Calibrating a hydrological model robustly to rain perturbations with stochastic surrogates

Katarina Radišić, Claire Lauvernet, Arthur Vidard

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Claire Lauvernet[1], Arthur Vidard[2]

[1]INRAE, RiverLy, Lyon-Villeurbanne

[2]Univ. Grenoble-Alpes, Inria, CNRS, Grenoble-INP, LJK

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Liberté
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Context

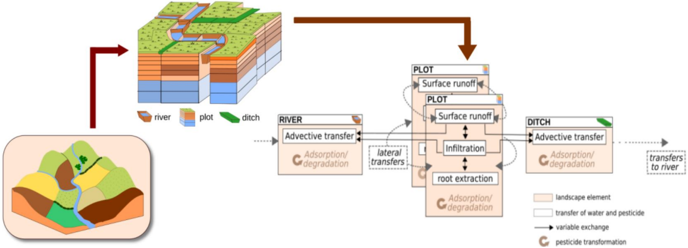

Figure: PESHMELBA[a], a process-based, spatially distributed water and pesticide transfer model, representing dynamical behavior of pesticides in agricultural catchments. Semi-conceptual, semi-physically based model, highly non-linear.

[a] Emilie Rouzies et al. (June 2019). "From agricultural catchment to management scenarios: A modular tool to assess effects of landscape features on water and pesticide behavior". en. In: *Science of The Total Environment* 671, pp. 1144–1160.

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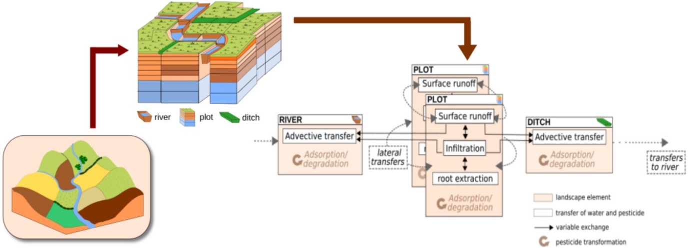

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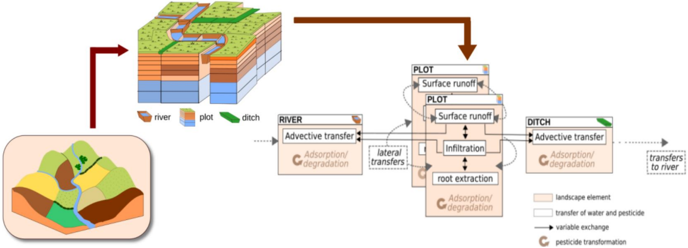

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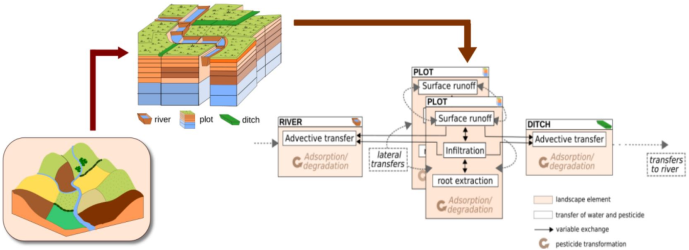

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- Impact of external uncertainties on the calibration results

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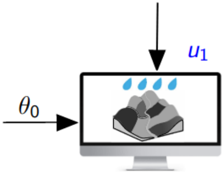

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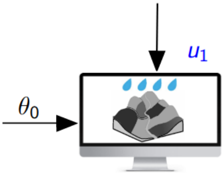

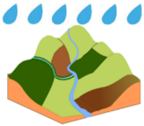

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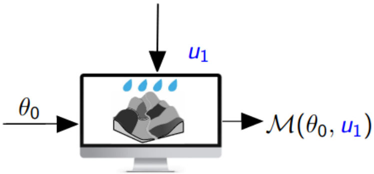

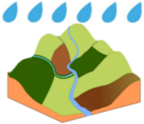

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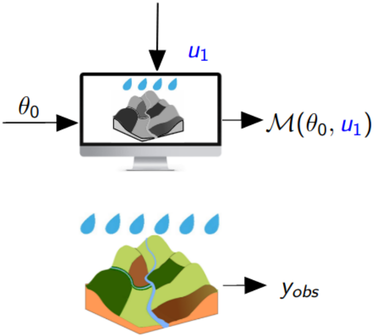

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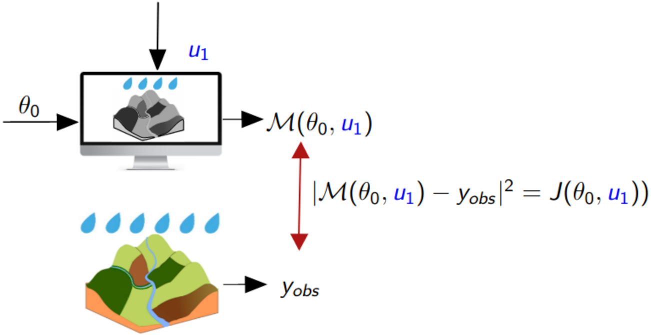

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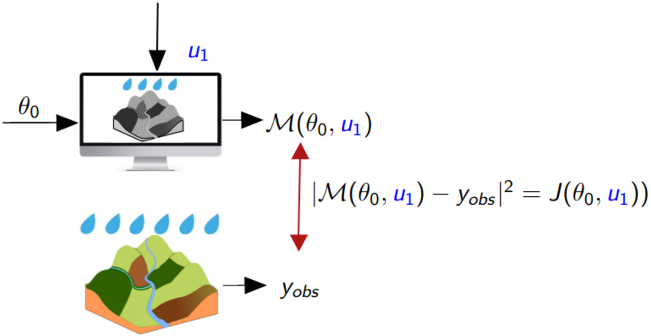

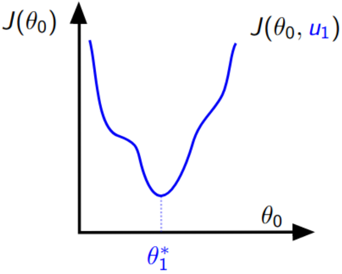

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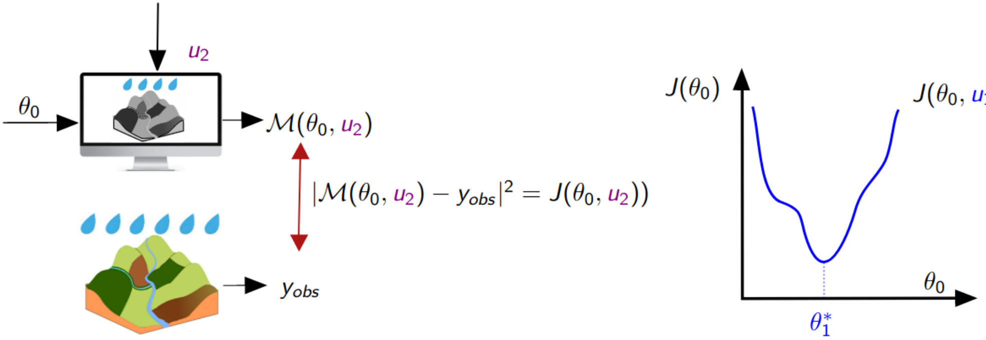

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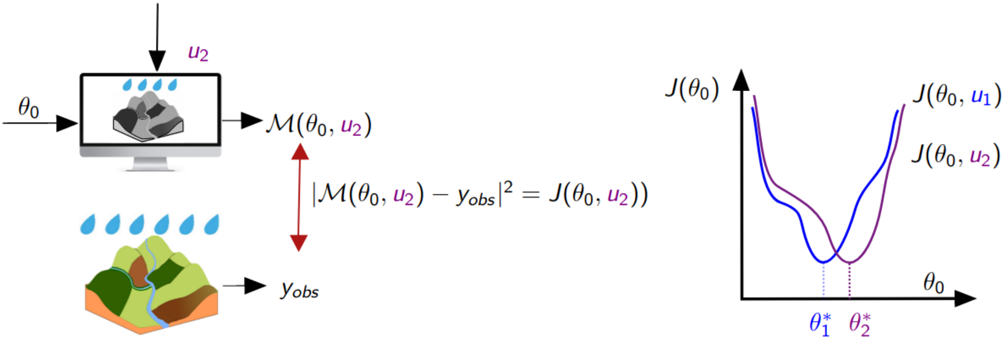

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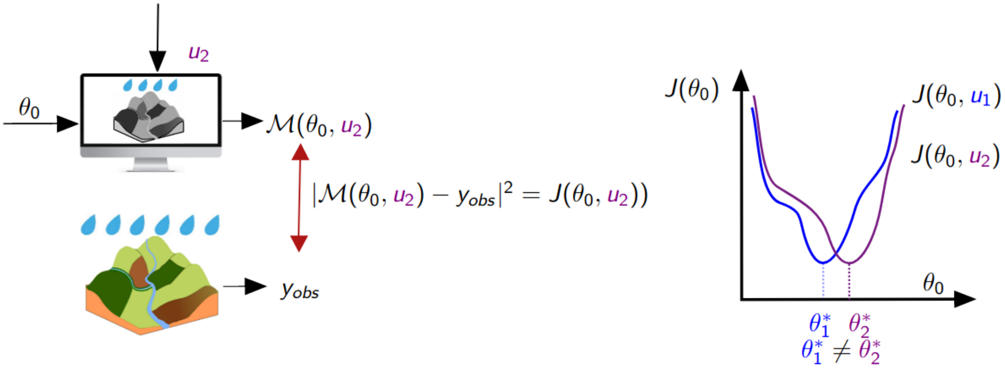

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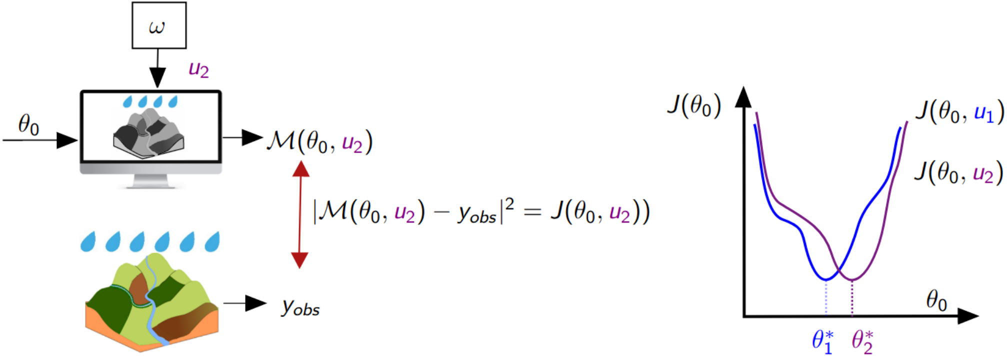

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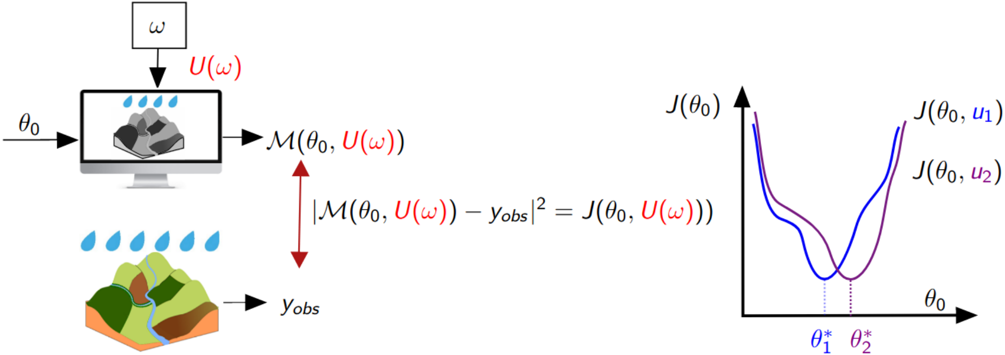

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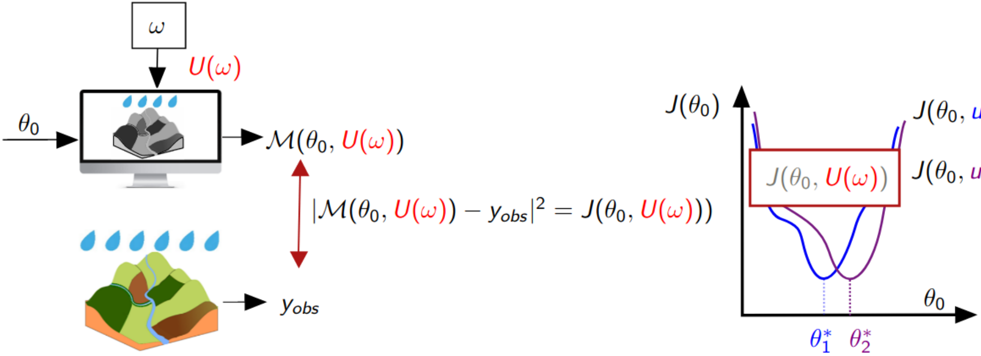

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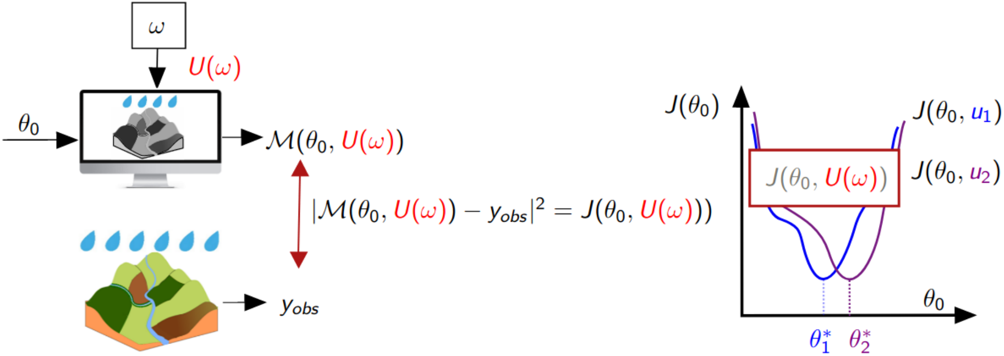
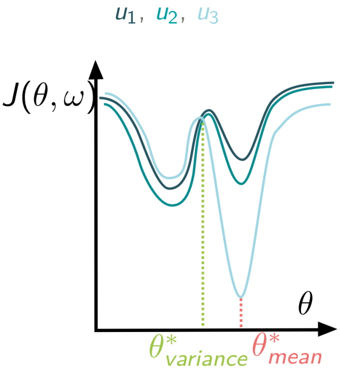


What does it mean to find a *robust* minimizer ?

Methods: Robust estimators



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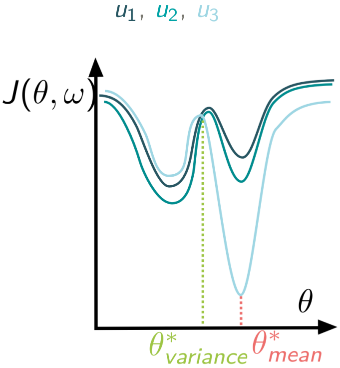

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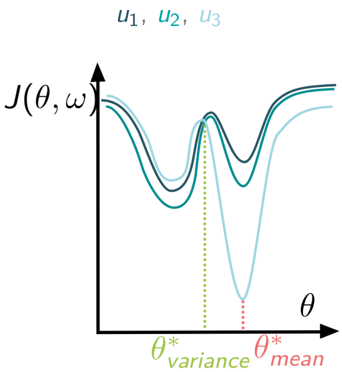

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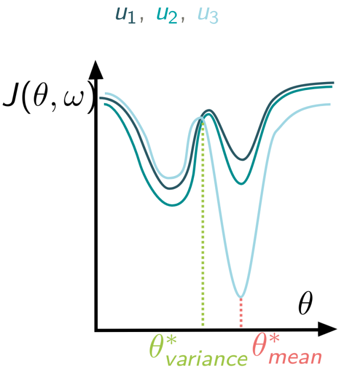

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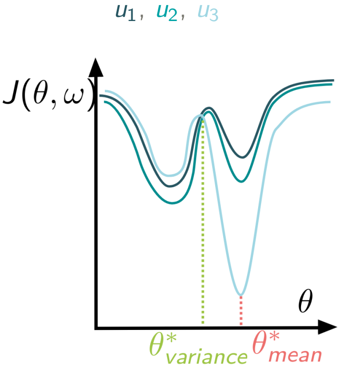

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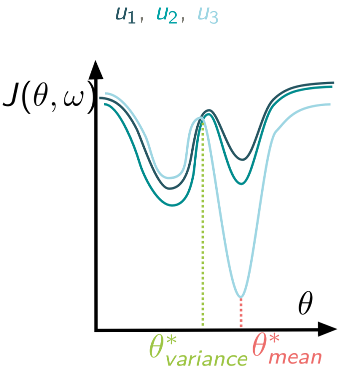

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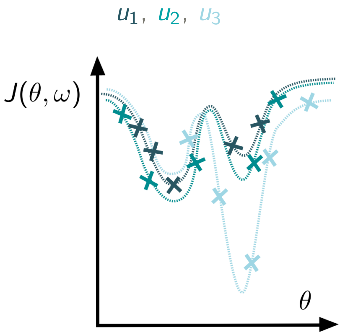

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[a] Nora Lüthen, Stefano Marelli, and Bruno Sudret (Mar. 2023). "A spectral surrogate model for stochastic simulators computed from trajectory samples". en. In: *Computer Methods in Applied Mechanics and Engineering* 406, p. 115875.

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- representation of the impact of the variability of the rain on the cost function through a random variable in the latent space
- the mean and variance are analytically available and independent of the distribution of Z

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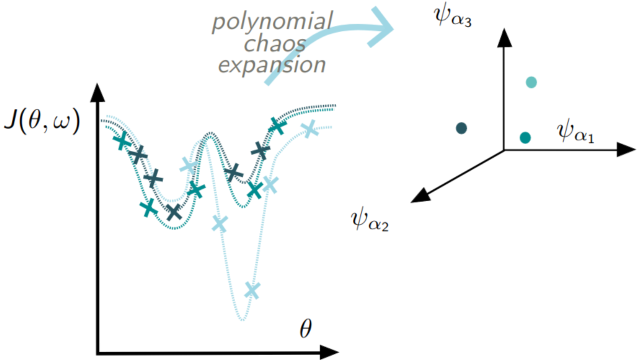

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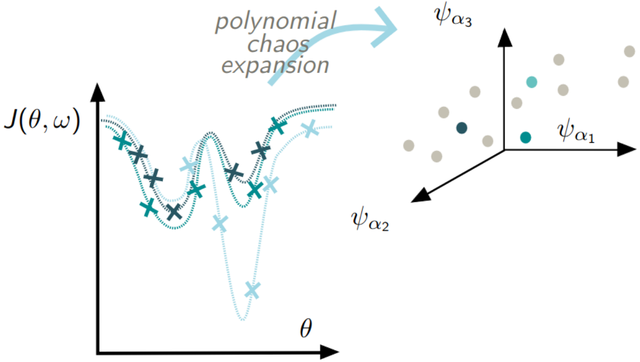

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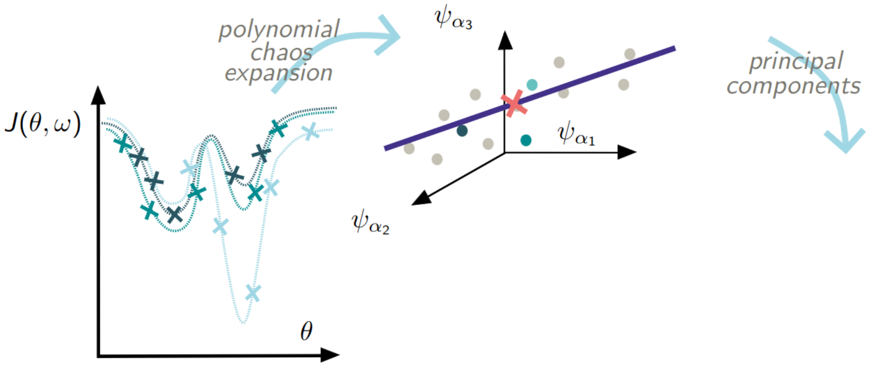

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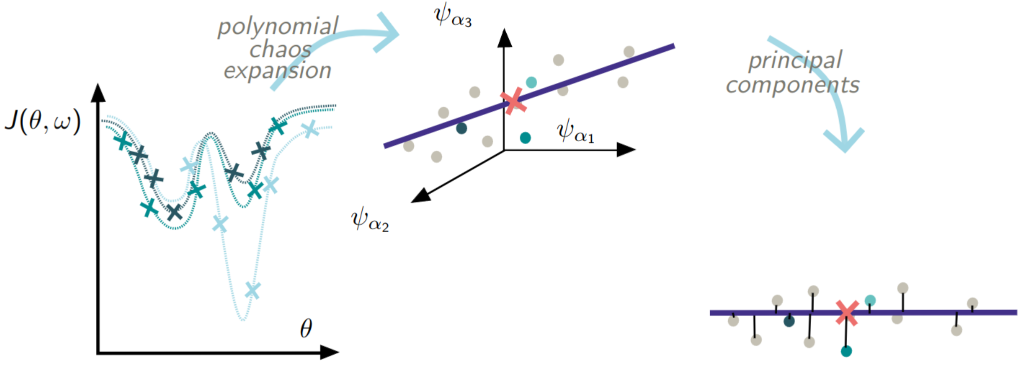

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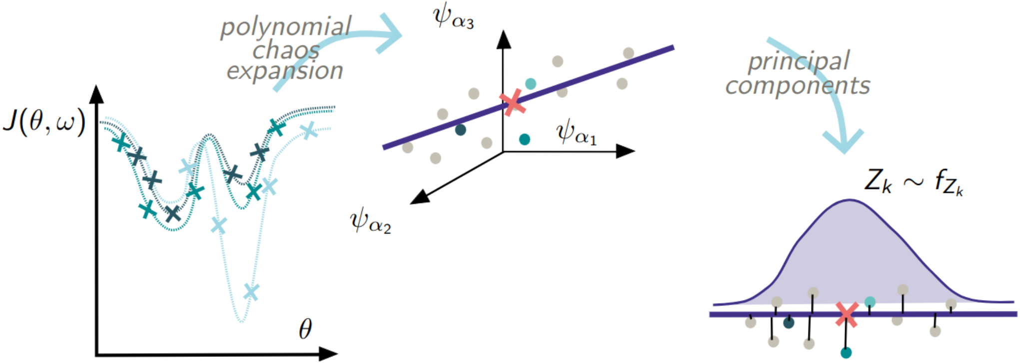

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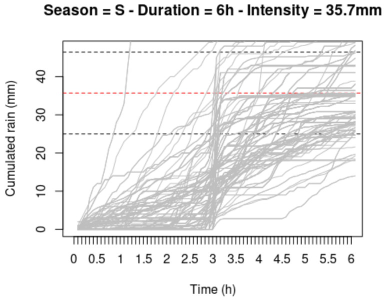
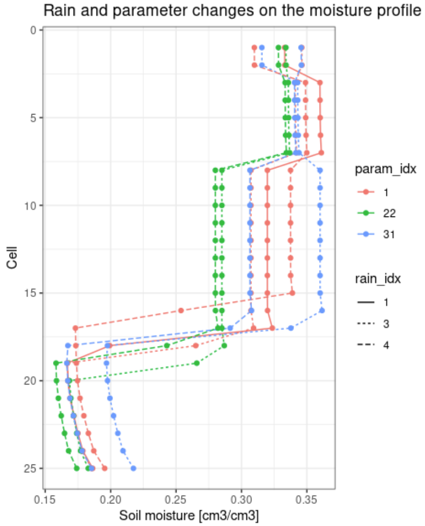
Case study: Moisture profile observations, twin experience

$$J(\boldsymbol{\theta}, u) = (\mathcal{M}(\boldsymbol{\theta}, u) - y_{true})^2$$
$$\boldsymbol{\theta} \in \mathbb{R}^6$$
$$y_{true} \in \mathbb{R}^{25}$$





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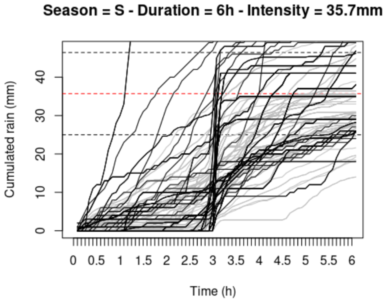

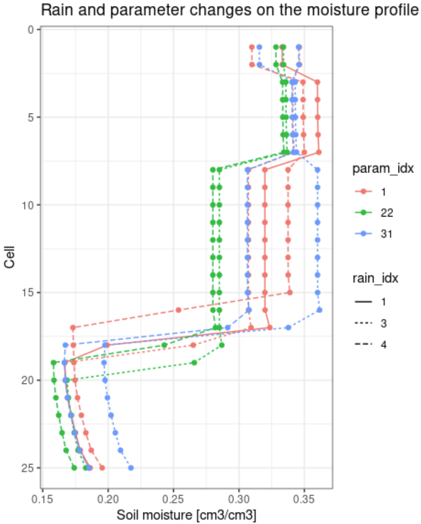

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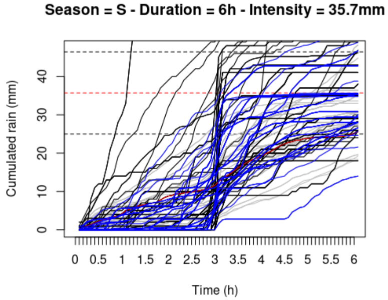

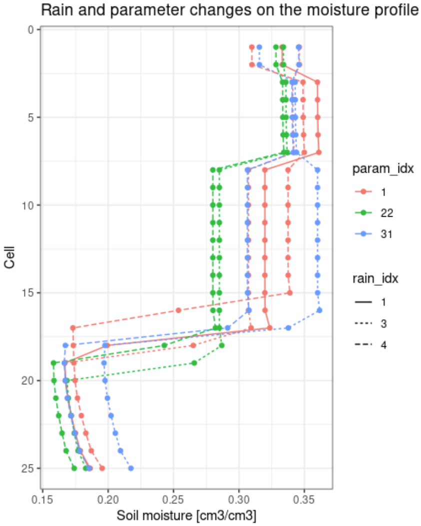

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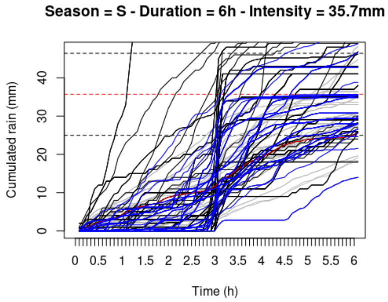
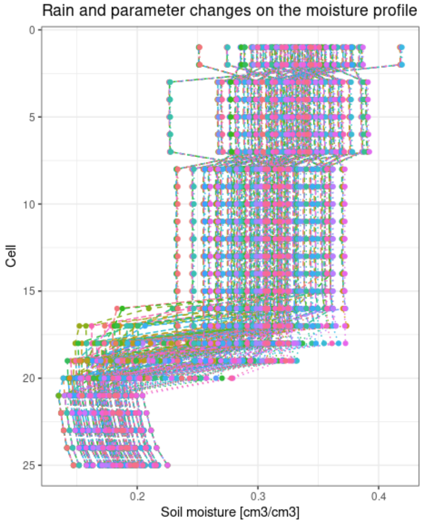




Results: Conditional minimization

- PCE constructed conditionally to each train rain realization.
- Determination coefficients $R^2 > 0.95$
- Minimization BFGS conditionally to each rain realization.

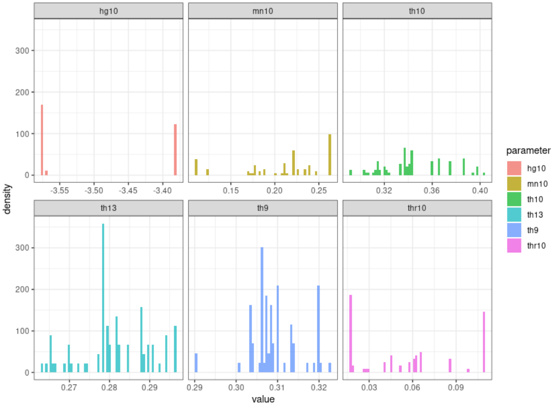


Figure: Histogram of conditional minimizers to each train rain realization.

Results: Validation of the emulator

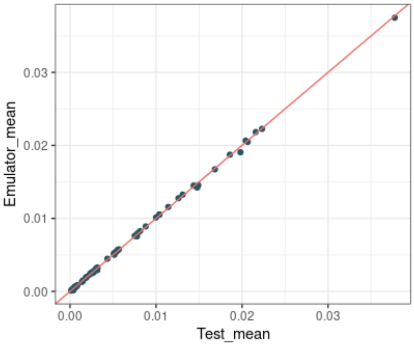


Figure: Comparison of the **train** and the **test** means $\mathbb{E}_U[J(\theta, U)]$.

$$\hat{J}(\theta, U(\omega)) = \hat{\mu}(\theta) + \sum_{k=1}^{K} \sqrt{\lambda_k} Z_k(\omega) \Big(\sum_{\alpha \in \mathcal{A}} b_\alpha^{(k)} \psi_\alpha(\theta) \Big)$$

- The emulator mean is a good estimator of the true mean.

Results: Validation of the emulator

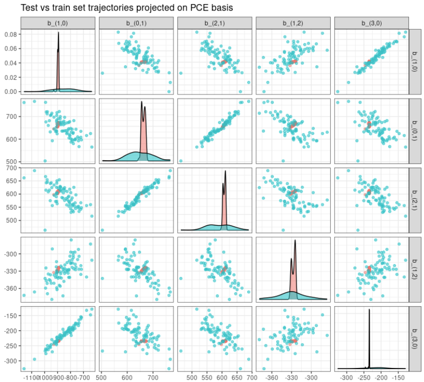


Figure: Comparison of the **train** and the **test** trajectories of PESHMELBA simulations, projected on the PCE basis.

$$\hat{J}(\boldsymbol{\theta}, U(\omega)) = \hat{\mu}(\boldsymbol{\theta}) + \sum_{k=1}^{K} \sqrt{\lambda_k} Z_k(\omega) \Big(\sum_{\alpha \in \mathcal{A}} b_\alpha^{(k)} \psi_\alpha(\boldsymbol{\theta}) \Big)$$

- The emulator mean is a good estimator of the true mean.
- The **train** set and the **test** set do not present the same variabilities, thus the emulator does not reproduce correctly the impact of rain perturbations on the cost function.

Results: Validation of the emulator

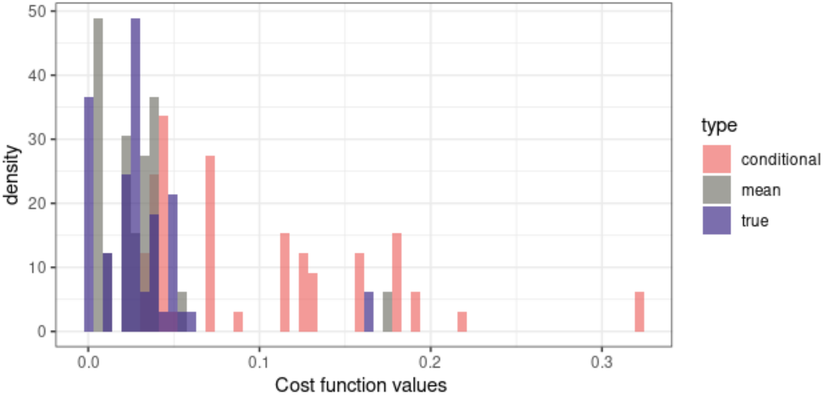


Figure: Cost function evaluated at the test rains, the simulations performed with the minimizer of the mean have a lower mean and variance than the one obtained with the minimizer conditioned on one rain realization.

Conclusion

- The PCE approximations on each conditioned rains have a determination coefficient $R^2 > 0.95$ and the approximation of the metamodel mean is good.
- The minimizer of the mean has lower cost function on unseen rains than a randomly chosen conditional minimizer.
- The variance of the metamodel is not a good estimate

What next ?

→ work on the estimation of the variance

→ study the Pareto-optimal minimizers

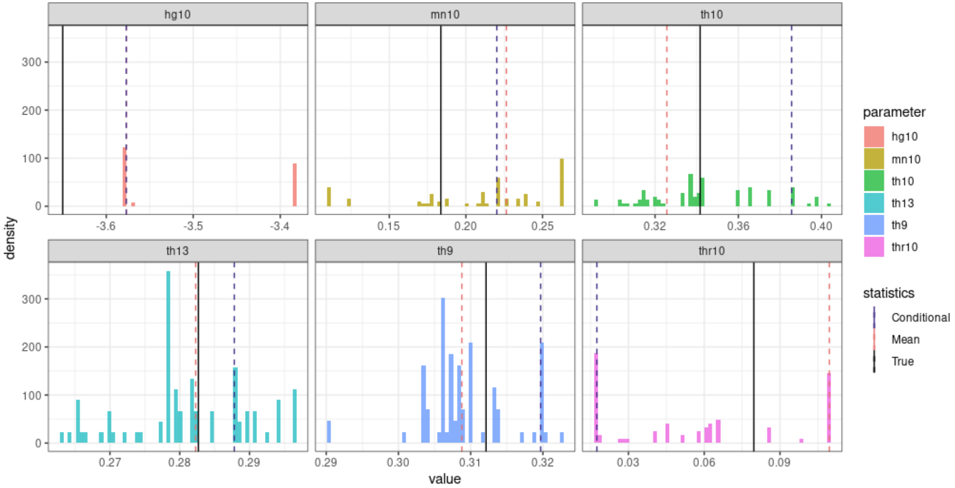
→ augment rain perturbations

→ minimize mean and variance with Gaussian Process based Efficient Global Optimization, compare the precision and number of model evaluations needed.

→ observe another output, for example pesticide quantities in the river, interaction will be added.

→ up the domain to the catchment scale

Thank you for your attention !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mn10
th10
th13
th9
thr10
density
value
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-3.5
-3.4
0.15
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0.09
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100
200
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parameter
hg10
mn10
th10
th13
th9
thr10
statistics
Conditional
Mean
True