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

Emilie Rouzies, Claire Lauvernet, Bruno Sudret, Arthur Vidard

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[3]ETH Zürich, Institute of Structural Engineering, Zürich

Introduction
Context

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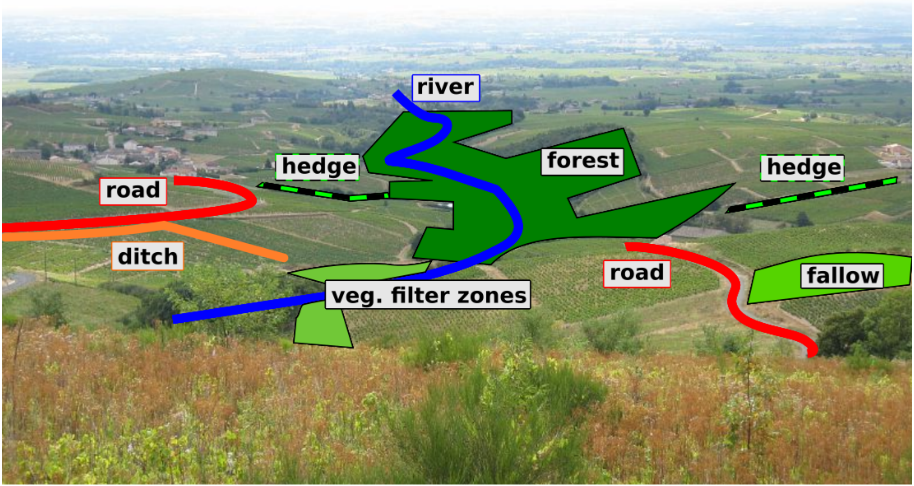
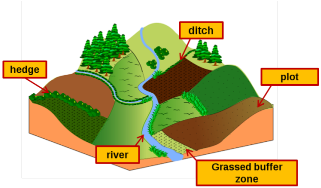
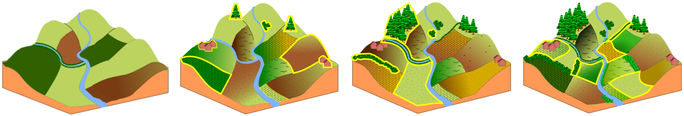


Development of the **PESHMELBA** model (Rouzies et al. 2019) to simulate pesticide transfers and fate on small agricultural catchments

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



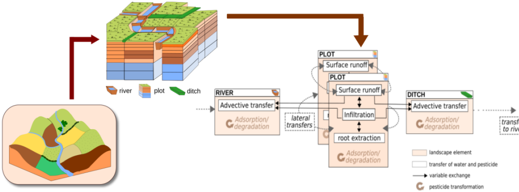
- ✓ Modular structure to explore landscape management scenarios



Introduction

The PESHMELBA model

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



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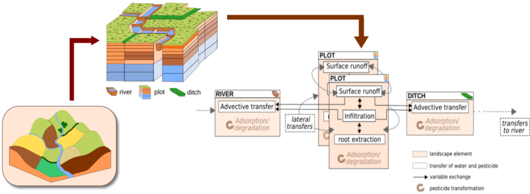
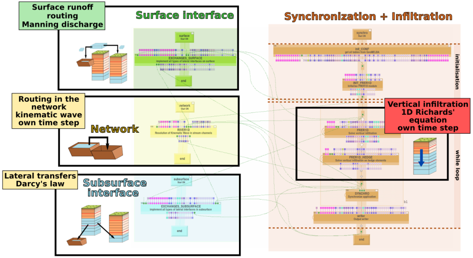


- ✓ One module ≡ one process or ensemble of processes on a landscape element
- ✓ Coupling of modules within the OpenPALM coupler (Buis, Piacentini, and Déclat 2006) turning the structure flexible



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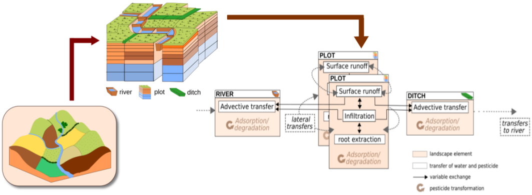

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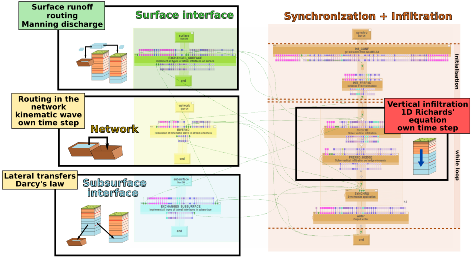

⇒ Complex structure may lead to additionnal difficulties to diagnose model behavior!

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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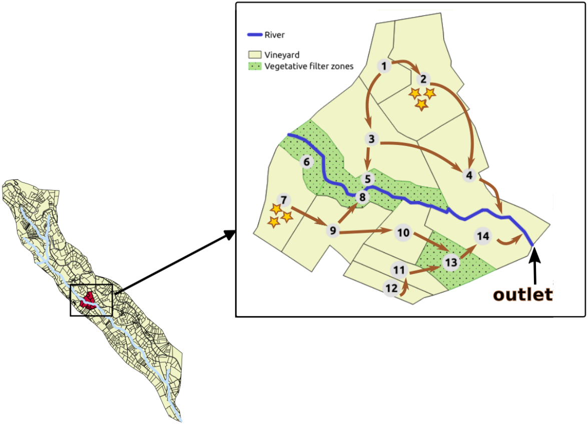
PhD objectives

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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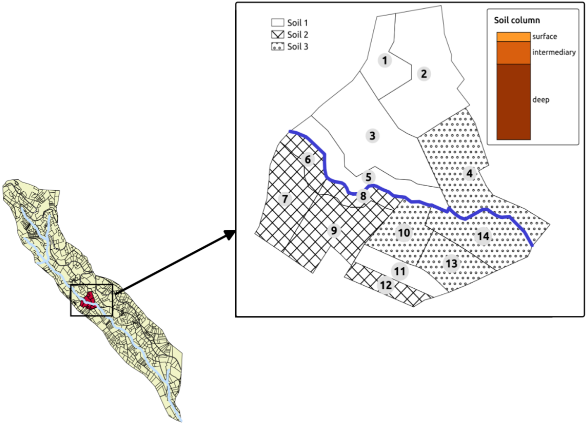

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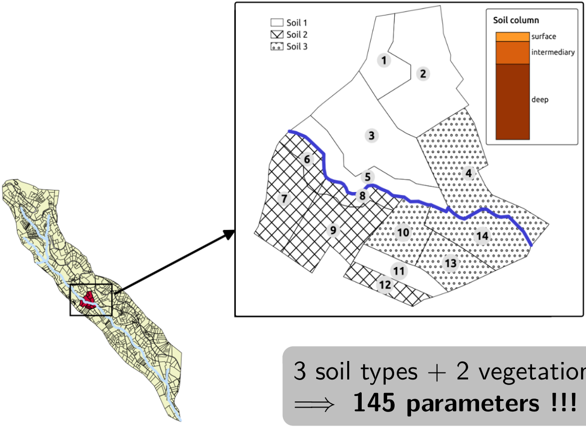

3 soil types + 2 vegetation types + ...
$\Longrightarrow$ **145 parameters !!!**

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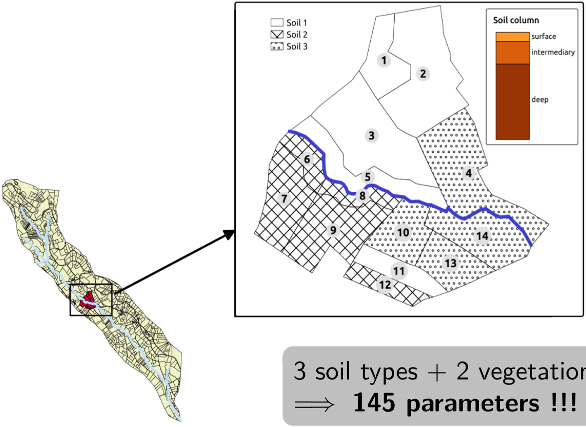
Which method to address sensitivity of such a process-oriented, spatialized model?



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GSA methods

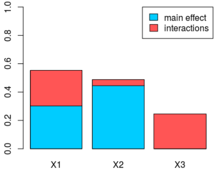
Notations $Y = f(X_1, X_2, ..., X_k)$

Variance-based Sobol method **(Sobol 1993)**
Decomposition of the output variance in conditional variances.

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

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

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



Sobol indices for Ishigami function

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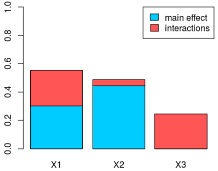


Sobol indices for Ishigami function

Classical Sobol sampling $>$ 75000 model runs, impossible!
$\Rightarrow$ Sobol indices obtained with Polynomial Chaos Expansion surrogate model (Wiener 1938) from 4000 simulation runs using UQLab (Marelli and Sudret 2014).

GSA methods

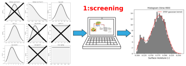
Alternative methods

- **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)

  $\Rightarrow$ **Screening method (De Lozzo and Marrel 2014)**



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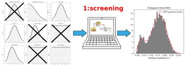
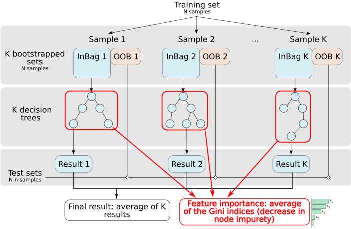
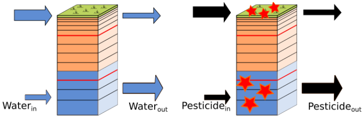


- **Random Forest**



Target variables

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



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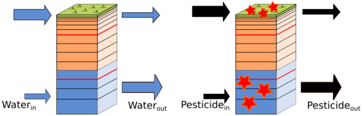
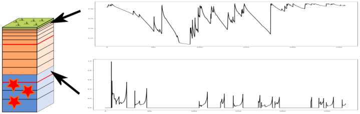


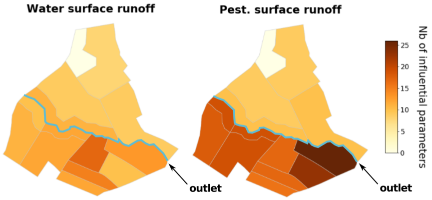
✓ **Temporal series**: target variables for DA: surface moisture,mean moisture in first 100 cm, water table pest. conc., water flow and pest. conc. at the outlet



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

After screening:

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



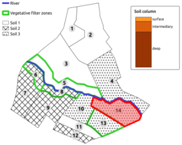
Number of parameters per HU after screening

✓ High number of influential parameters remaining after screening: method not discriminant enough? Many physical processes at stake?

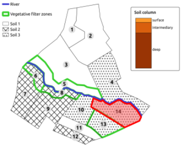
✓ Spatial heterogeneities consistent with heterogeneities in physical processes activation

Results

Scalar variables - ranking



Ranking for cumulated pesticide mass transferred in surface runoff



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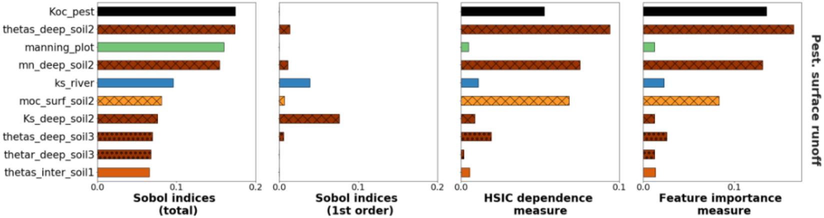

✓ Discrepancies in ranking between the 3 methods

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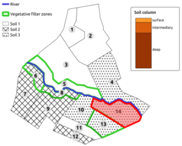

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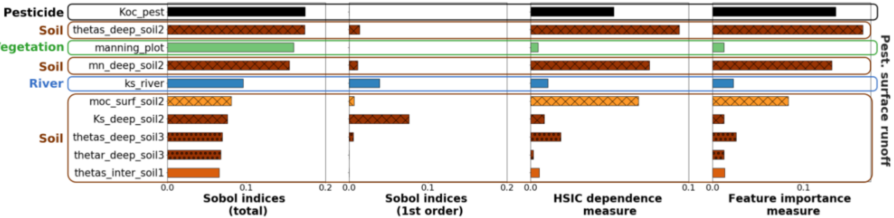
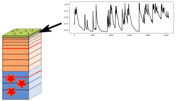
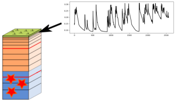


- ✓ Discrepancies in ranking between the 3 methods
- ✓ Pesticide transfers at surface result from the interaction of several physical processes.



Random Forest feature importance for surface moisture on HU 4



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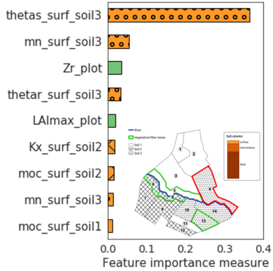
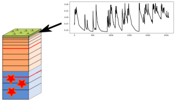


✓ Uncertainty on influential parameters will be reduced during the DA process

Results

Surface moisture time serie - ranking



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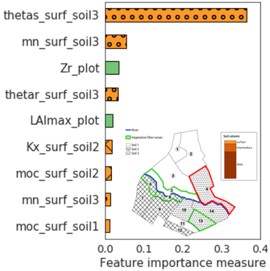

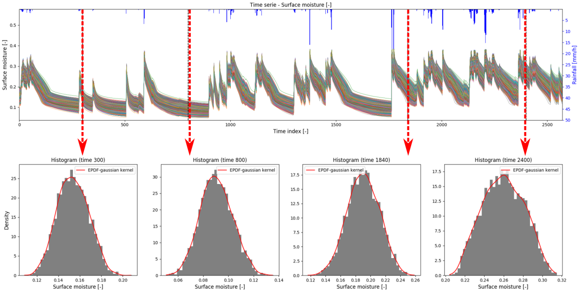

- ✓ Uncertainty on influential parameters will be reduced during the DA process
- ✓ Variable mainly gaussian along the simulation: valuable info to choose DA method

Conclusion

- ✓ PESHMELBA specificities turn sensitivity analysis a challenging task $\Longrightarrow$ 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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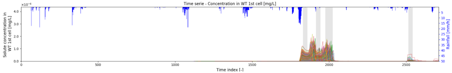
To be further explored:
Sensitivity analysis on temporal series may be improved, especially for pesticide concentration series $\Rightarrow$ On-going test of PCA-PCE analysis.



Conclusion

Thanks for your attention