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Sensitivity Analysis of a Spatio-Temporal Hydrological Model for Pesticide Transfers

Supervisors : Emilie Rouzies,
Claire Lauvernet, Arthur Vidard

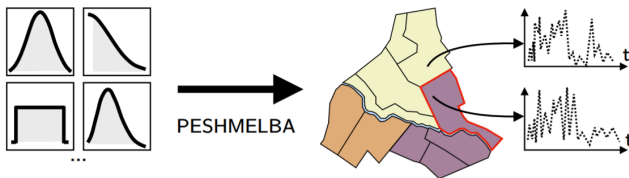
Katarina Radišić

30 November 2021

Introduction

PESHMELBA model

INRAE Lyon currently developing PESHMELBA model [Rouzies et al. 2019].



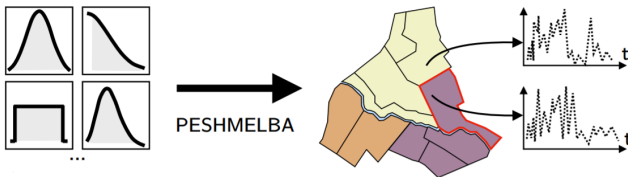
Simulates water and pesticide transfers on a watershed scale, while considering the heterogeneity of landscape elements (plots).

Type of output studied : surface moisture outputs.

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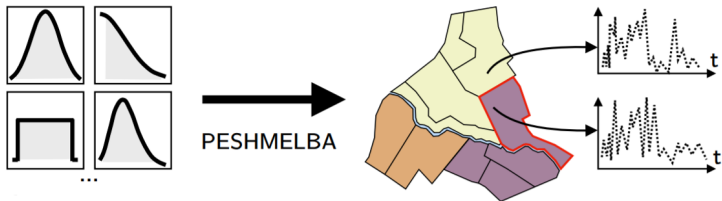
Simulates water and pesticide transfers on a watershed scale, while considering the heterogeneity of landscape elements (plots).

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Perform a **sensitivity analysis** on PESHMELBA outputs while taking into consideration both the **temporal** and the **spatial** aspect.

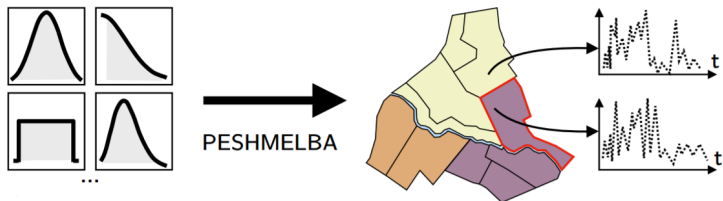
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Challenges on PESHMELBA



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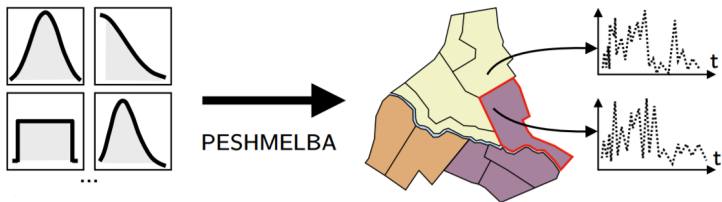


$$\begin{bmatrix} Y^{(1)}(t) \\ Y^{(2)}(t) \\ \vdots \\ Y^{(M)}(t) \end{bmatrix} = \mathcal{M}(\mathbf{X}, t), \quad t \in \mathcal{T}$$

where M is the number of areal units.

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Challenges on PESHMELBA



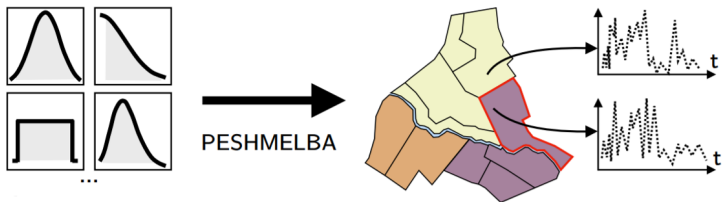
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- time dependent outputs

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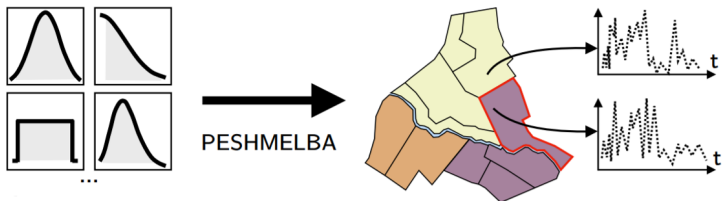
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- time dependent outputs
- spatial interactions

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- time dependent outputs
- spatial interactions
- high number of input parameters (145)

1 Screening

2 Temporal aspect

- Generalisation of Sobol' indices
- Estimation of Sobol' indices
- Results for Sobol' indices on one areal unit at a time

3 Spatial aspect

- Vector projections
- Comparison between Gamboa and Xu approach

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2. Screening

Morris method : computationally cheap, classifies input parameters in two groups, **influential and non-influential**.

2. Screening

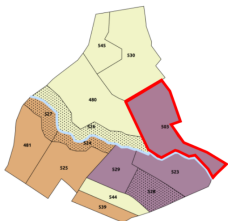
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Developed for **scalar outputs**.

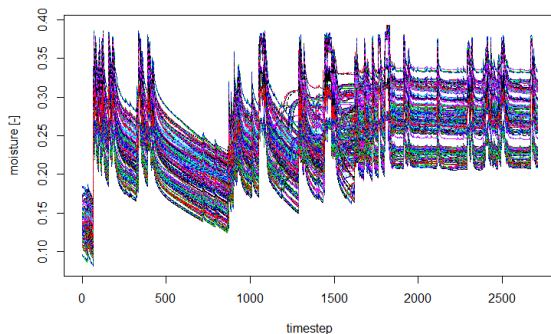
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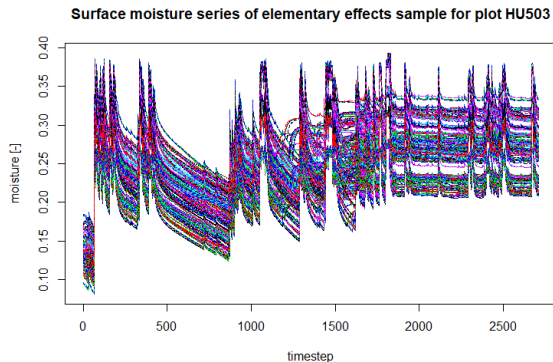
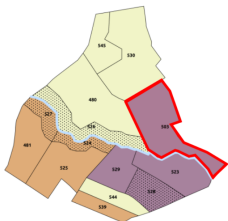
Surface moisture series of elementary effects sample for plot HU503



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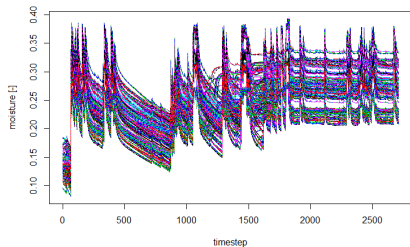
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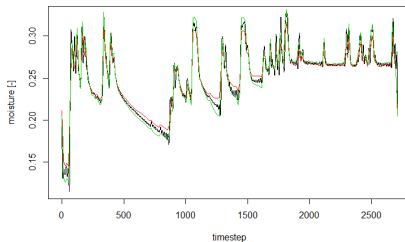
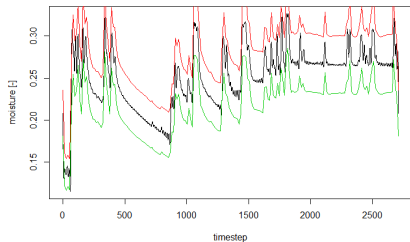
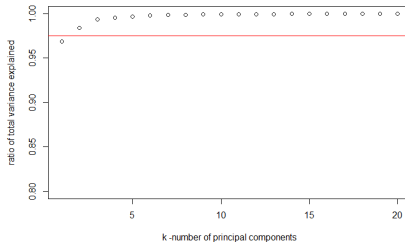
Apply the Morris method to the scores on the **functional principal components** of one areal unit at a time.

1. Screening

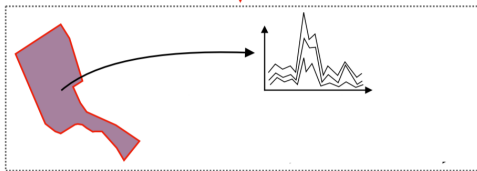
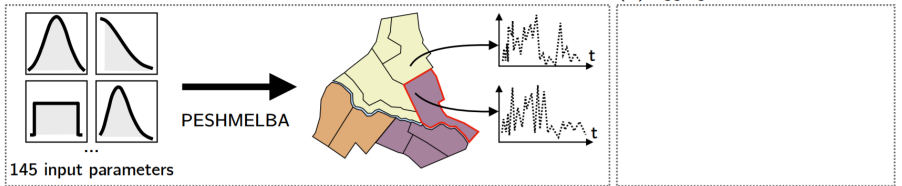
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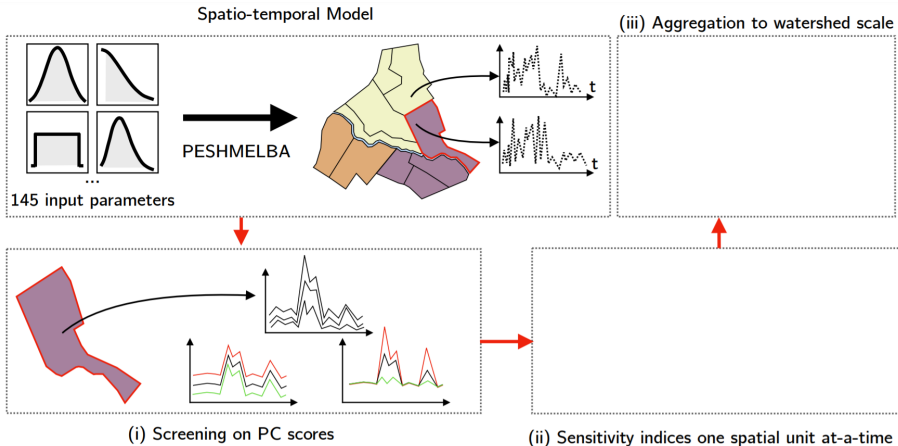


Screplot for elementary effects sample of HU503



Spatio-temporal Model





Input parameters reduced from 145 to 52 influential parameters at the watershed scale.

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2. Temporal aspect

2.1. Generalisation of Sobol' indices [Lamboni et al. 2010]

How to generalize Sobol' indices to functional outputs?

$$Y(t) = \mathcal{M}(\mathbf{X}, t), \quad t \in \mathcal{T}, \quad m \in \{1..M\}$$

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The output is scalar now, we fall back into the classical formulation for Sobol' indices calculation.

2. Temporal aspect

2.2. Estimation of Sobol' indices [Sudret 2008]

Polynomial Chaos Expansion (PCE) metamodel :

$$Y = \sum_{\alpha \in \mathbb{N}^K} y_{\alpha} \Psi_{\alpha}(\mathbf{X})$$

where K is the number of input parameters.

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Sobol' indices are obtained analytically from PCE :

$$S_i = \sum_{\alpha \in \mathcal{I}_i} y_{\alpha}^2 / D$$

$$\mathcal{I}_i = \left\{ \alpha \in \mathbb{N}^K : \alpha_i > 0, \alpha_{j \neq i} = 0 \right\}$$

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2.2. Estimation of Sobol' indices [Sudret 2008]

Polynomial Chaos Expansion (PCE) metamodel :

$$Y = \sum_{\alpha \in \mathcal{A}_q^{K,p}} y_\alpha \Psi_\alpha(\mathbf{X}) + \epsilon_{\text{truncation}}$$

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Sobol' indices are obtained analytically :

$$\hat{S}_i = \sum_{\alpha \in \mathcal{I}_i^*} y_\alpha^2 / D$$

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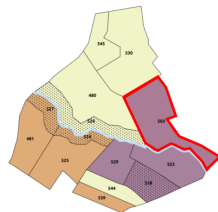
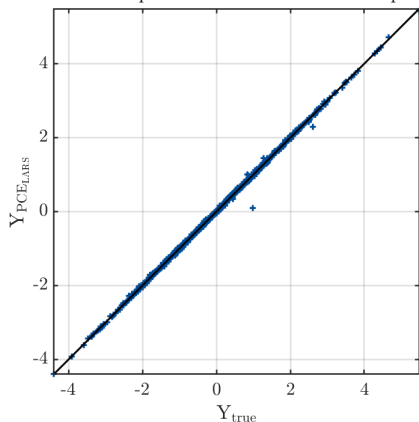
$$\mathcal{I}_i^* = \left\{ \alpha \in \mathcal{A}_q^{K,p} : \alpha_i > 0, \alpha_{j \neq i} = 0 \right\}$$

The precision of the Sobol' indices obtained depends on the precision of the PCE metamodel w.r.t. the real model \mathcal{M} .

3. Temporal aspect

3.3. Results for Sobol' indices on one areal unit at a time

Metamodel vs. true response on the validation set for fpc1+fpc2 of 503

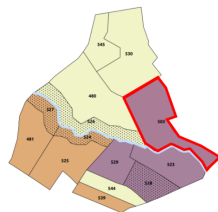
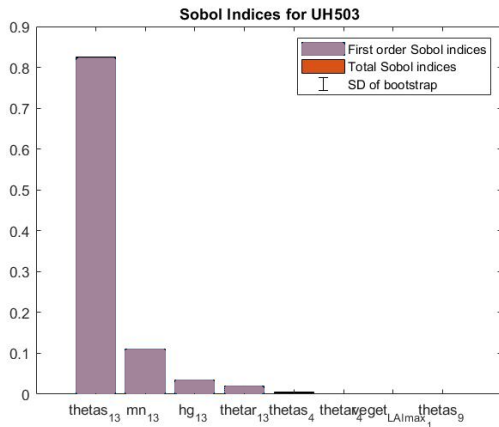


Quality of the PCE metamodel :
 $R^2 > 0.95$ on validation set.

Figure – Validation set metamodel output vs PESHMELBA simulation.

3. Temporal aspect

3.3. Results for Sobol' indices on one areal unit at a time



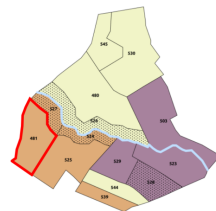
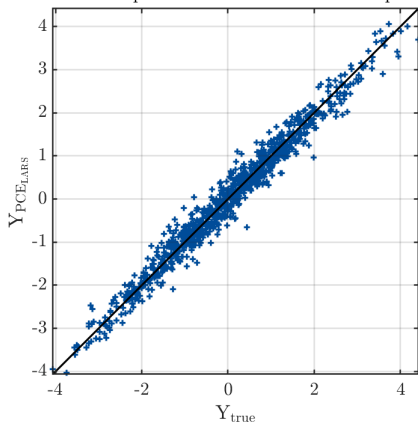
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Figure – Sobol' indices for areal unit UH503. Bar colours refer to soil types.

2. Temporal aspect

2.3. Results for Sobol' indices on one areal unit at a time

Metamodel vs. true response on the validation set for fpc1+..fpc4 of 481

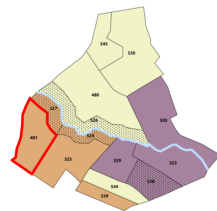
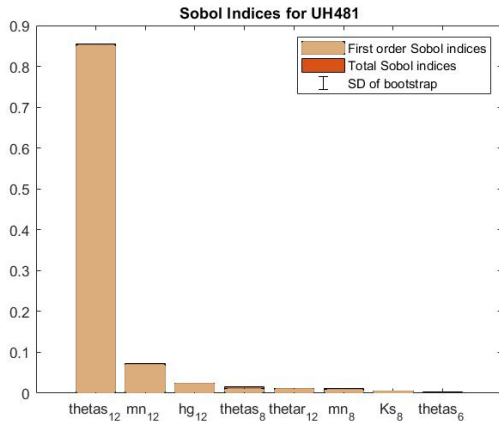


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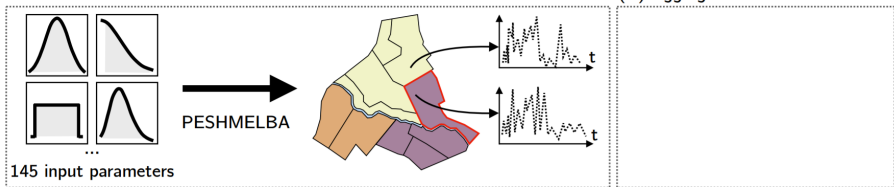
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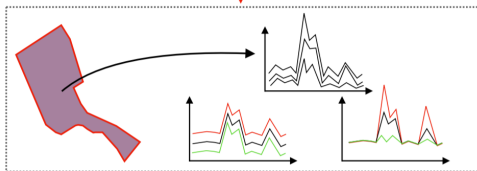
Quality of the PCE
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Figure – Sobol' indices for areal unit UH481. Bar colours refer to soil types.

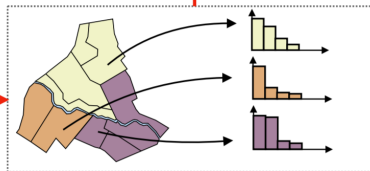
Spatio-temporal Model



(iii) Aggregation to watershed scale



(i) Screening on PC scores



(ii) Sensitivity indices one spatial unit at-a-time

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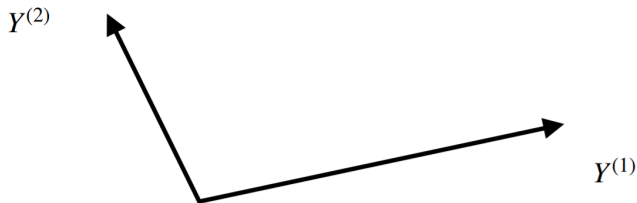
3. Spatial aspect

3.1. Vector projections [Xu et al. 2019]



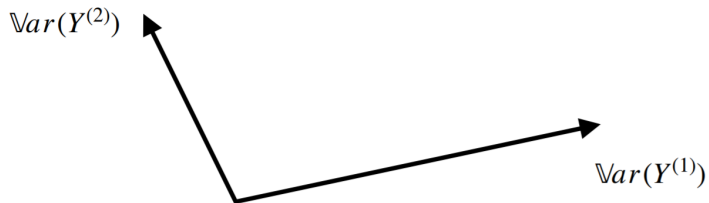
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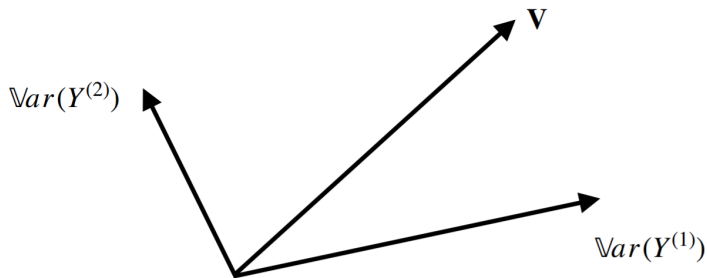
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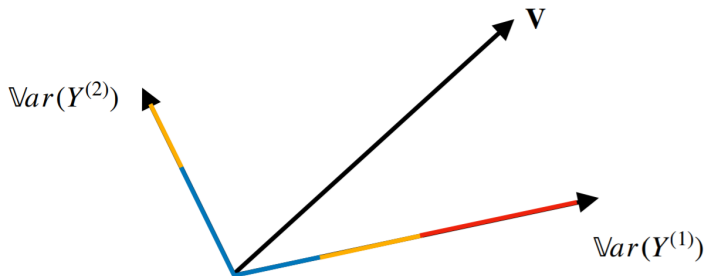
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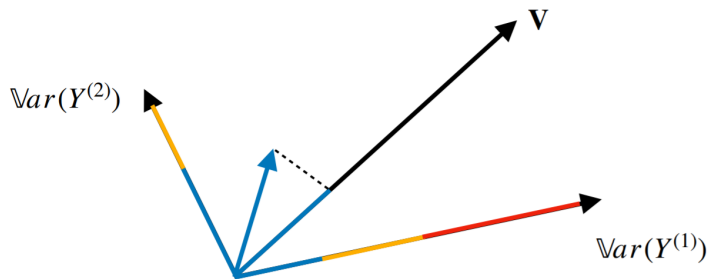


$$\mathbb{V}ar(Y^{(1)}) = \mathbb{V}ar(\mathbb{E}[Y^{(1)}|X_1]) + \mathbb{V}ar(\mathbb{E}[Y^{(1)}|X_2]) +$$

$$\mathbb{V}ar(\mathbb{E}[Y^{(1)}|X_1, X_2]) - \mathbb{V}ar(\mathbb{E}[Y^{(1)}|X_1]) - \mathbb{V}ar(\mathbb{E}[Y^{(1)}|X_2])$$

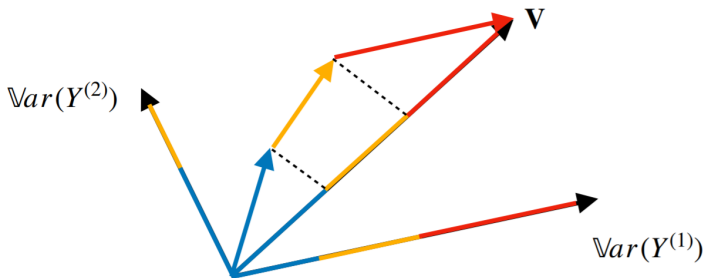
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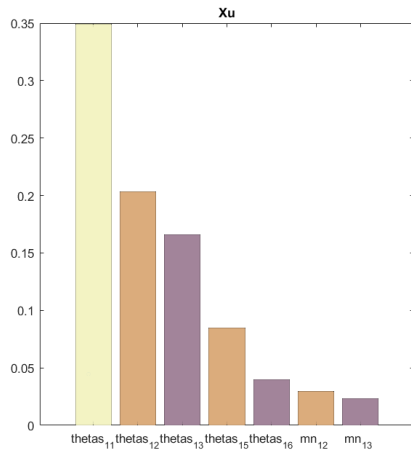
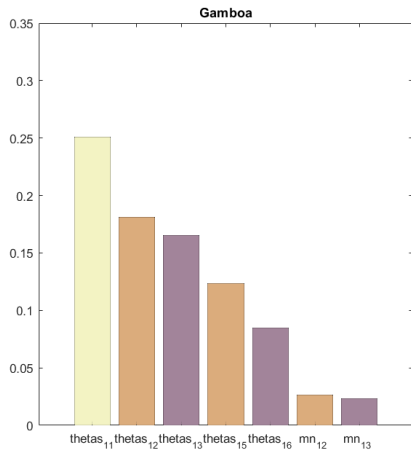
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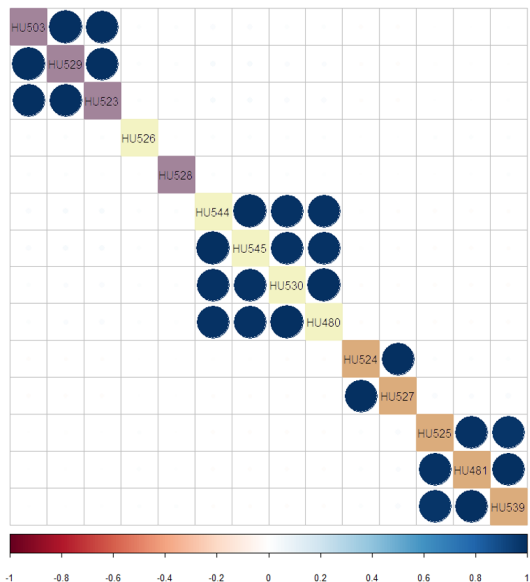
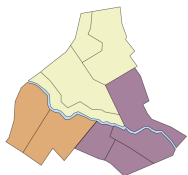
3. Spatial aspect

3.2. Gamboa vs. Xu, aggregation to the watershed scale

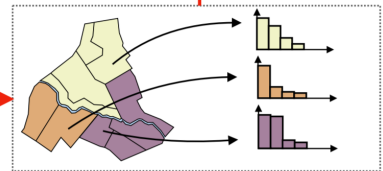
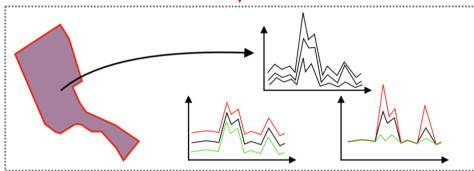
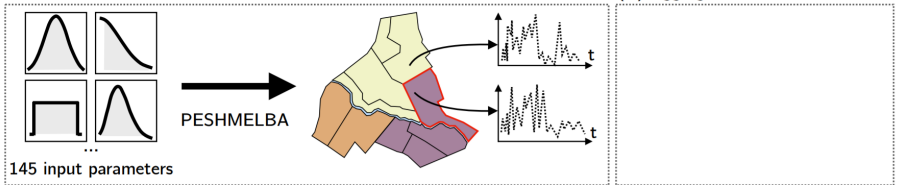


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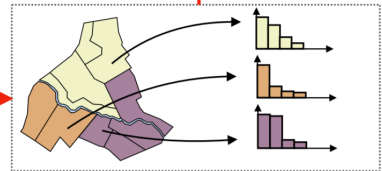
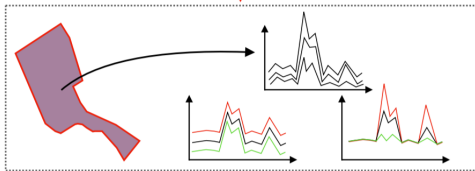
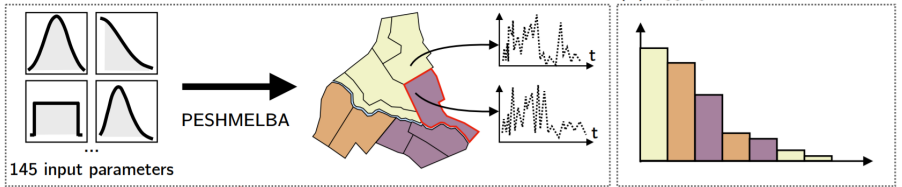
3.3. Correlations among outputs



Spatio-temporal Model



Spatio-temporal Model



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- The methodology was tested on pesticide mass outputs.
 - Due to the complexity of the physical processes the PCE metamodels need a bigger basis and become too expensive.
 - Further adaptations : replace polynomial chaos expansion metamodel with more flexible metamodels (random forests).

Merci de votre attention !

- M. Lamboni, H. Monod, and D. Makowski. Multivariate sensitivity analysis to measure global contribution of input factors in dynamic models. *Reliability Engineering System Safety*, 96(4) :450–459, April 2011.
- E. Rouzies, C. Lauvernet, C. Barachet, T. Morel, F. Branger, I. Braud, and N. Carluer. From agricultural catchment to management scenarios : A modular tool to assess effects of landscape features on water and pesticide behavior. *Science of The Total Environment*, 671 :1144–1160, June 2019.
- L. Xu, Z. Lu, and S. Xiao. Generalized sensitivity indices based on vector projection for multivariate output. *Applied Mathematical Modelling*, 66 :592–610, February 2019.