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UNCECOMP 2021
4th International Conference on Uncertainty Quantification in
Computational Sciences and Engineering

How can we quantify and reduce the uncertainty
of a watershed-scale pesticide transfer model? A
comparison of several approaches.

Emilie Rouzies¹, Claire Lauvernet¹, Bruno Sudret³, Arthur Vidard²

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Introduction

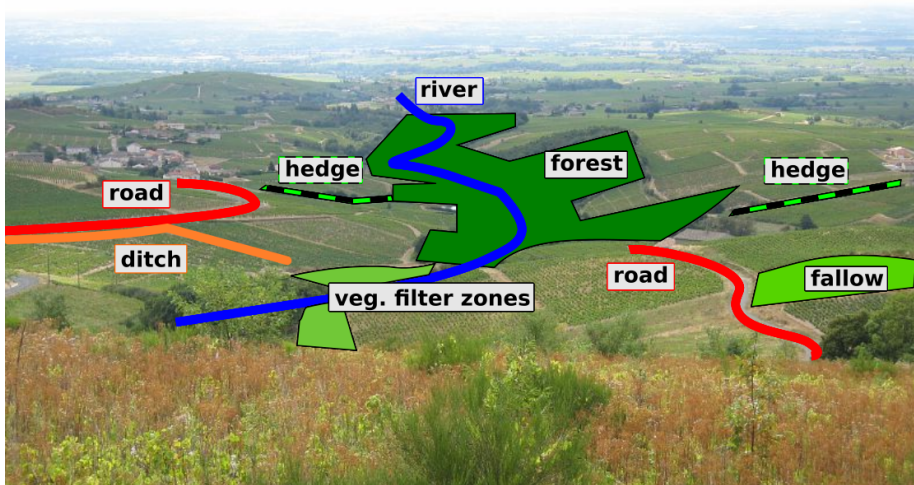
Context



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Introduction

Context

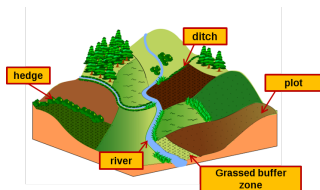


Introduction

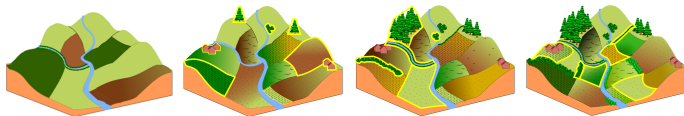
The PESHMELBA model

Development of the **PESHMELBA** model (Rouzies et al. 2019) to simulate pesticide transfers and fate on small agricultural catchments

- ✓ Simulations of heterogenous landscapes composed of plots, vegetative filter zones, hedges, ditches and rivers



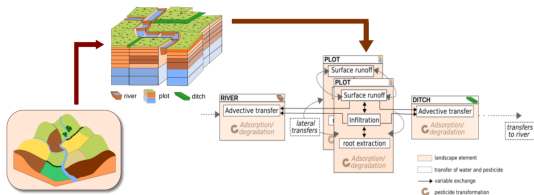
- ✓ Modular structure to explore landscape management scenarios



Introduction

The PESHMELBA model

- ✓ Process-oriented, fully spatialized model
- ✓ Water transfers on surface and subsurface + pesticide advection, adsorption and degradation



Introduction

PhD Objectives



We have a dream that one day PESHMELBA will be used as a decision-making tool to set up management scenarios and to identify an optimal landscape configuration for pesticide transfer mitigation.

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*This is our objective...but before, it is necessary to **quantify** and **reduce** the uncertainty associated to PESHMELBA output variables.*

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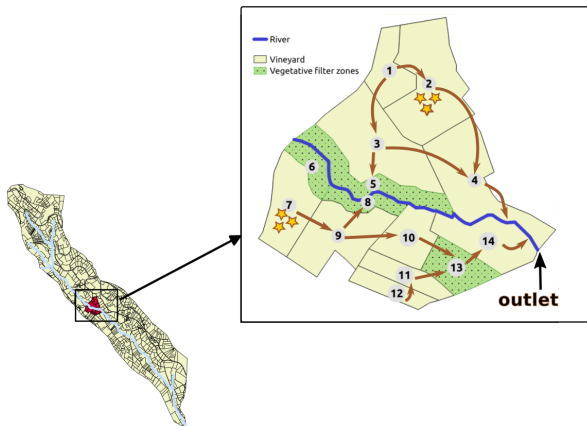
*This is our objective...but before, it is necessary to **quantify** and **reduce** the uncertainty associated to PESHMELBA output variables.*

PhD objectives

1. **Quantify**: performing an uncertainty analysis and a sensitivity analysis of the model
2. **Reduce**: performing data assimilation to integrate different sources of data: soil moisture images, ERT measurements and in-situ data of pesticide concentration

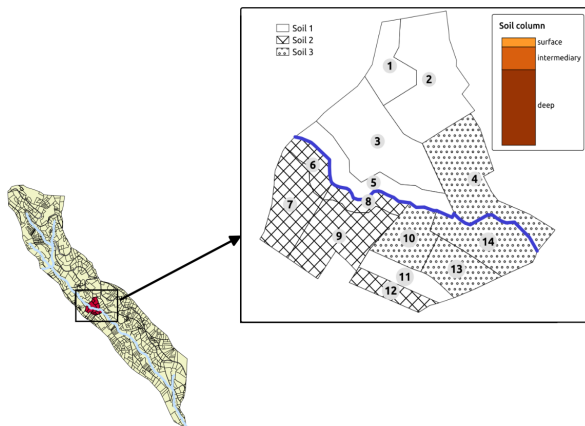
Case study

First GSA of PESHMELBA: let's keep it simple...but realistic! (types of landscape elements, number of parameters, climate conditions...)



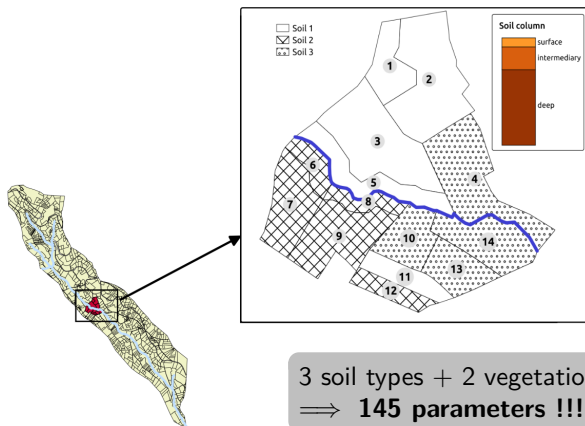
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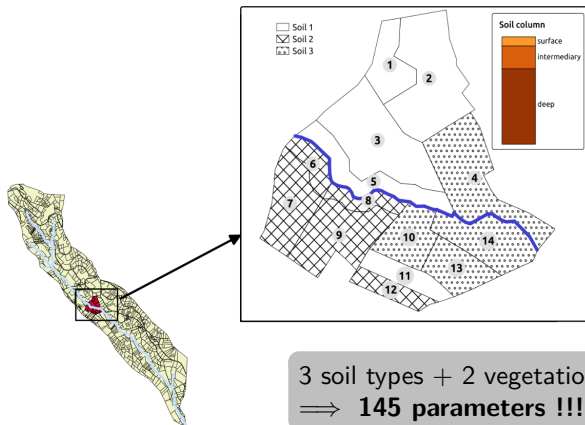


3 soil types + 2 vegetation types + ...
⇒ **145 parameters !!!**

Case study

First GSA of PESHMELBA: let's keep it simple...but realistic! (types of landscape elements, number of parameters, climate conditions...)

Which method to address sensitivity of such a process-oriented, spatialized model?



Notations $Y = f(X_1, X_2, \dots, X_k)$

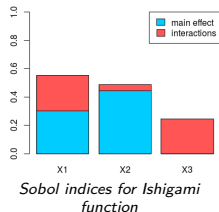
Variance-based Sobol method (Sobol 1993)

Decomposition of the output variance in conditional variances.

$S_i = \frac{V_i}{V(Y)}$ main effect of i^{th} parameter

$S_{ij} = \frac{V_{ij}}{V(Y)}$ interaction effect due to the i^{th} and the j^{th} factors

$S_{T_i} = S_i + \sum S_{ij} + \dots + \sum S_{1,\dots,k}$ overall output sensitivity



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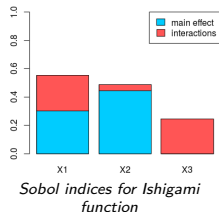
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Classical Sobol sampling > 75000 model runs, impossible!

⇒ Sobol indices obtained with Polynomial Chaos Expansion surrogate model (Wiener 1938) from 4000 simulation runs using UQLab (Marelli and Sudret 2014).

Alternative methods

■ HSIC dependence measure (Da Veiga 2015)

Main idea: describe the similarity between P_Y and $P_{Y|X_i}$ by using a dependence measure d

$$S_i^d = \mathbb{E}_{X_i}(d(P_Y, P_{Y|X_i}))$$

Chosen dependence measure: Hilbert-Schmidt independence criterion (HSIC) (Gretton et al. 2005)

⇒ **Screening method (De Lozzo and Marrel 2014)**



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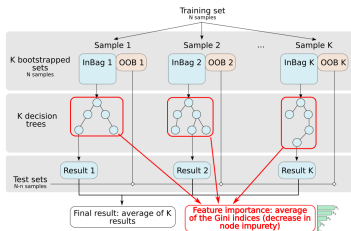
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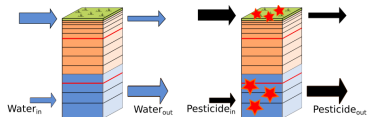


■ Random Forest



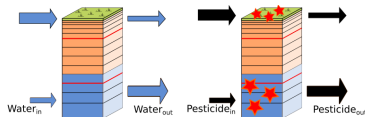
Target variables

- ✓ **Scalar variables:** informative variables: cumulated water volume and pesticide mass transferred from each HU by subsurface lateral transfers and by surface runoff.

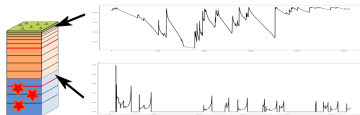


Target variables

- ✓ **Scalar variables:** informative variables: cumulated water volume and pesticide mass transferred from each HU by subsurface lateral transfers and by surface runoff.



- ✓ **Temporal series:** target variables for DA: surface moisture, mean moisture in first 100 cm, water table pest. conc., water flow and pest. conc. at the outlet



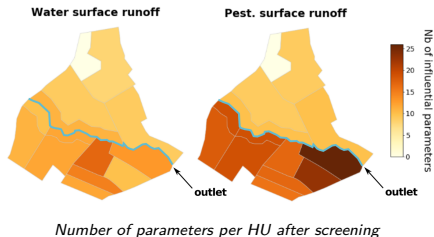
Results

Scalar variables - screening

Screening: independance test based on HSIC measure (power of the test $\alpha=1\%$)

After screening:

- Water surface runoff: 43 parameters
- Pesticide surface runoff: 45 parameters



- ✓ High number of influential parameters remaining after screening: method not discriminant enough? Many physical processes at stake?
- ✓ Spatial heterogeneities consistent with heterogeneities in physical processes activation

Results

Scalar variables - ranking



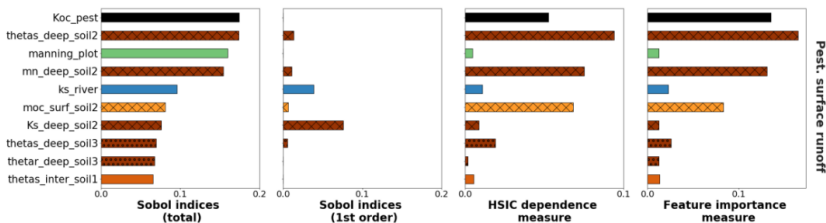
Ranking for cumulated pesticide mass transferred in surface runoff

Results

Scalar variables - ranking



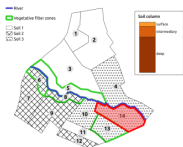
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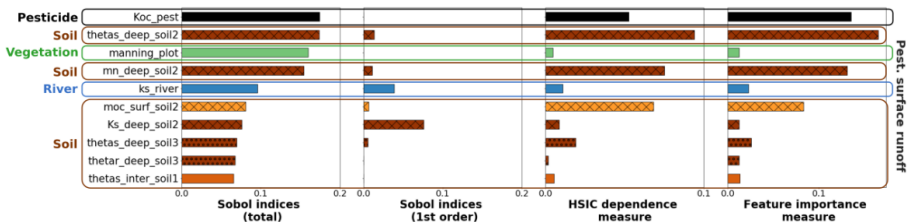
✓ Discrepancies in ranking between the 3 methods

Results

Scalar variables - ranking



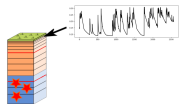
Ranking for cumulated pesticide mass transferred in surface runoff



- ✓ Discrepancies in ranking between the 3 methods
- ✓ Pesticide transfers at surface result from the interaction of several physical processes.

Results

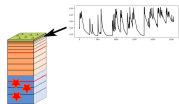
Surface moisture time serie - ranking



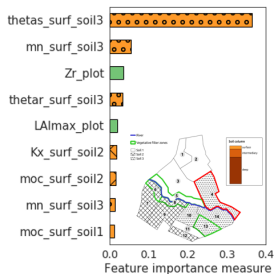
Random Forest feature importance for surface moisture on HU 4

Results

Surface moisture time serie - ranking



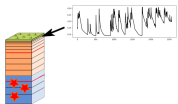
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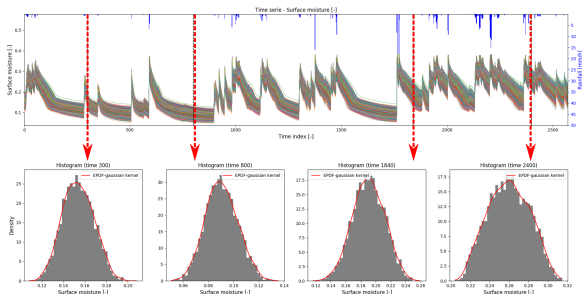
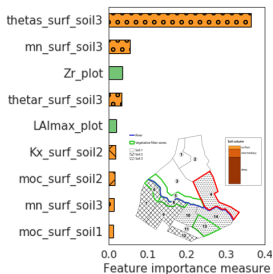
- ✓ Uncertainty on influential parameters will be reduced during the DA process

Results

Surface moisture time serie - ranking



Random Forest feature importance for surface moisture on HU 4



- ✓ Uncertainty on influential parameters will be reduced during the DA process
- ✓ Variable mainly gaussian along the simulation: valuable info to choose DA method

Conclusion

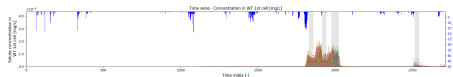
- ✓ PESHMELBA specificities turn sensitivity analysis a challenging task \implies need for adapted tools: Sobol' indices from PCE, HSIC, Random Forest
- ✓ Sensitivity analysis provides valuable information about hydrological processes activation and interaction for a given scenario
- ✓ Uncertainty/Sensitivity analysis are a necessary preliminary task for data assimilation (which parameters could be estimated? which method can be used ?)

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To be further explored:

Sensitivity analysis on temporal series may be improved, especially for pesticide concentration series \implies On-going test of PCA-PCE analysis.



Thanks for your attention