How can we quantify and reduce the uncertainty of a watershed-scale pesticide transfer model? Application to the PESHMELBA model.

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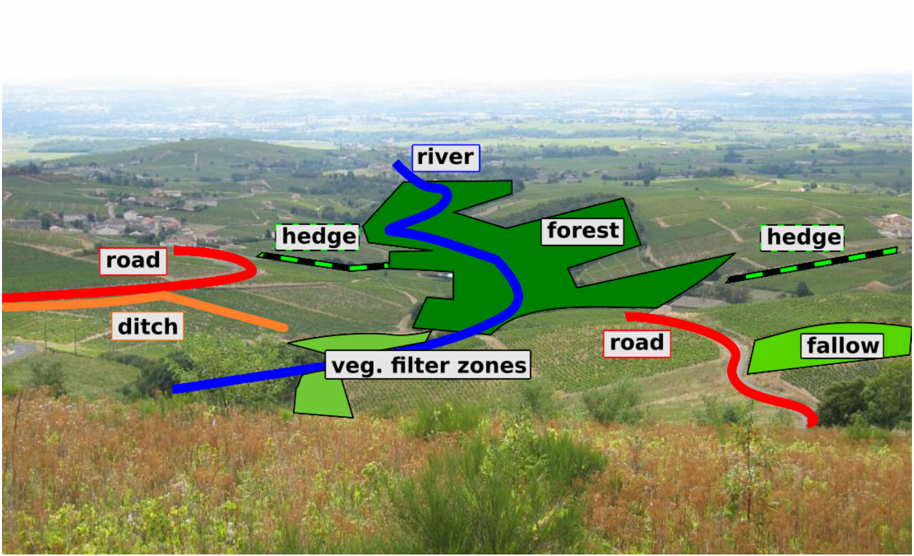
PhD supervised by Arthur Vidard (LJK/Inria, France) and Claire Lauvernet (Inrae, France)

Introduction

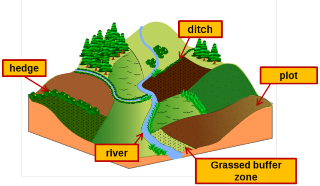
Context



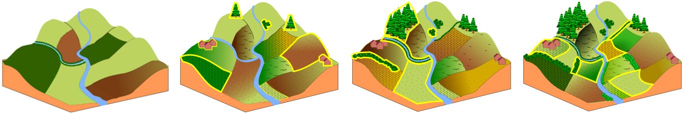
river
hedge
forest
hedge
road
ditch
road
fallow
veg. filter zones

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



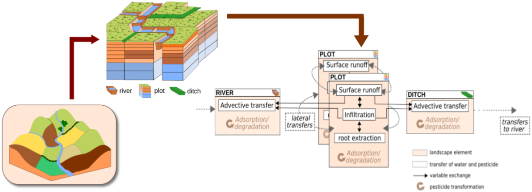
✓ Modular structure to explore landscape management scenarios



Introduction

The PESHMELBA model

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



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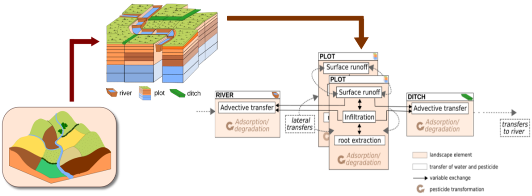
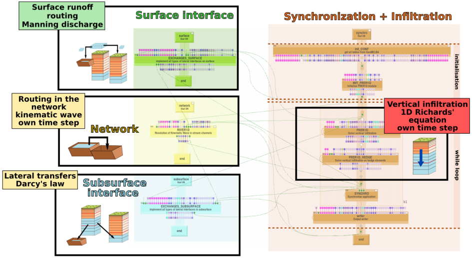


- ✓ One module ≡ one process or ensemble of processes on a landscape element
- ✓ Coupling of modules within the OpenPALM coupler (Buis et al. 2006) turning the structure flexible



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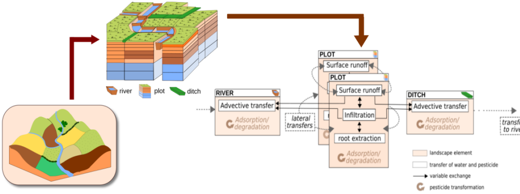

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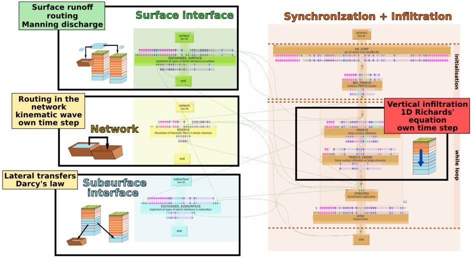

⇒ **Complex structure may lead to additionnal difficulties to diagnose model behavior!**

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PhD objectives

1. Quantify: performing 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

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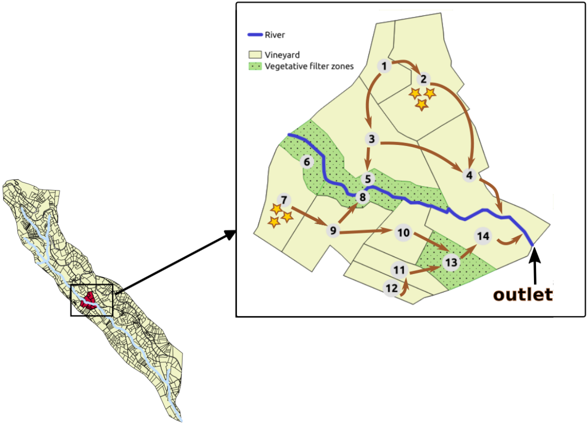
First attempt of GSA and DA in the PESHMELBA model: let's keep it simple...but realistic! (types of landscape elements, number of parameters, climate conditions...)



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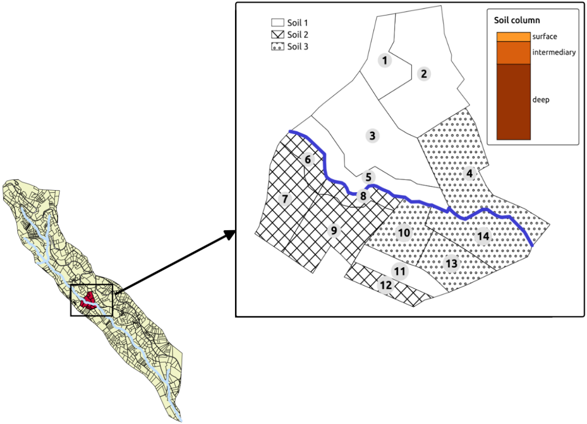

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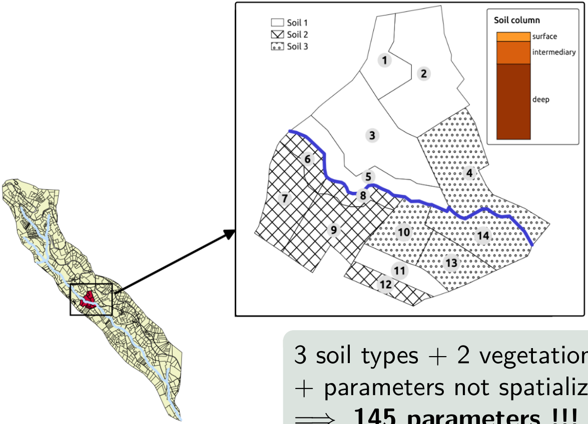


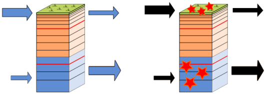
3 soil types + 2 vegetation types + ...
+ parameters not spatialized
$\Longrightarrow$ **145 parameters !!!**

⚠ parameters are assumed independent

Uncertainty quantification

Objectives

✓ Get insight into the (recent) model functioning



- ✓ Get insight into the (recent) model functioning **GSA on integrated variables**

Integrated variables: cumulated water volume and pesticide mass transferred from each HU by subsurface lateral transfers and by surface runoff.

Uncertainty quantification

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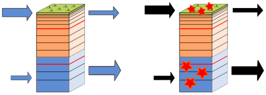

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- ✓ Get insight into the (recent) model functioning **GSA on integrated variables**
- ✓ Identify the parameters that may be estimated by data assimilation (most influential)

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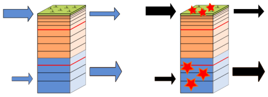
Objectives

- ✓ Get insight into the (recent) model functioning **GSA on integrated variables**
- ✓ Identify the parameters that may be estimated by data assimilation (most influential) **GSA on time series ⇒ see next talk (Katarina)**



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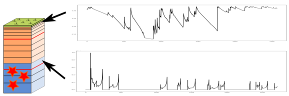


Target variables for DA: surface moisture,mean moisture in first 100 cm, water table pest. conc., water flow and pest. conc. at the outlet

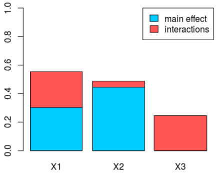
Notations $Y = f(X_1, X_2, ..., X_k)$

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

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

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

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



Sobol indices for Ishigami function

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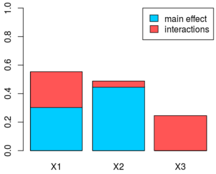


Sobol indices for Ishigami function

Classical Sobol sampling $>$ 75,000 model runs, impossible!
$\Rightarrow$ Sobol indices obtained with Polynomial Chaos Expansion surrogate model (Wiener 1938) using UQLab (Marelli and Sudret 2014).

Uncertainty quantification

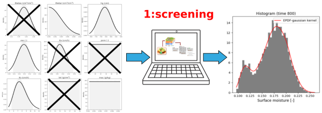
GSA methods

- **HSIC dependence measure** **(Da Veiga 2015)**
  Dependence measures: aim at quantifying, from a probabilistic point of view, the dependence between X_i and Y with the property that the measure equals zero if and only if X_i and Y are independent.

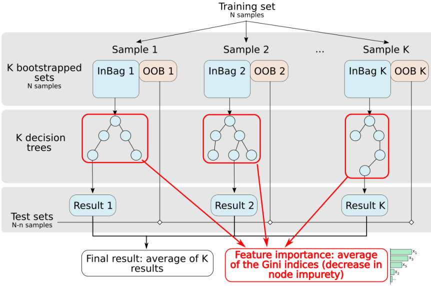
  $\Rightarrow$ Chosen dependence measure: **Hilbert-Schmidt independence criterion (HSIC)** (Gretton et al. 2005): calculate the cross-correlation between any non-linear transformations of some input factor X_i and the output Y.

$$HSIC(\mathrm{X}_i, \mathrm{Y})_{\mathcal{F}_i,\mathcal{G}} = ||C[\mathcal{G}\mathcal{F}_i]||^2_{HS}$$

Also used as a **screening** method based on an independence test (De Lozzo and Marrel 2014)



Feature importance from Random Forest (Breiman 2001)



Feature importance measures: an input parameter X_i is considered important if when breaking the link between X_i and the output Y by permutation, the RF prediction error increases.

Uncertainty quantification

Workflow for scalar variables

Case study

PESHMELBA
=
vertical infiltration
+
surface runoff
+
lateral exchanges
+
pest. degradation
+
pest. adsorption

→ 145 input parameters

Spatialized scalar output:

- ✓ water/pest. surface runoff
- ✓ water/pest. subsurface flow

1 Screening (4,000-pts LHS)

Independence test based on HSIC measure

$$p\text{-val}_B = \frac{1}{B}\sum_{b=1}^{B} \mathbb{1}_{\widehat{HSIC}^{[b]}(X_i,Y) > \widehat{HSIC}(X_i,Y)}$$

2 Ranking (1,000-pts LHS)

a. Site indices: one GSA per HU

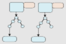
- ✓ Sobol' indices from PCE

$$S_{i_1,\ldots,i_s} = \frac{V_{i_1,\ldots,i_s}}{\mathrm{Var}[Y]}$$

- ✓ HSIC dependence measures

$$HSIC(X_i, Y)_{\mathcal{F}_i,\mathcal{G}} = ||C[\mathcal{G}\mathcal{F}_i]||^2_{HS}$$

- ✓ RF feature importance measures



b. Aggregated indices: one GSA for the whole catchment

- ✓ Aggregated Sobol indices (Gamboa 2014)

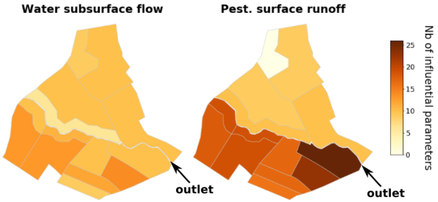
$$S_u = \frac{\sum_{j=1}^{d} \mathrm{Var}[Y_j] S_{u,j}}{\sum_{j=1}^{d} \mathrm{Var}[Y_j]}$$

- ✓ Aggregated HSIC indices
- ✓ Aggregated RF indices

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

After screening:

- Water lateral transfer: 42 parameters
- Pesticide surface runoff: 45 parameters



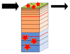
Number of parameters per HU after screening

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

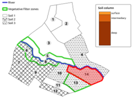
✓ Spatial heterogeneities consistent with heterogeneities in physical processes activation

Uncertainty quantification

Results - ranking (scalar variables)



Ranking for cumulated pesticide mass transferred in surface runoff



Uncertainty quantification

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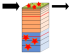

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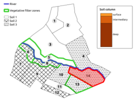
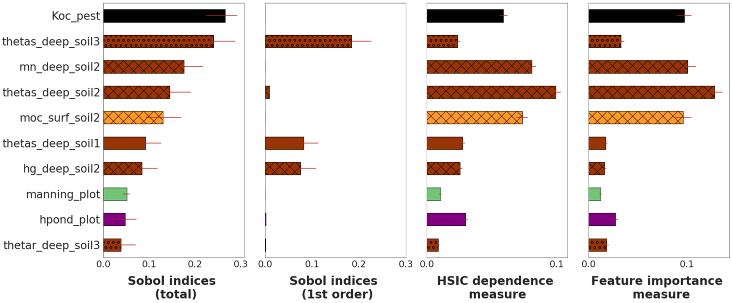
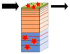




- ✓ Rankings from Sobol' **total** indices, HSIC and RF measures are mainly consistent
- ✓ Quantitative differences due to the contrasts in *Sensitivity* definition
- ✓ Uncertainty + on Sobol' indices: PCE estimation quality ?



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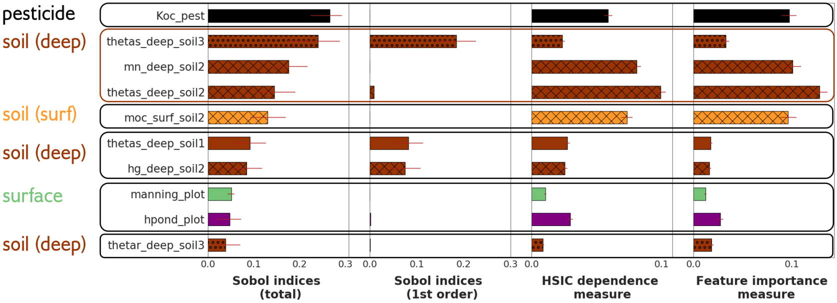
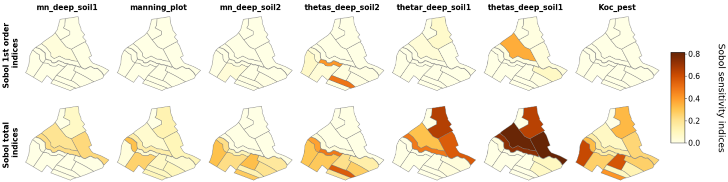
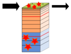


- ✓ Influential parameters relate to various physical processes of transfers **and** transformation: adsorption, overland flow, vertical infiltration...
- ✓ This ranking reflects the interactions of physical processes in PESHMELBA

Ranking for cumulated pesticide mass transferred in surface runoff

Site sensitivity indices





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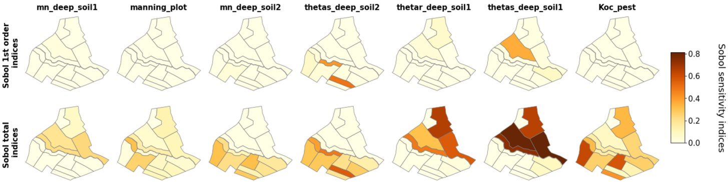

✓Detailed insights into the model sensitivity but computationally costly

Uncertainty quantification

Results - landscape analysis (scalar variables)

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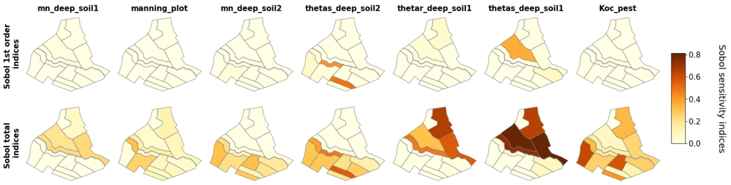

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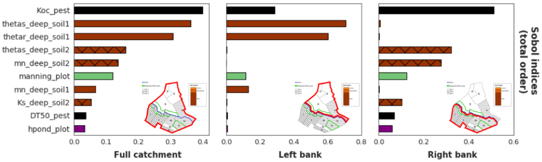
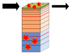
Aggregated sensitivity indices





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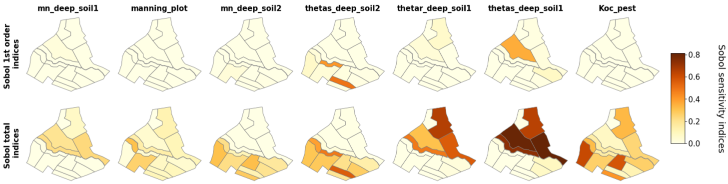

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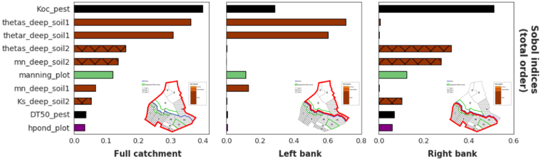

- ✓ Summary of overall sensitivity
- ✓ Hillslope scale used as an intermediary scale to mantain physical interpretation of aggregated indices

- Rankings mainly consistent for hydro. variables
- Differences for more complex pest. variables due to differences in "*sensitivity*" definitions
- Sobol aggregated indices at intermediary scale provide valuable information about the physics + overall summary on sensitivity
- We choose Sobol indices as they capture interactions but HSIC and RF should not be discarded for "simple" variables (many advantages).
- How could we transpose the methodology to real catchments ? ⇒ New challenges: spatialized, dependent input parameters ? choice of a relevant intermediary scale to guarantee physical interpretability of results ?