m)}(\mathbf{X})$$

$$\approx \mathcal{M}_{PC1, PCE}^{(m)}(\mathbf{X})$$

$$H_2^{(m)} = \mathcal{M}_{PC2}^{(m)}(\mathbf{X})$$

$$\approx \mathcal{M}_{PC2, PCE}^{(m)}(\mathbf{X})$$



## 1 Case study

## 2 Methodology

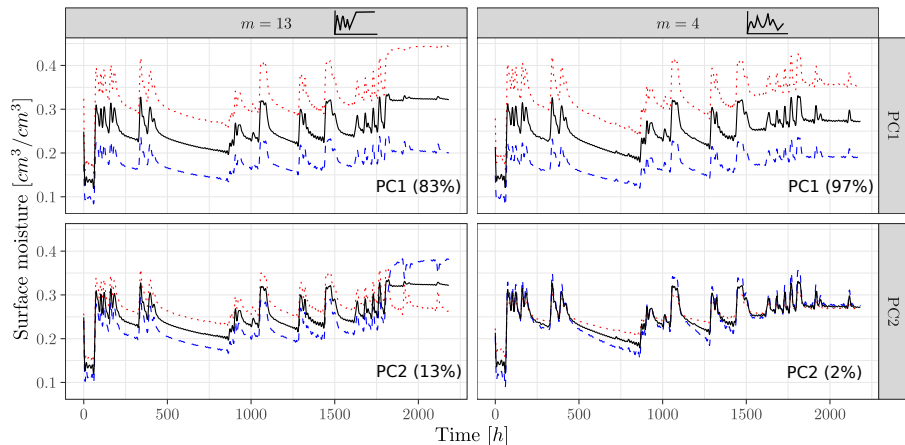
- Sobol' indices and PCE metamodels
- Functional principal components

## 3 Results

- Interpretation of principal components
- Validation of metamodels
- Sobol' indices

# 3. Results

## 3.1. Interpretation of principal components



$$\text{— } \mu^{(m)} \quad \text{... } \mu^{(m)} + 3\sqrt{\lambda_1^{(m)}} \mathbf{v}_1^{(m)} \quad \text{- - } \mu^{(m)} - 3\sqrt{\lambda_2^{(m)}} \mathbf{v}_2^{(m)}$$

# 3. Results

## 3.2 Validation of metamodels

$m$	$\mathcal{M}_{PC1,PCE}^m$	$\mathcal{M}_{PC2,PCE}^m$
1	1.00	NA
2	0.99	0.80
3	0.99	0.77
4	0.99	0.99
5	0.99	NA
6	0.99	0.97
7	0.99	0.82
8	1.00	NA
9	0.99	0.80
10	0.99	0.98
11	1.00	NA
12	0.99	0.95
13	0.98	0.78
14	0.99	0.99

$$Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)} \mathbf{v}_1^{(m)}(t) + H_2^{(m)} \mathbf{v}_2^{(m)}(t)$$

$$H_1^{(m)} \approx \mathcal{M}_{PC1,PCE}^{(m)}(\mathbf{X})$$

$$H_2^{(m)} \approx \mathcal{M}_{PC2,PCE}^{(m)}(\mathbf{X})$$

$R^2$  of the metamodels built on PC1 and PC2.

# 3. Results

## 3.2 Validation of metamodels

$m$	$\mathcal{M}_{PC1,PCE}^m$	$\mathcal{M}_{PC2,PCE}^m$	$\mathcal{G}$
1	1.00	NA	$\mathcal{G}_{no\_plateau}$
2	0.99	0.80	$\mathcal{G}_{plateau}$
3	0.99	0.77	$\mathcal{G}_{plateau}$
4	0.99	0.99	$\mathcal{G}_{no\_plateau}$
5	0.99	NA	$\mathcal{G}_{no\_plateau}$
6	0.99	0.97	$\mathcal{G}_{no\_plateau}$
7	0.99	0.82	$\mathcal{G}_{plateau}$
8	1.00	NA	$\mathcal{G}_{no\_plateau}$
9	0.99	0.80	$\mathcal{G}_{plateau}$
10	0.99	0.98	$\mathcal{G}_{no\_plateau}$
11	1.00	NA	$\mathcal{G}_{no\_plateau}$
12	0.99	0.95	$\mathcal{G}_{no\_plateau}$
13	0.98	0.78	$\mathcal{G}_{plateau}$
14	0.99	0.99	$\mathcal{G}_{no\_plateau}$

$$Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)} \mathbf{v}_1^{(m)}(t) + H_2^{(m)} \mathbf{v}_2^{(m)}(t)$$

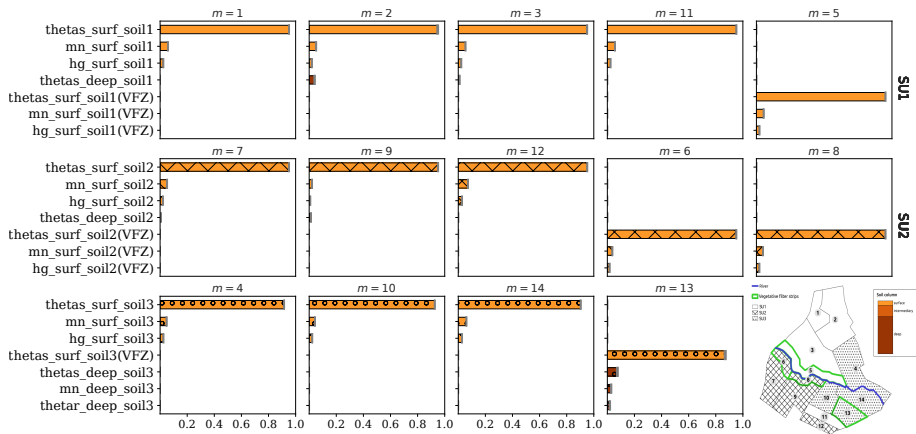
$$H_1^{(m)} \approx \mathcal{M}_{PC1,PCE}^{(m)}(\mathbf{X})$$

$$H_2^{(m)} \approx \mathcal{M}_{PC2,PCE}^{(m)}(\mathbf{X})$$

$R^2$  of the metamodels built on PC1 and PC2.

# 3. Results

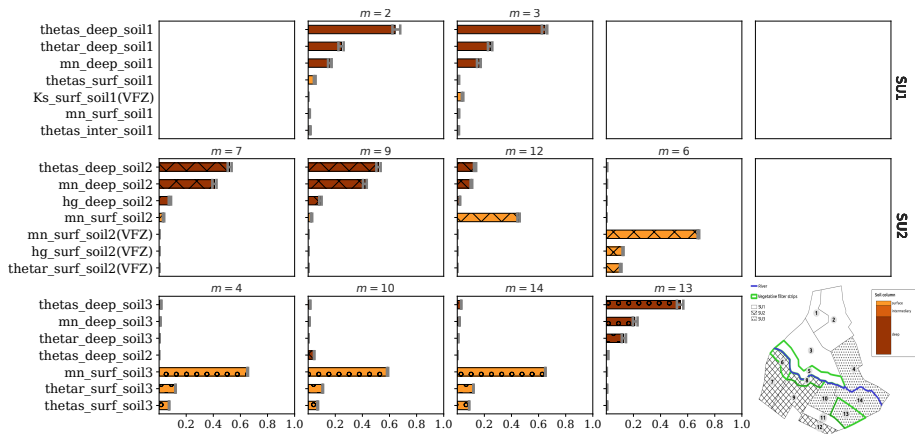
## 3.3 Sobol' indices



Total Sobol' indices on **PC1** per landscape unit with bootstrap confidence limits.

# 3. Results

## 3.3 Sobol' indices



Total Sobol' indices on **PC2** per landscape unit with bootstrap confidence limits.

- Successful application to surface moisture outputs.
  - Sobol' indices obtained with high precision.
  - Meaningful physical interpretations, increased comprehension of model behaviour.
  - information on the surface runoff type (infiltration excess runoff, saturation excess overland flow)
- Further adaptations
  - Cluster based SA for landscape units  $\in \mathcal{G}_{plateau}$
  - Replace polynomial chaos expansion metamodel with more flexible metamodels (random forests or deep GP Gaussian processes)