

Data assimilation: overview and constraints for agro-ecology modelling

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Avec le soutien de :

Plan

Introduction

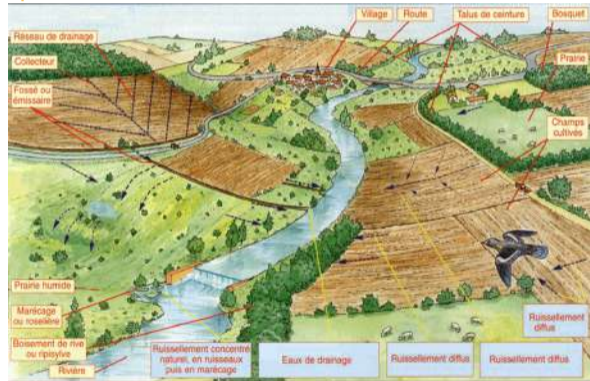
Data assimilation

An example of data assimilation in spatialized model

Context : How to improve the water quality ?

⇒ a better understanding of water and pesticide transfer in soil

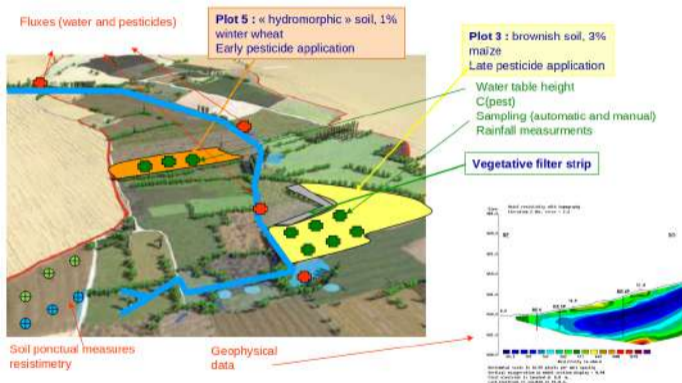
- Spatial heterogeneity of the soils, at all scales
- Soil and agricultural practices are more and more diverse
- Processes that drive the pesticide fate at the catchment scale are complex :
 - Hydrological transfer
 - adsorption
 - degradation



Spatially and temporally heterogeneous data...

Availability, quality, quantity of data are heterogeneous in space and time :

- remote sensing images
- field data (lysimeters in soil, water table and river measurements)
- geophysical data



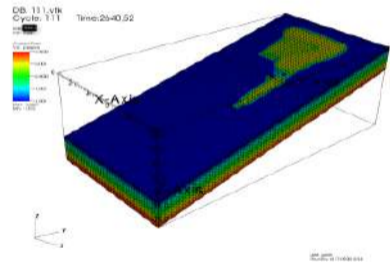
BUT without heavy experiments, this is very difficult to get the pesticides dynamics

Spatially and temporally heterogeneous data...

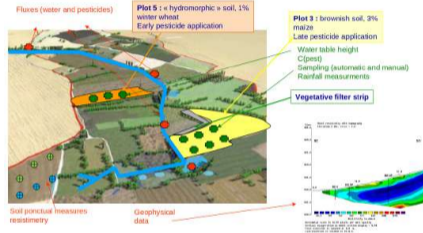
... and pesticides modeling at several scales and several complexity degrees

- based on non linear equations and/or conceptual
- unknown boundary and initial conditions
- a large set of spatialized parameters that are difficult to measure/estimate
- many processes affecting pesticide transfer are not (well) represented (e.g., pref. flows)

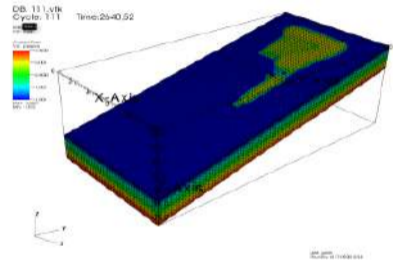
⇒ a high uncertainty (when we it is considered !)



Spatially heterogeneous data...



... and spatialized modeling



⇒ merging information from the available data and from the model to get as close as possible to the “true” state

Data Assimilation techniques (or *model-data fusion*)

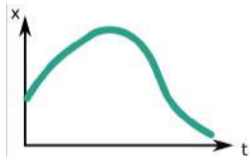
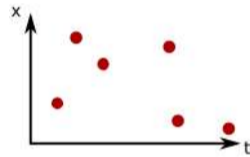
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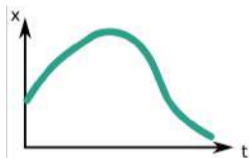
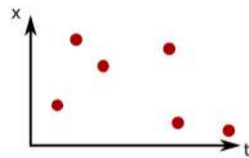
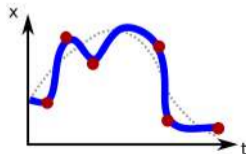
Data assimilation

An example of data assimilation in spatialized model

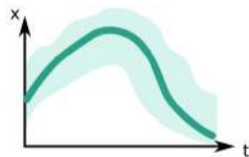
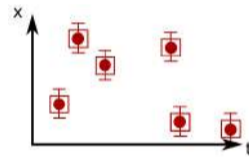
- the systematic use of data to constrain a numerical model
- first used in the 1960s in numerical weather forecasting models for short-term predictions of meteorological conditions
- in the 1970s, development in numerical ocean general circulation models (OGCMs)
- poorly developed in other domains (hydrology)

**Model****Observations**

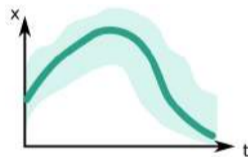
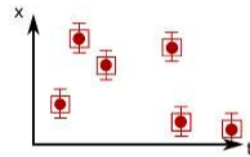
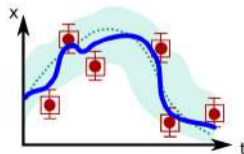
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Data assimilation

The ingredients

$\mathbf{x} = (\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N)^T$ represents the state of system:
streamflow at the outlet, soil moisture, dissolved oxygen concentration in the river, etc.
We don't know it, but we do have information from :

- **the dynamical model** $x_k = M_{k-1 \rightarrow k}[x_{k-1}, param] + \eta_k$

η_k the model error of covariance matrix P_k

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- **the observation model** $y_k = H_k[x_k] + \varepsilon_k$

y_k is the observation/data at time k

ε_k the observation error, of covariance matrix R_k , e.g. instrumental error, representativeness

$H : \mathcal{R}^m \rightarrow \mathcal{R}^d$ the observation operator that projects from model space to observational space

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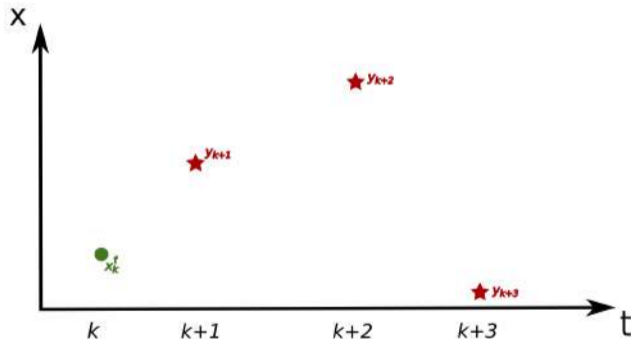
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- **the dynamical model** $x_k = M_{k-1 \rightarrow k}[x_{k-1}, param] + \eta_k$
- **the observation model** $y_k = H_k[x_k] + \varepsilon_k$
- We assume that model and obs. errors are random variables \rightarrow described by pdf

\Rightarrow Bayesian framework \Rightarrow The Kalman Filter

The Kalman Filter (Kalman 1960) : estimate the optimal state at each observation

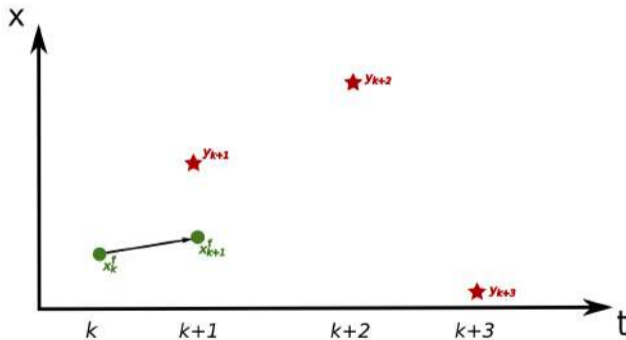
- ★ observation
 - forecast/prior for next step
 - analysis
- time



0. At time k : x_k^f

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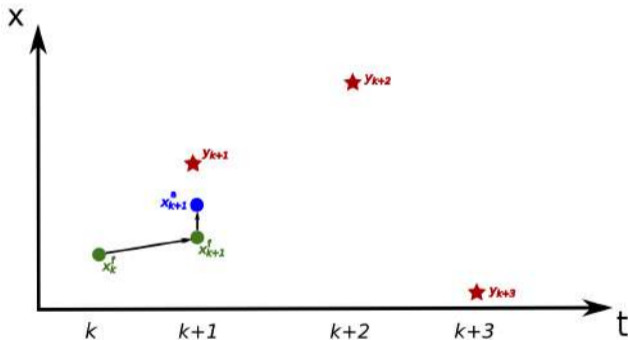
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1. Forecast step: $\mathbf{x}_{k+1}^f = \mathbf{M}\mathbf{x}_k^f$

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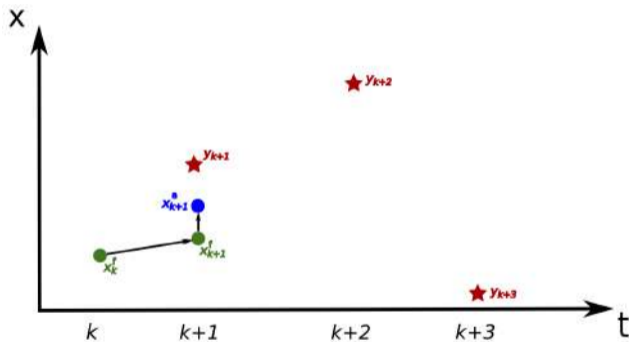
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2. Analysis step: $X_{k+1}^a = X_{k+1}^f + K_{k+1}(Y_{k+1} - H_{k+1}X_{k+1}^f)$

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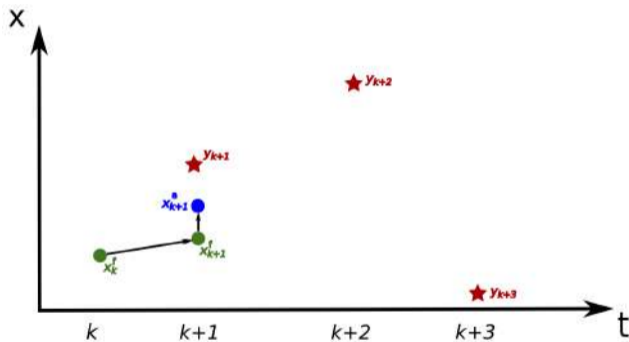
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 with $\mathbf{K}_{k+1} = \mathbf{P}_{k+1}^f \mathbf{H}_{k+1}^T [\mathbf{H}_{k+1} \mathbf{P}_{k+1}^f \mathbf{H}_{k+1}^T + \mathbf{R}_{k+1}]^{-1}$

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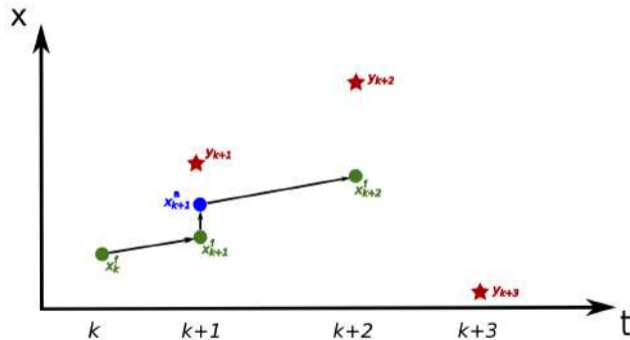


2. Analysis step: $\mathbf{X}_{k+1}^a = \mathbf{X}_{k+1}^f + \mathbf{K}_{k+1}(\mathbf{Y}_{k+1} - \mathbf{H}_{k+1}\mathbf{X}_{k+1}^f)$

$$\mathbf{P}_{k+1}^a = \mathbf{P}_{k+1}^f - \mathbf{K}_{k+1}\mathbf{H}_{k+1}\mathbf{P}_{k+1}^f$$

The Kalman Filter (Kalman 1960) : estimate the optimal state at each observation

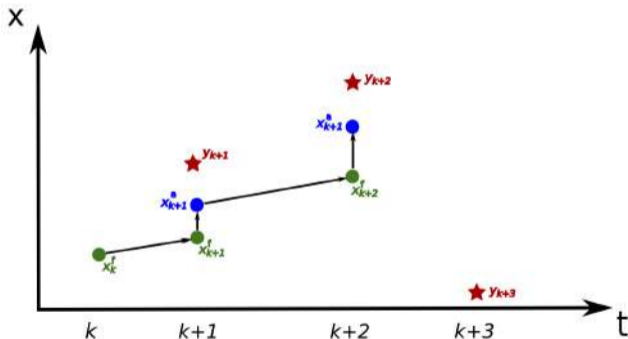
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time ● analysis



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time

The KF assumes that:

- ✓ all sources of errors are gaussian
- ✓ both the observational and dynamical models are linear

→ not realistic in most cases !

Data assimilation

The method for data assimilation should be suited to spatialized models

- models are physically-based but:
 - highly nonlinear equations (Richards, ...)
 - some are more/less conceptual
=> discontinuities, thresholds
- **definitely not gaussian !**
- **Ensemble filter approaches**

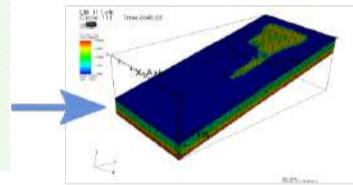
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$$\begin{aligned} S_w S_w \frac{\partial \theta}{\partial t} + \theta \frac{\partial S_w}{\partial t} &= \nabla [K_r K_r (\nabla \theta + \eta_w)] + q_w \\ \frac{\partial Q}{\partial t} + \alpha \frac{\partial Q}{\partial s} - D_s \frac{\partial^2 Q}{\partial s^2} + c_s q_s(h, \theta) \\ \frac{\partial \theta c}{\partial t} &= \nabla \cdot (-\vec{U}c + D \nabla c) + q_{pc} \\ \frac{\partial Q_m}{\partial t} + c_s \frac{\partial Q_m}{\partial s} &= D_s \frac{\partial^2 Q_m}{\partial s^2} + c_s q_{ms} \end{aligned}$$

CATHY-Pesticides

Camporese et al., 2010

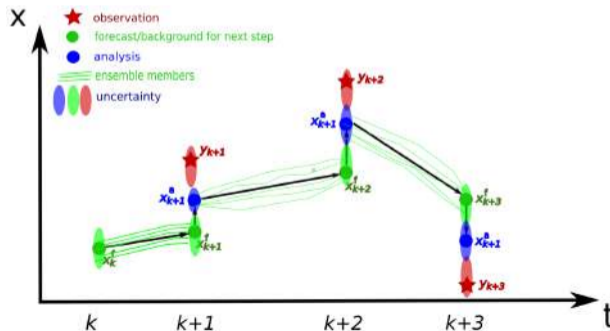
Gatel et al., 2019



Data assimilation

Ensemble-based methods (Evensen 2003)

- a version of the Kalman filter for nonlinear problems at large dimension
- the state variable distribution is represented by an ensemble of state vectors x_k
- the error covariance matrices are represented by the ensemble covariance



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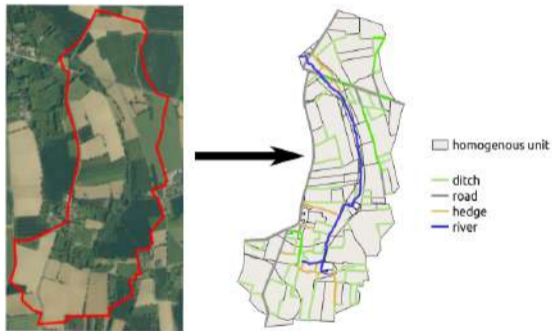
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The PESHMELBA model (Rouzies et al. 2019)

PESticides et Hydrologie: Modélisation à l'EcheLle du BAssin versant

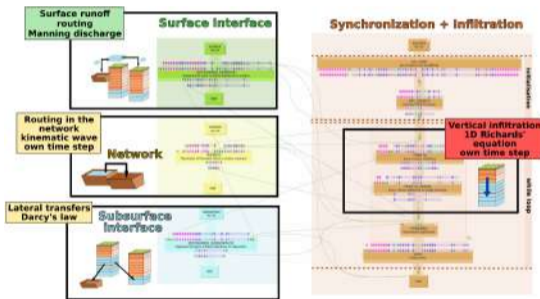
- ✓ Simulation of heterogenous landscapes composed of plots, vegetative filter zones, hedges, ditches and rivers
- ✓ Water transfers on surface and subsurface
- ✓ Solute advection, adsorption and degradation



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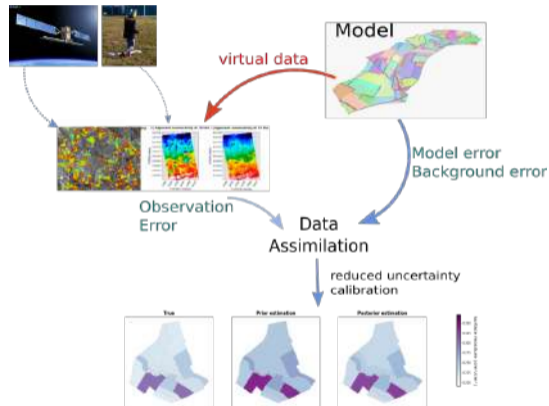
- ✓ Simulation of heterogenous landscapes composed of plots, vegetative filter zones, hedges, ditches and rivers
- ✓ Water transfers on surface and subsurface
- ✓ Solute advection, adsorption and degradation
- ✓ One module \equiv one process or ensemble of processes on a landscape element
- ✓ Coupling of modules within the OpenPALM coupler (Fouilloux and Piacentini 1999) turning the structure flexible



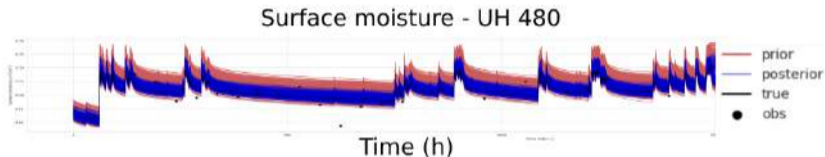
Twin experiments

A virtual experiment where we know the true state : an output of the model

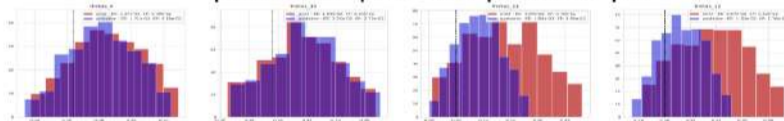
- obs $y = x^{true} + error$
- “data” = images of surface soil moisture => virtual data
- model = PESHMELBA
- errors are gaussian



Twin experiments with PESHMELBA



parameter prior and posterior pdf



Twin experiments with PESHMELBA










Conclusion

- the twin experiment show the feasibility of DA in pesticide transfer modeling
- assimilate other images than at surface
- define the spatial (and temporal?) correlation in obs. error (E. Rouzies PhD)
- test with real images \Rightarrow scale the model to the data (observation operator)
- combine images with in situ data to improve the water quality predictions
- development on the CATHY model, purely physics-based (less discontinuities?)

\Rightarrow data assimilation = an optimal way to merge information

Thank you!

Any questions ?

-  Camporese, M. et al. (2010). "Surface-subsurface flow modeling with path-based runoff routing, boundary condition-based coupling, and assimilation of observation data". In: *Water Resources Research* 46.2.
-  Evensen, Geir (2003). "The Ensemble Kalman Filter: theoretical formulation and practical implementation". In: *Ocean Dynamics* 53.4, pp. 343–367.
-  Fouilloux, A. and A. Piacentini (1999). "The PALM Project: MPMD Paradigm for an Oceanic Data Assimilation Software". In: *Euro-Par'99 Parallel Processing: 5th International Euro-Par Conference Toulouse, France, August 31 - September 3, 1999 Proceedings*. Berlin, Heidelberg: Springer Berlin Heidelberg, pp. 1423–1430.
-  Gatel, Laura, Claire Lauvernet, Nadia Carluer, Sylvain Weill, and Claudio Paniconi (2019). "Sobol Global Sensitivity Analysis of a Coupled Surface/Subsurface Water Flow and Reactive Solute Transfer Model on a Real Hillslope". In: *Water* 12.1, p. 121.
-  Gatel, Laura, Claire Lauvernet, Nadia Carluer, Sylvain Weill, Julien Tournebize, et al. (2019). "Global evaluation and sensitivity analysis of a physically based flow and reactive transport model on a laboratory experiment". In: *Environmental Modelling & Software* 113, pp. 73–83.
-  Kalman, Rudolph Emil (1960). "A New Approach to Linear Filtering and Prediction Problems". In: *Transactions of the ASME—Journal of Basic Engineering* 82.Series D, pp. 35–45.
-  Rouzies, Emilie et al. (2019). "From agricultural catchment to management scenarios: A modular tool to assess effects of landscape features on water and pesticide behavior". In: *Science of The Total Environment* 671, pp. 1144–1160.