# Introduction to Geostatistics - Metamodeling with Gaussian processes

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# Main stakes of uncertainty management

- **Modeling phase**
  - Improve the model
  - Explore the best as possible different input combinations
  - Identify the predominant inputs and phenomena in order to priorize R&D

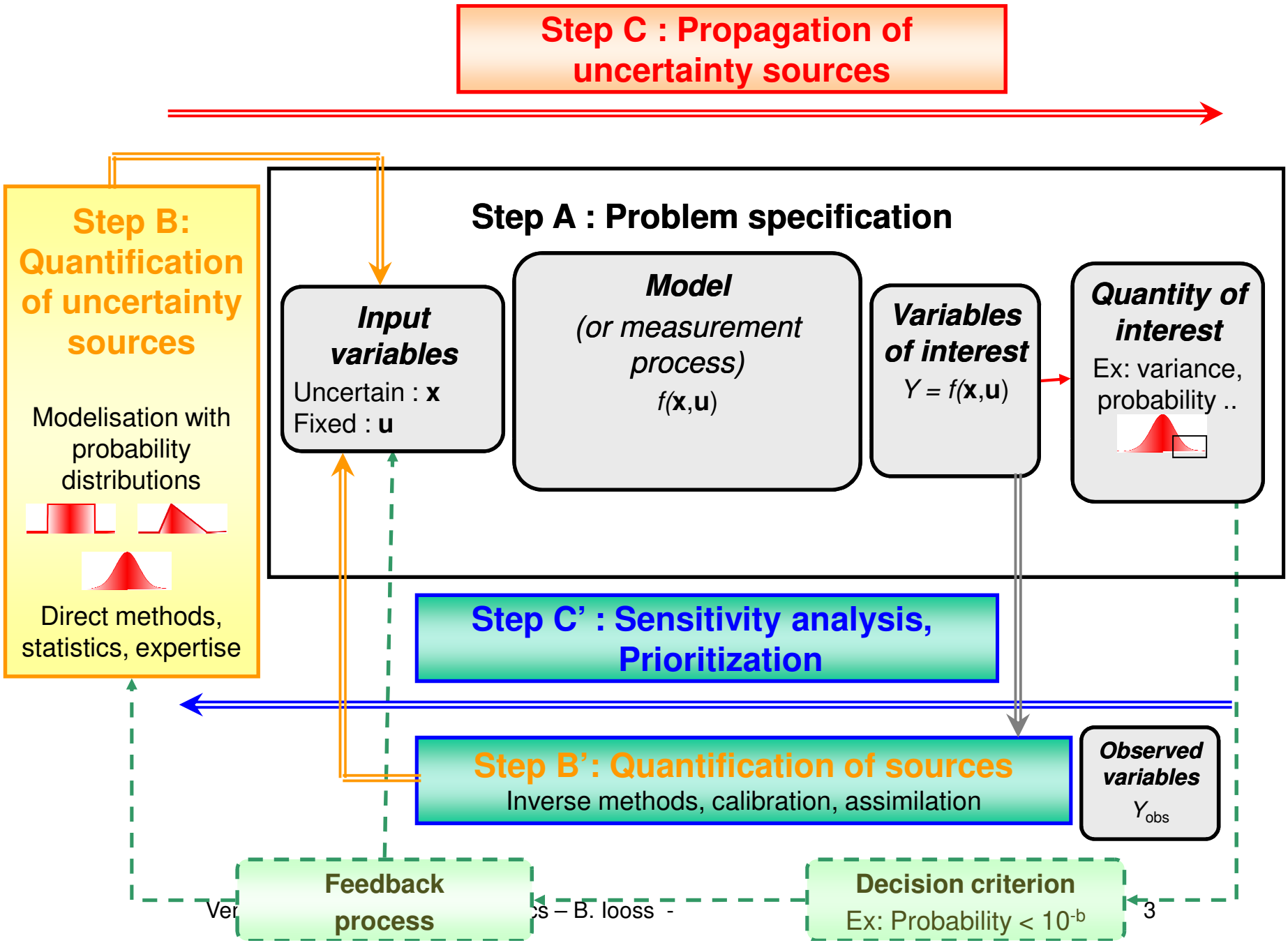
- **Validation phase**
  - Reduce prediction uncertainties
  - Calibrate the model parameters

- **Practical use of a model**
  - **Safety studies:** assess a risk of failure (rare events)
  - **Conception studies:** optimize system performances and robustness

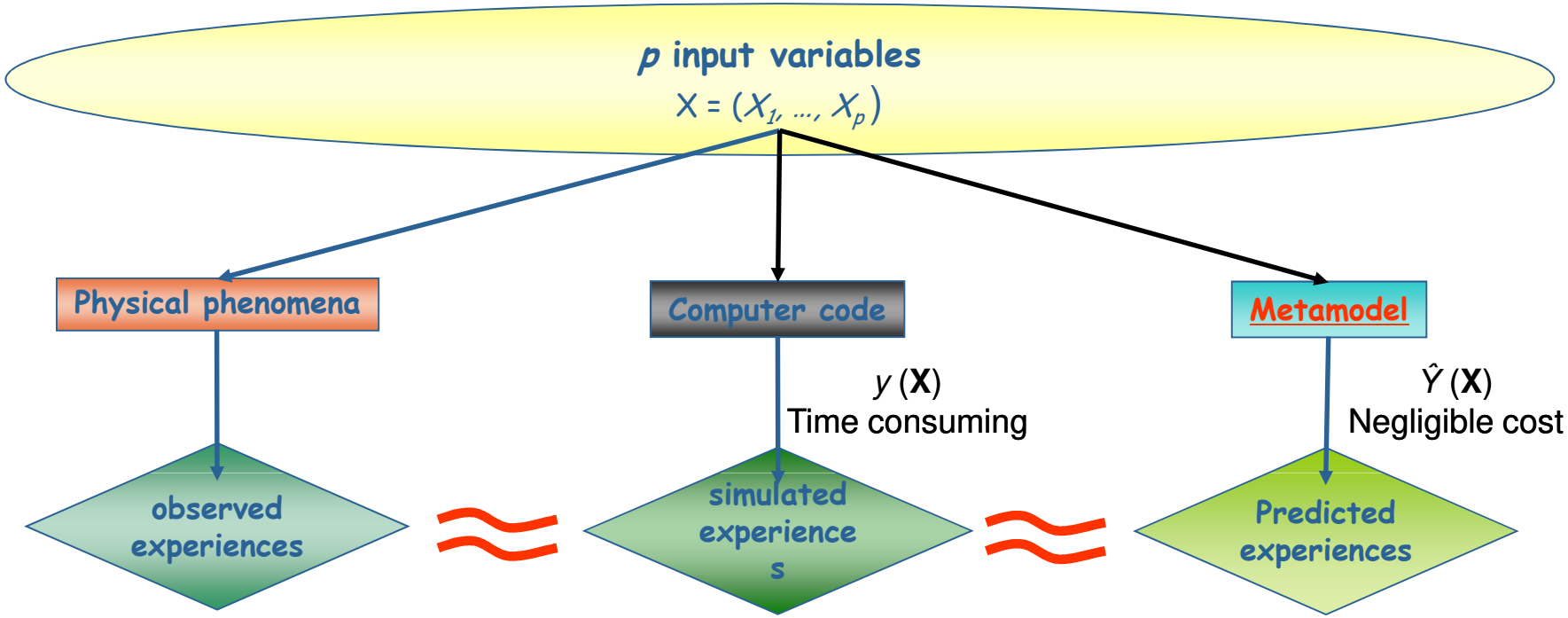
Advantages of a probabilistic approach

- to propagate the uncertainties, to perform global sensitivity analysis
- to design/optimize the system taking into account uncertainties
- to give rigorous safety margins, …

# Uncertainty management - The generic methodology

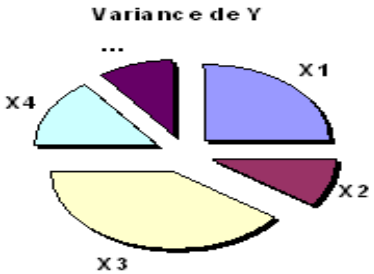


# Uncertainties management for cpu time consuming models

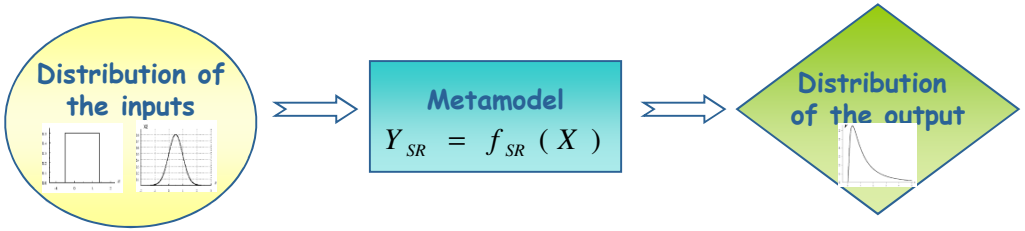



## Use of the metamodel :

- C':Sensitivity analysis




- C:Uncertainty propagation (via Monte Carlo methods)




- B':Calibration

Identification of input parameters values

Adequation between observed and simulated experiences

# Metamodel : definition

*[ Kleijnen 70's ]*

**A metamodel is a mathematical function**

- **which approximates the outputs of the model,**
- **with neglgible cpu cost,**
- **which allows to make new output predictions with a good accuracy**

• <u>Synonyms:</u>

- Response surface
- Simplified model
- Emulator
- Proxy model
- Surrogate model

# Metamodeling steps

**Design of experiments:**

Points to perform simulations

→

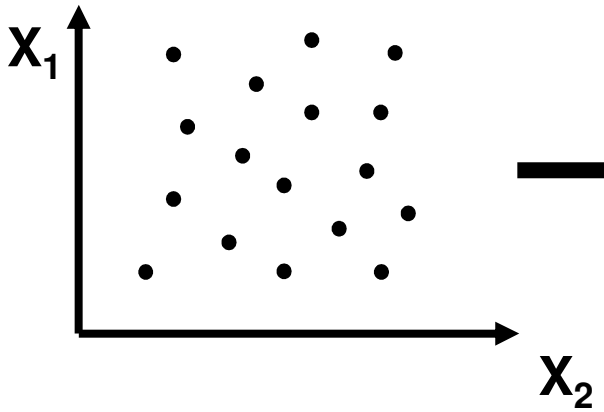
**Simulation :**

Performing simulations

→

**Metamodeling :**

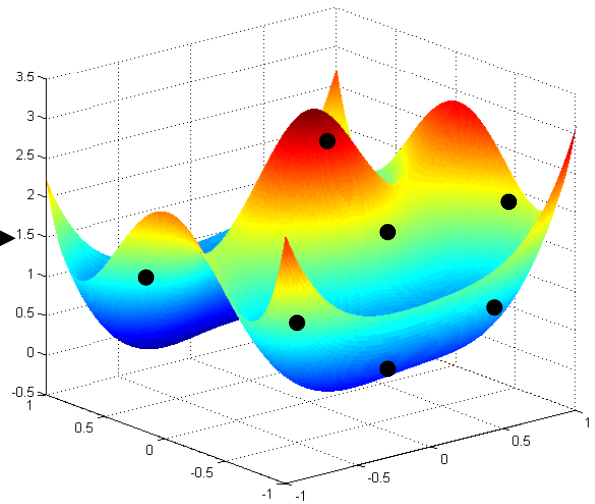
**Approximation of the computer code**




→

**Computer code**

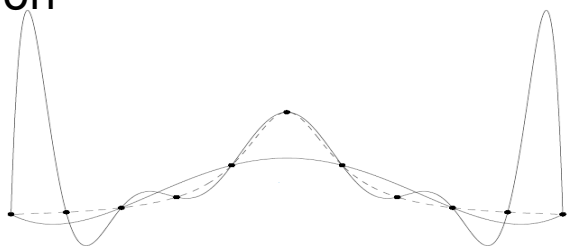
→

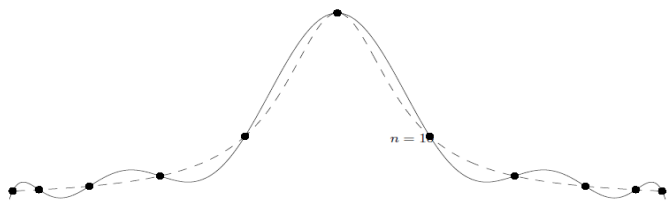


# Differents types of metamodels

[ Simpson et al. 2001 ]
[ Storlie & Helton 2008 ]

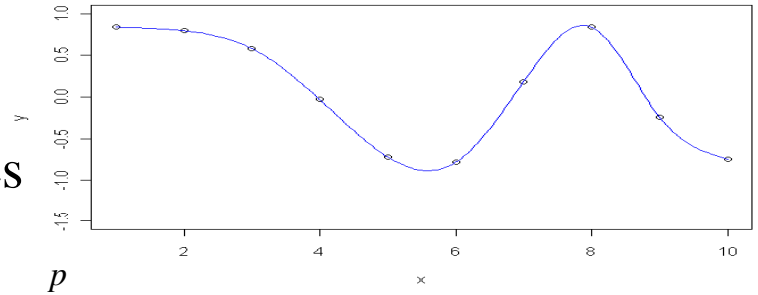
- Linear regression






- Polynomials

- Splines




$$\hat{G}(\mathbf{x}) = \sum_{k=1}^{K} \hat{\beta}_k B_k(\mathbf{x}) \text{ with } K \text{ the number of nodes}$$

- Additive models, GAM $\hat{G}(\mathbf{x}) = \sum_{i=1}^{p} s_i(x_i) + \sum_{i<j}^{p} s_{ij}(x_i, x_j) + \cdots$

- Regression trees $\hat{G}(\mathbf{x}) = \sum_{k=1}^{K} \hat{\beta}_k I_k(\mathbf{x})$

- Neural networks
- Chaos polynomials
- Support Vector Machines
- Kriging – Gaussian process

# Kriging metamodel

Kriging *[ Matheron 63 ]* for computer codes relies on the idea to interpolate the code outputs in dimension *p* *[ Sacks et al. 89 ]* as a spatial cartography

**Kriging (or Gaussian process) is interesting because:**

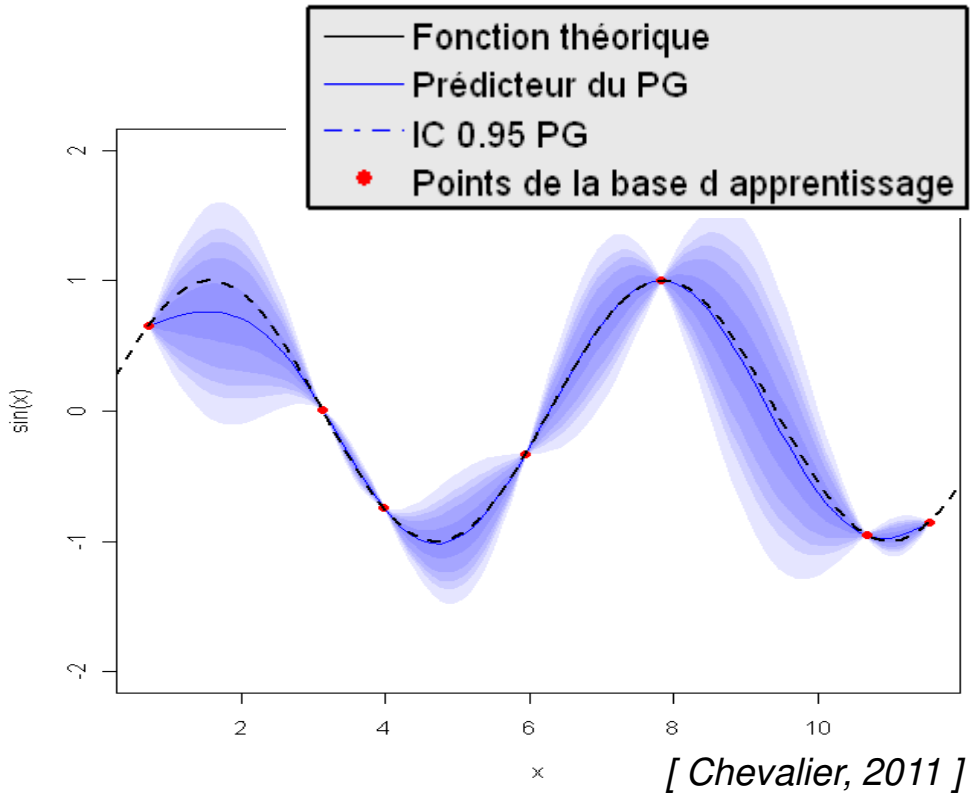
- **it interpolates the outputs,**
- **it gives predictor associated with confidence bands**

<u>Example in 1D :</u>

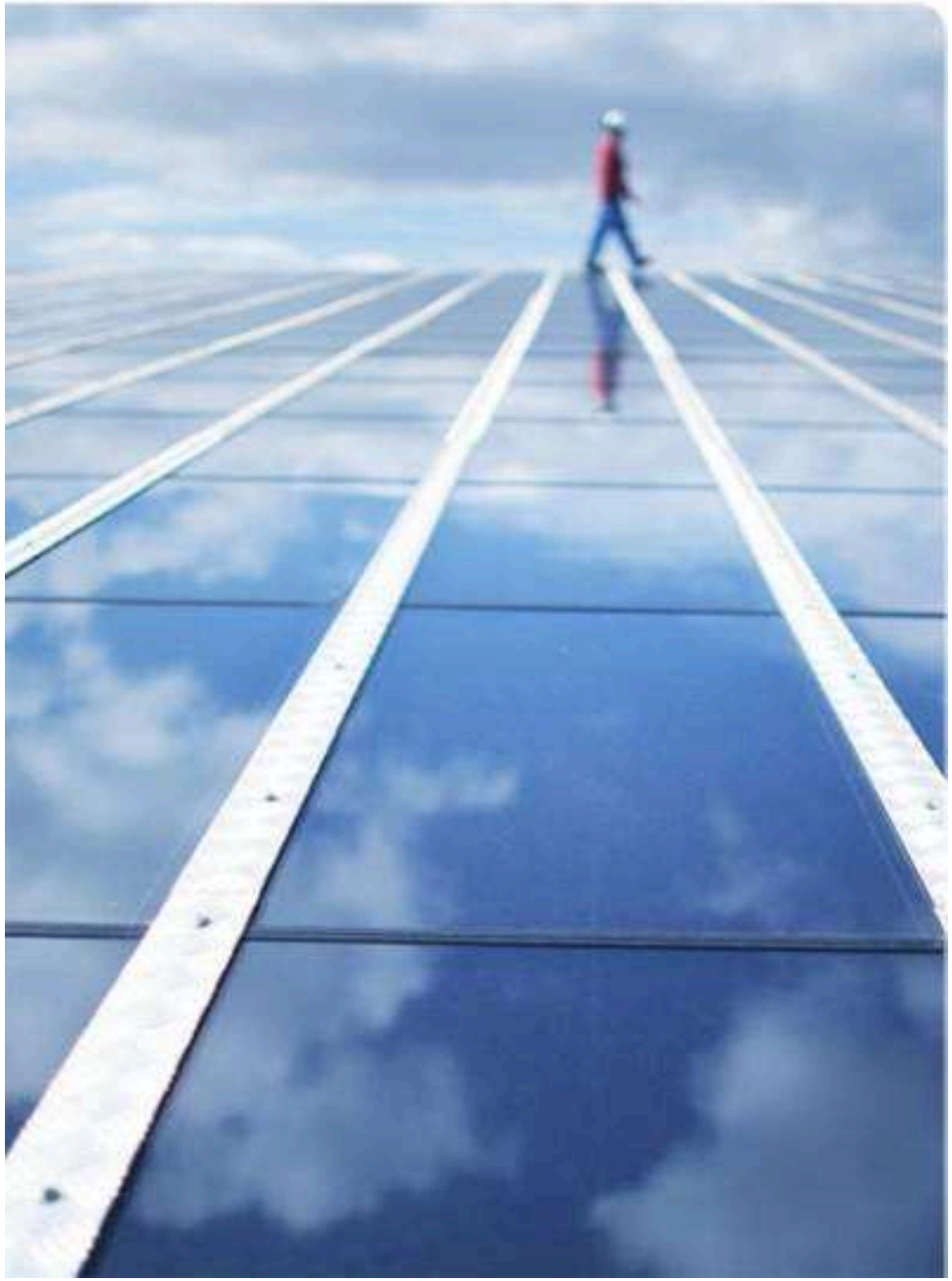
Theoretical function ($p$ =1) :

$$Y = f(X) = \sin(X)$$

Simulation of $N$ = 7 computation points




*[ Chevalier, 2011 ]*



# Introduction to Geostatistics

# Introduction to Geostatistics

Objectives : treatment of **numerical data** with **spatial support** (or temporal) with **uncertainty quantification**

**Principal aspects:**

- Taking into account the spatial structure of data,
- Dimension 1, 2, 3, …,
- Irregular sampling,
- Integrating external information

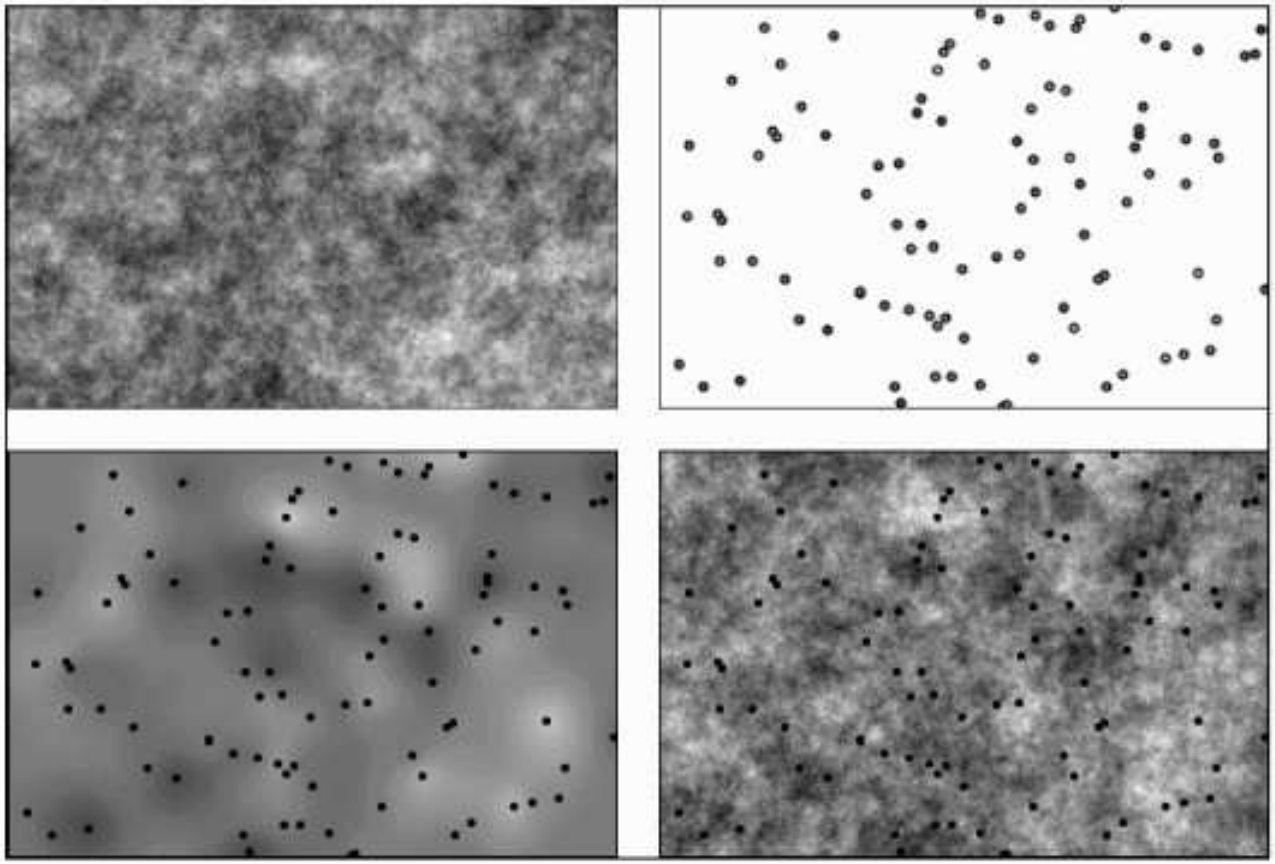
**2 types of methods:**

- **Estimation** (prediction, …) at a given point
- **Simulations** reproducing the variability of the phenomenon

# Example : porosity of a geological medium

Reality

Sample



Optimal prediction
(unique)

One conditional simulation

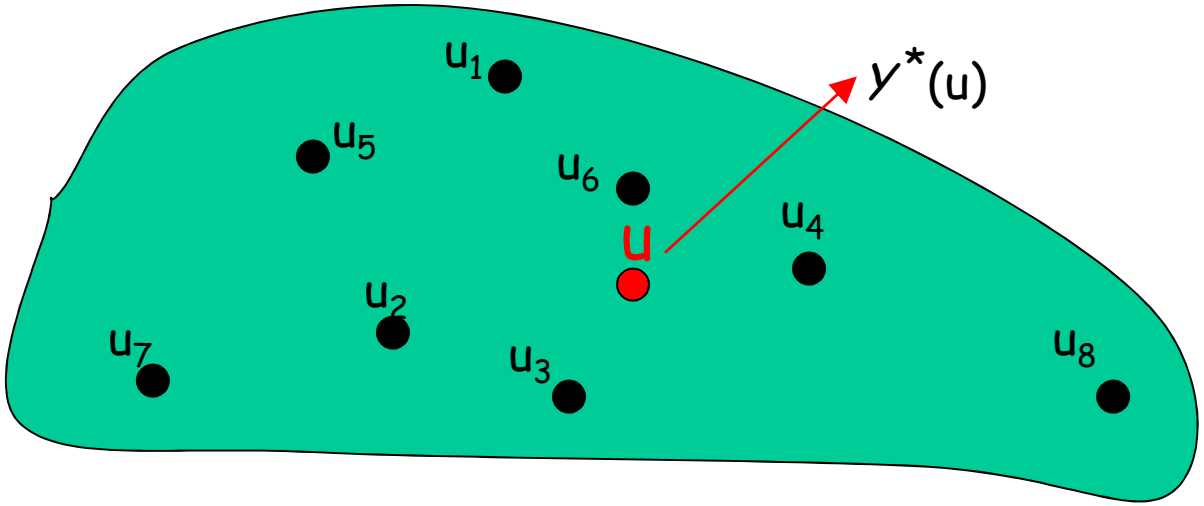
*[ Chilès ]*

# Spatial statistics: kriging interpolation

Linear combination of $N$ data:

$$Y^*(u) = \sum_{i=1}^{N} \lambda_i Y(u_i)$$

Kriging can take into account the data configuration, the distance between data and target, the spatial correlations and potential external information




**Probabilistic framework**

**Estimation without bias:** $E[\,Y^*(u) - Y(u)\,] = 0$

the mean of the errors is zero

**Estimation $Y^*(u)$ is optimal:** $Var[\,Y^*(u) - Y(u)\,]$ is minimal

the dispersion of the errors is reduced

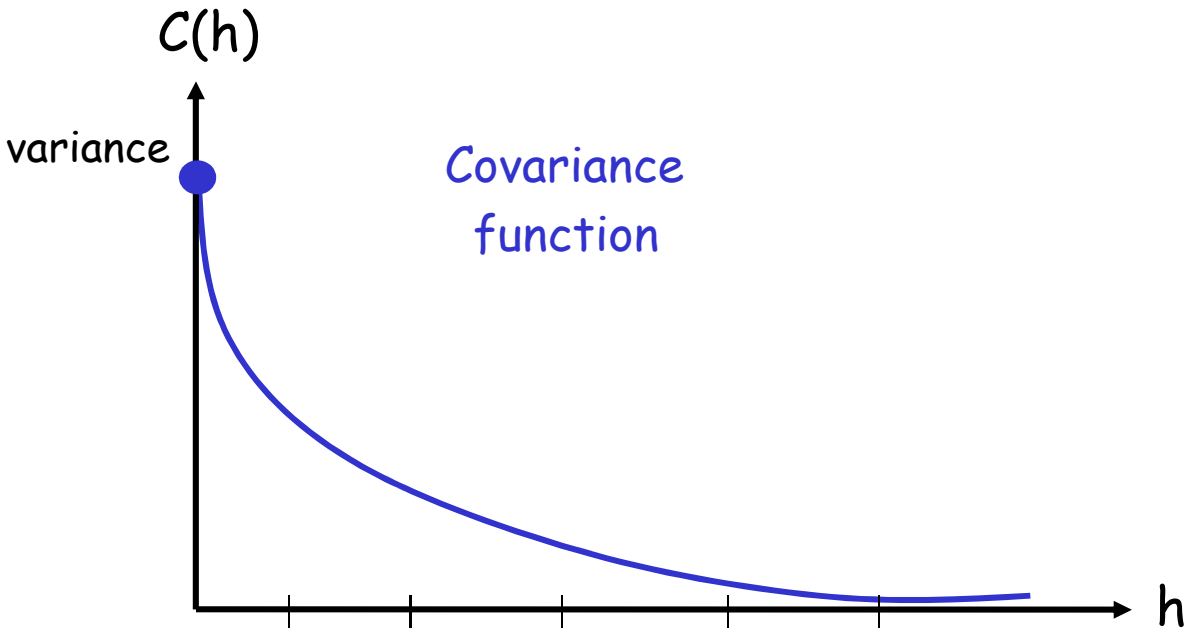
# Stochastic model for Y(x)

**The random field $Y(x)$, with $Y \in \Re$ and $x \in \Re^p$, is characterized by its mean and its covariance**

**$Y(x)$ is stationary of second order:**

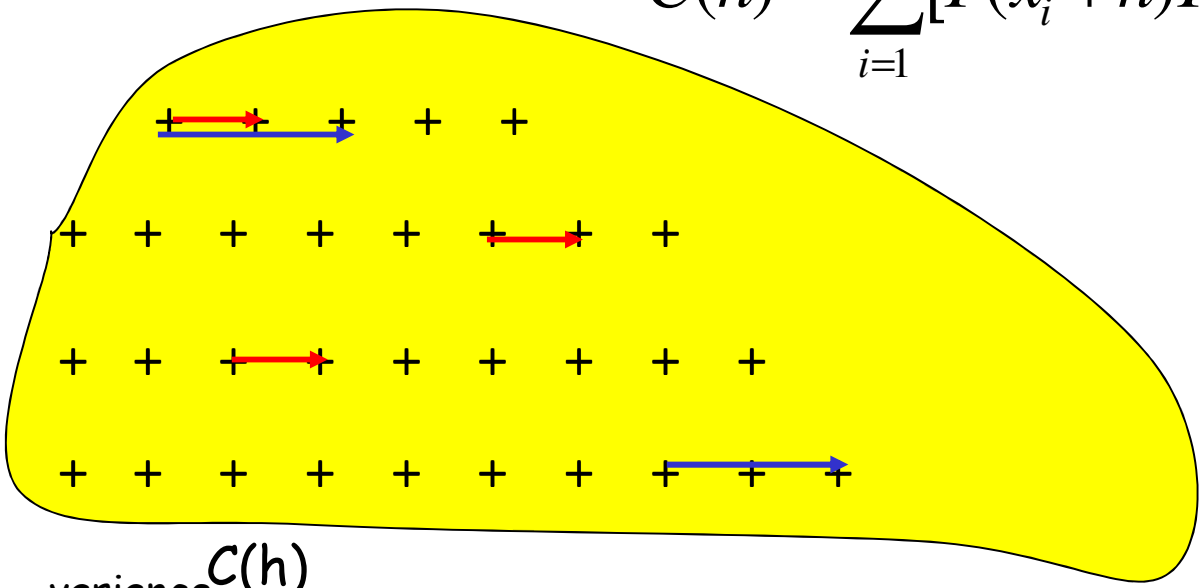
1. $E[Y(x)] = m$ does not depend on x
2. **Covariance:** $\mathrm{Cov}[Y(x), Y(x+h)] = \mathrm{E}[Y(x+h)Y(x)] - E[Y(x+h)]E[Y(x)] = C(h)$

does not depend on x



# In practice

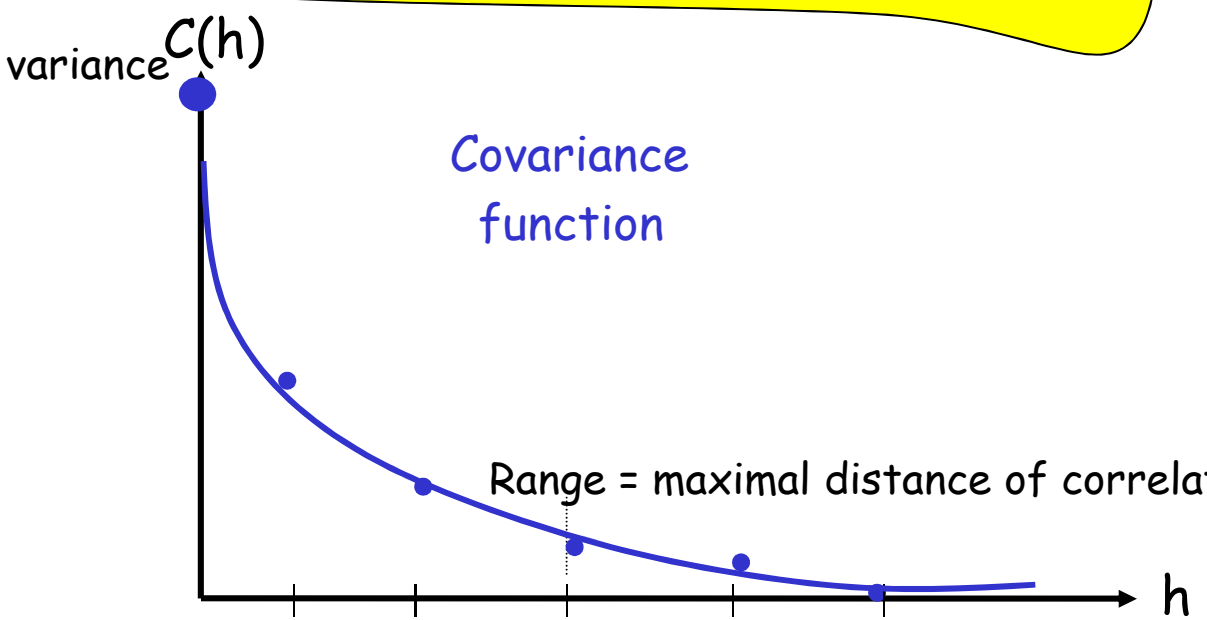
$$C(h) = \sum_{i=1}^{N(h)} \left[ Y(x_i + h) Y(x_i) \right] - m^2$$



Var[Y(x)] = C(0)

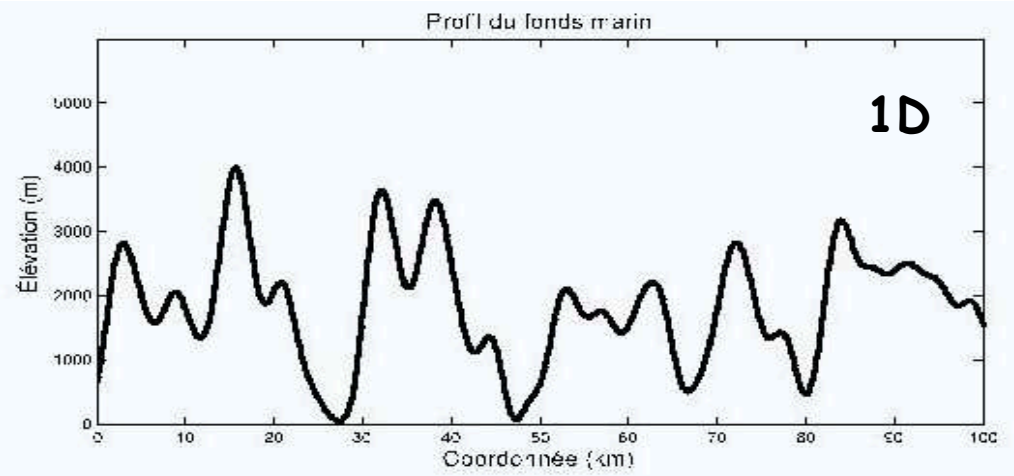
Y(x) → Y(x+h)

Y(x) → Y(x+2h)

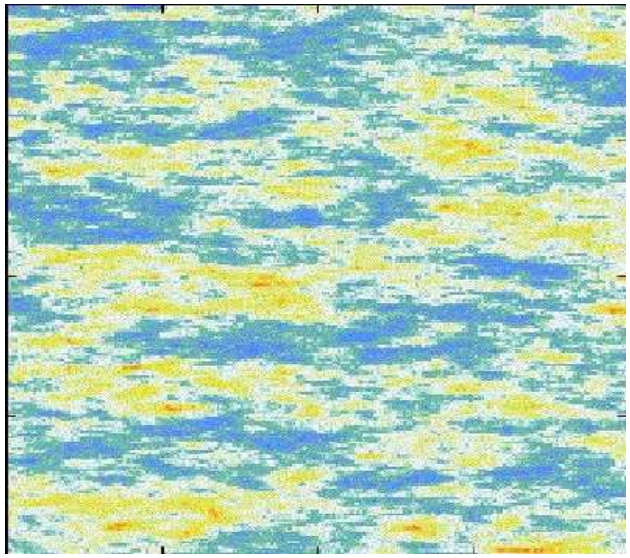



Range = maximal distance of correlation = correlation length

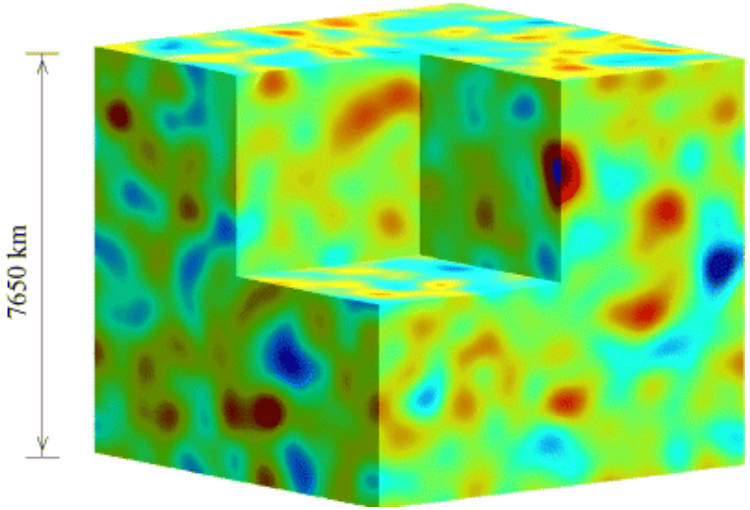
# Examples of stochastic processes (Gaussian)




*[ from: Marcotte ]*



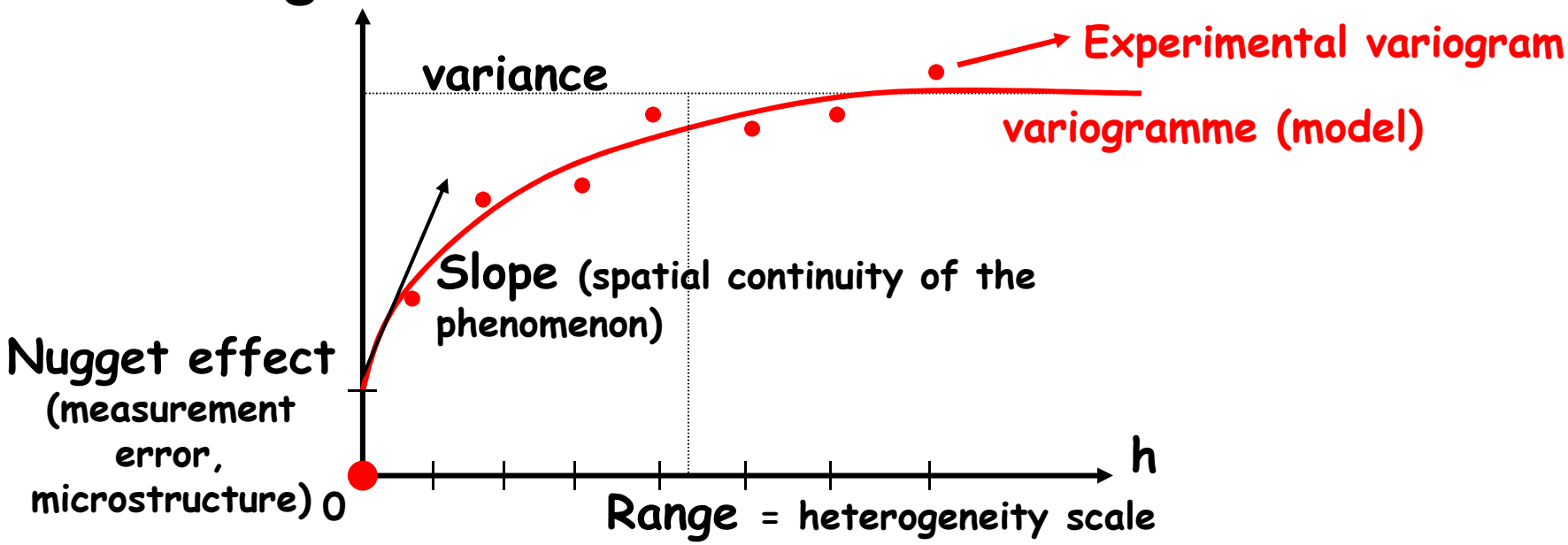
2D

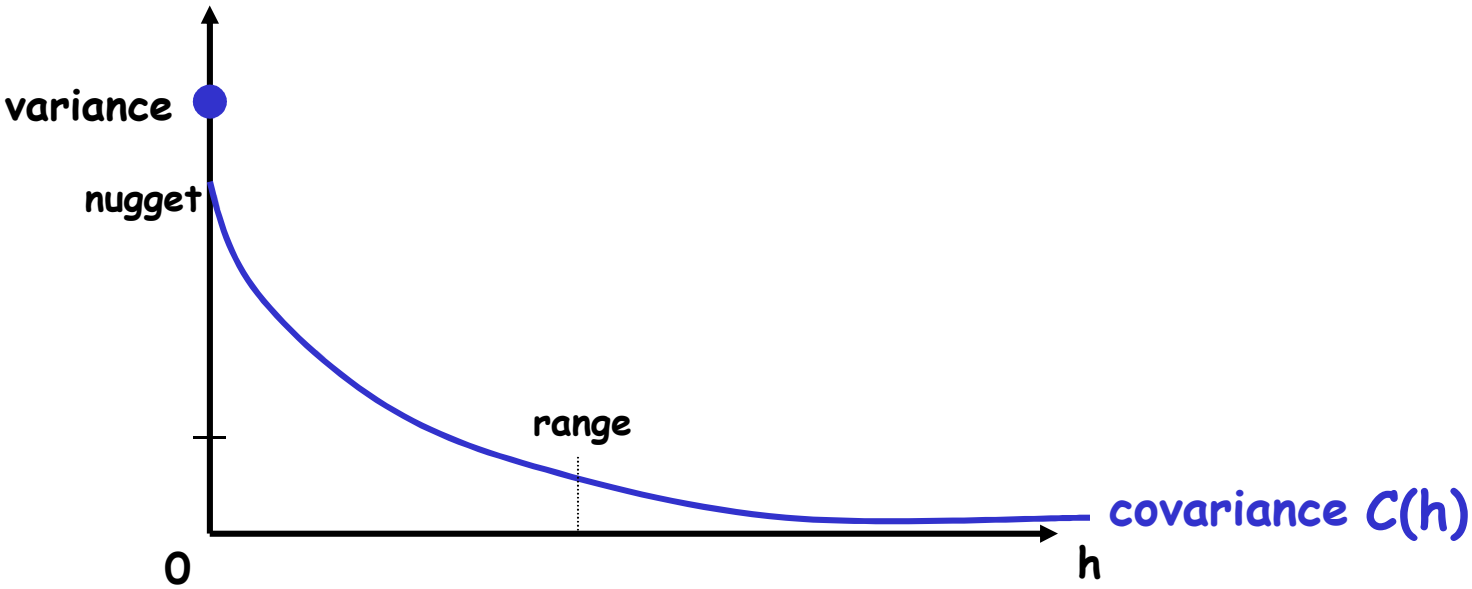



3D

*[ from: Baig, 2003 ]*

# The variogram



# Simple kriging (known mean)

$$Y^*(u) = \sum_{i=1}^{N} \lambda_i(u)\,[Y(u_i) - m] + m$$

($m$ = known constant)

Min { E [ $Y^*(u) - Y(u)$ ]$^2$ }
$\lambda_i$ ➡ multiple linear regression by least squares

**Best Linear Unbiased Predictor (BLUP)**

Kriging weights $\lambda_i(u)$ for $Y(u_i)$ are obtained by:

$$\left\{ \sum_{j=1}^{N} \lambda_j(u)\, C(u_i - u_j) = C(u_i - u) \qquad \forall\, i = 1 \ldots N \right.$$

System of $N$ linear equations with $N$ unknowns which have an unique solution (for non singular covariance matrix)

**Kriging variance (estimation error):** $\sigma_K^2(u) = C(0) - \sum_{i=1}^{N} \lambda_i(u)\, C(u_i - u)$
does not depend on the $Y$ values

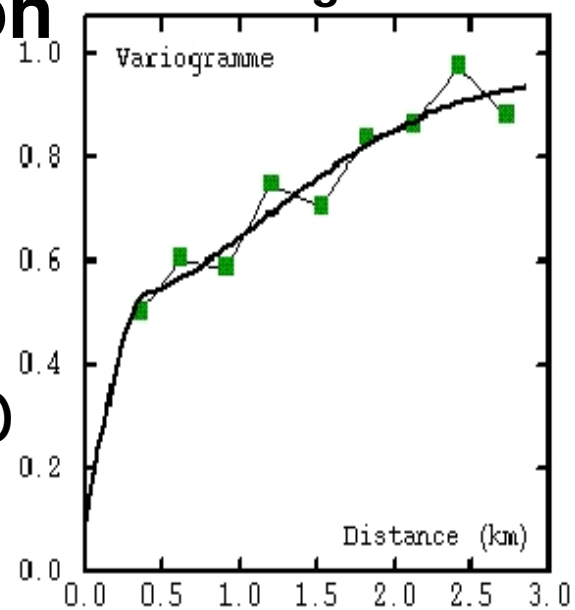
=> Visualisation of regions with imprecise estimations
=> Put new observation points in these regions

# Example : cartography of air pollution

73 measures of benzene concentration (Rouen, France)

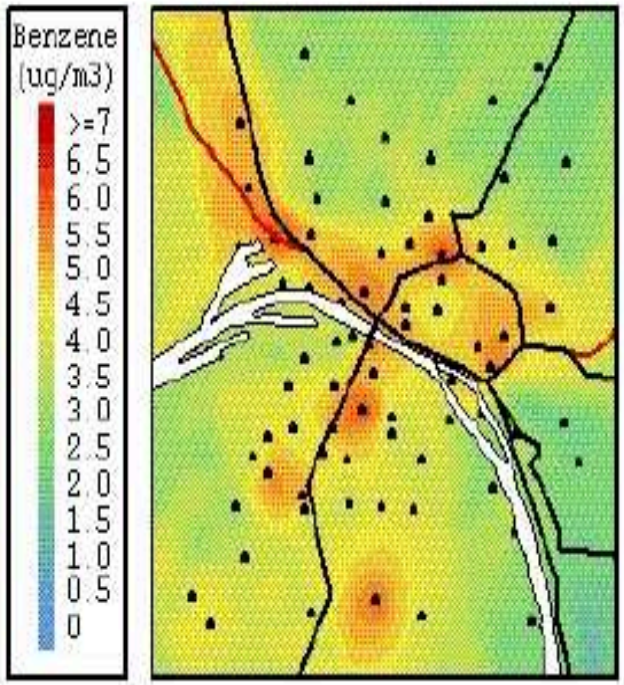
*[ from: Bobbia, Mietlicki & Roth, 2000 ]*

**Variogram**

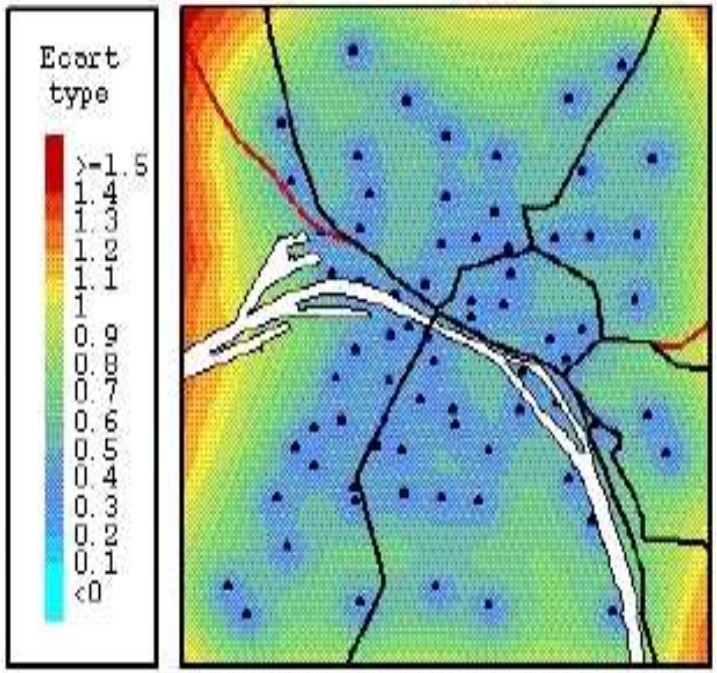



$$\gamma(h) = C(0) - C(h)$$

**Kriging mean**




**Kriging standard deviation**

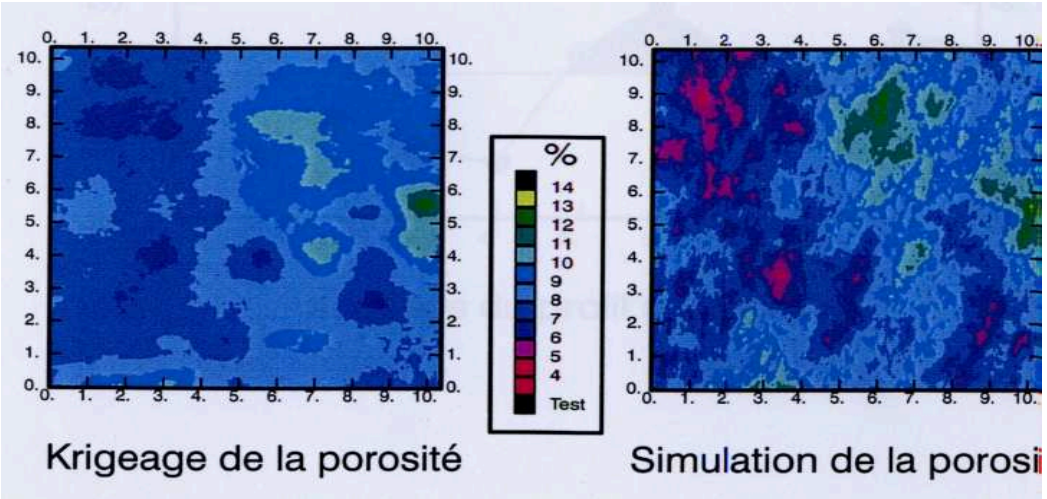


# Simulations

- **Kriging give the optimal estimation** (unbiased, minimal error variance) of the variable at any point, from experimental data

- **A simulation represents a possible realization** of the real phenomenon

  It reproduces its true **variability** (distribution, variogram), with respecy to experimental data **(conditional simulation)**




Main goal of simulation : quantify the uncertainty via sampling (as Monte Carlo)

Numerous methods of random fields simulation (LU decomposition, turning bands method, spectral method, Karhunen-Loève, etc.)

# Conditional simulations

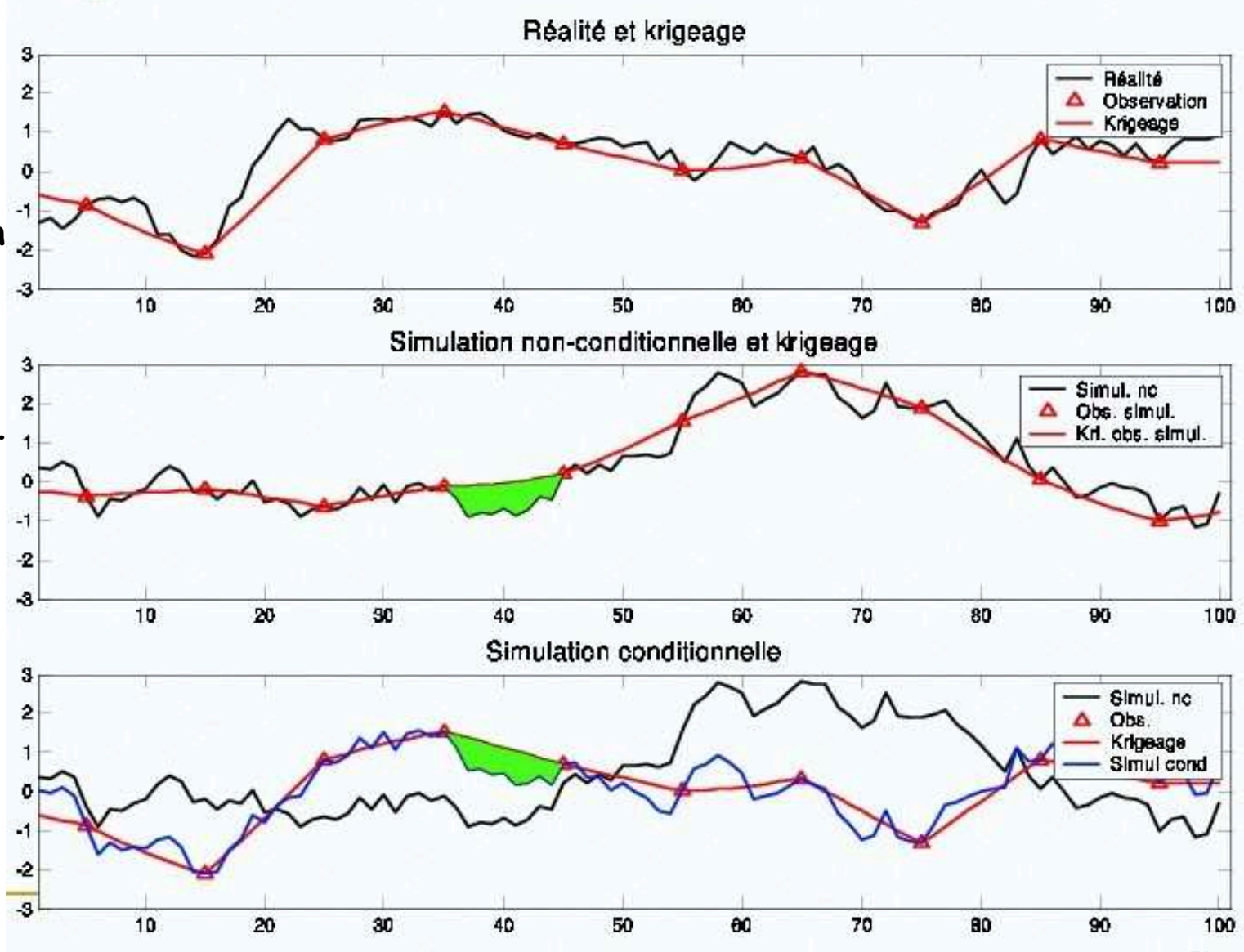
Kriging
of observation

+

Non cond. Simul.
-
Kriging of
non cond. simul

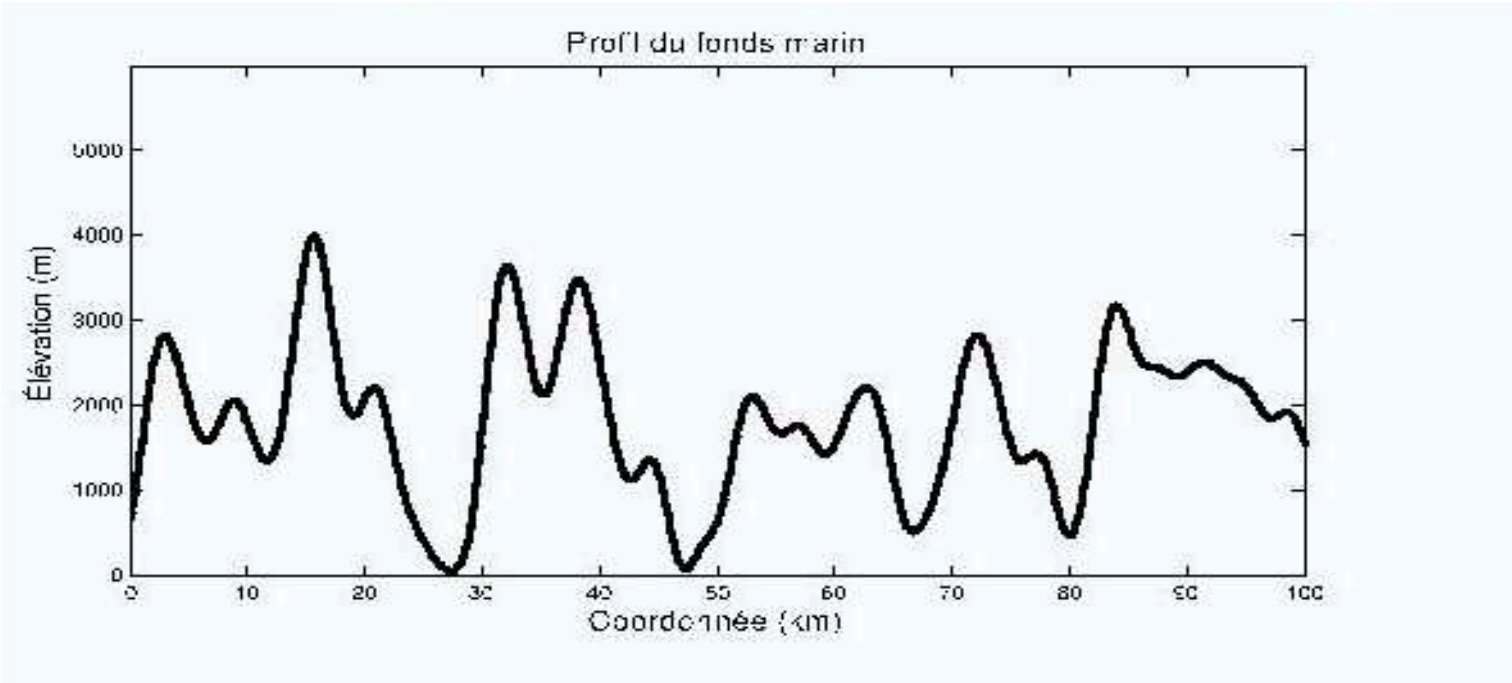
=

Conditional
simulation




*[ Marcotte, Cours EPM ]*

# Example : profile of ocean bottom (1/5)



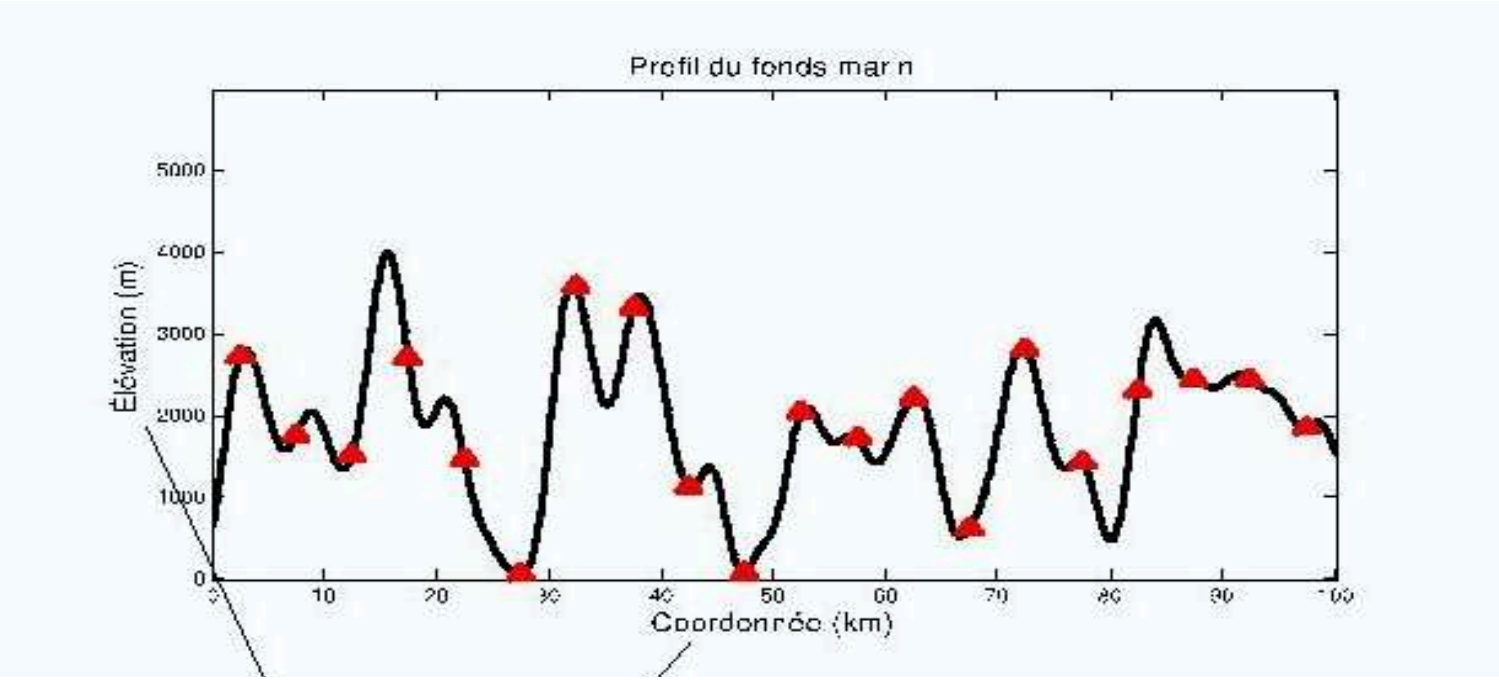

You have to put a cable on the ocean bottom

Question: what is the length of the cable?

*[ Marcotte, Cours EPM ]*

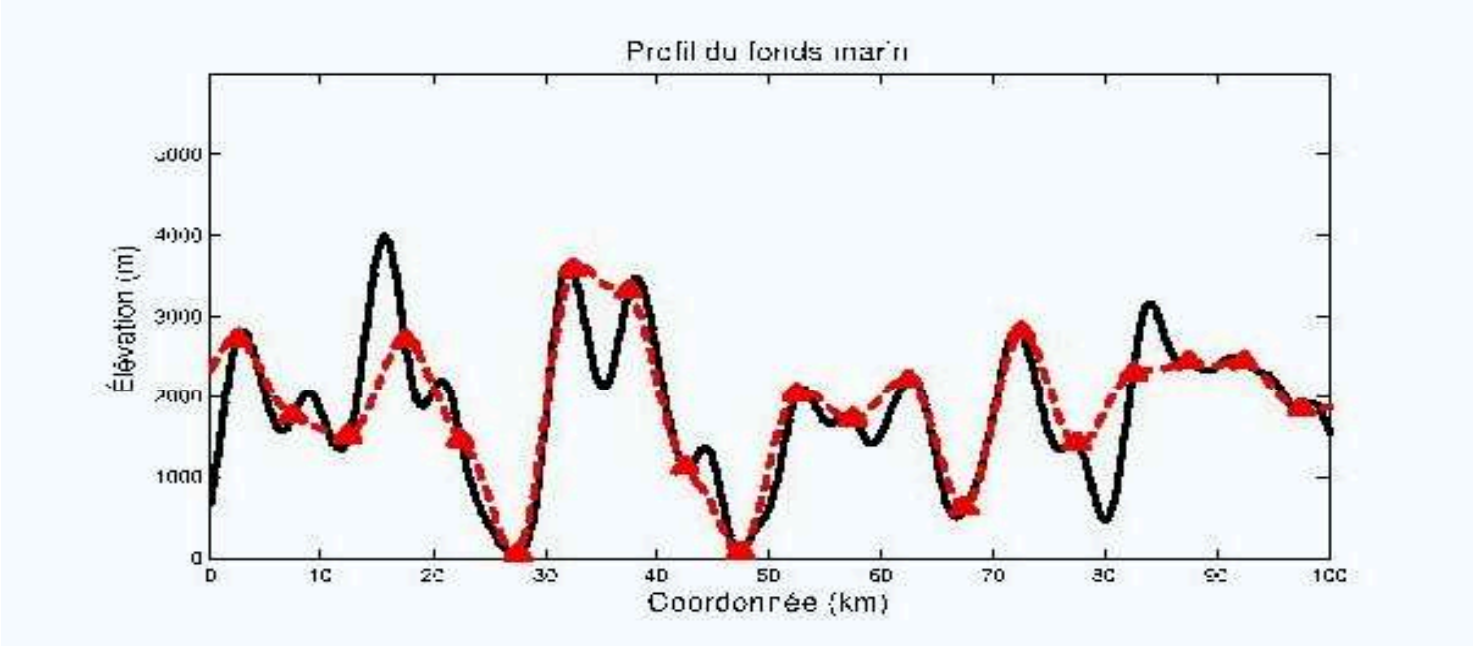
# Example : profile of ocean bottom (2/5)

The exact depth is uniquely known at the observation points (survey)



# Example : profile of ocean bottom (3/5)

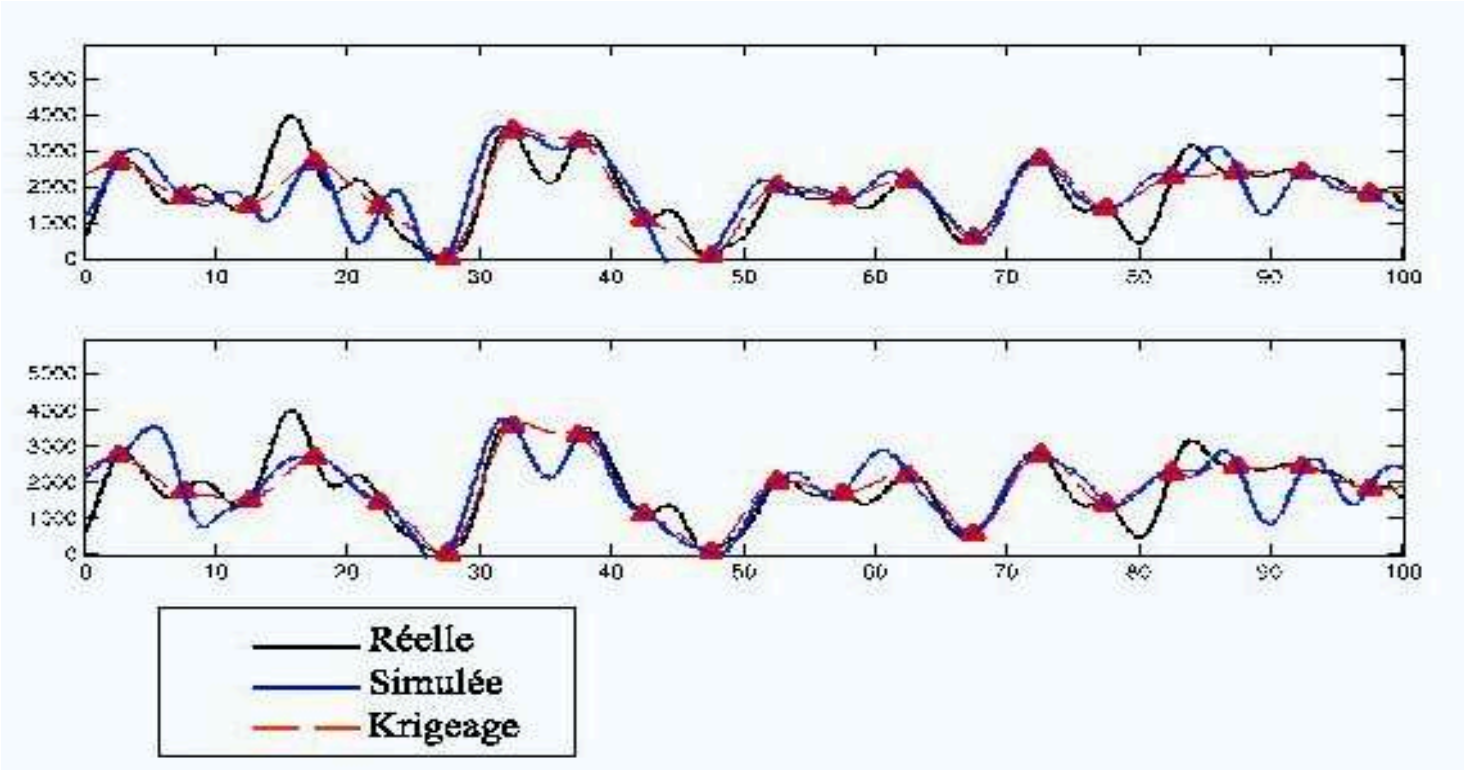
**Kriging of the ocean depth**



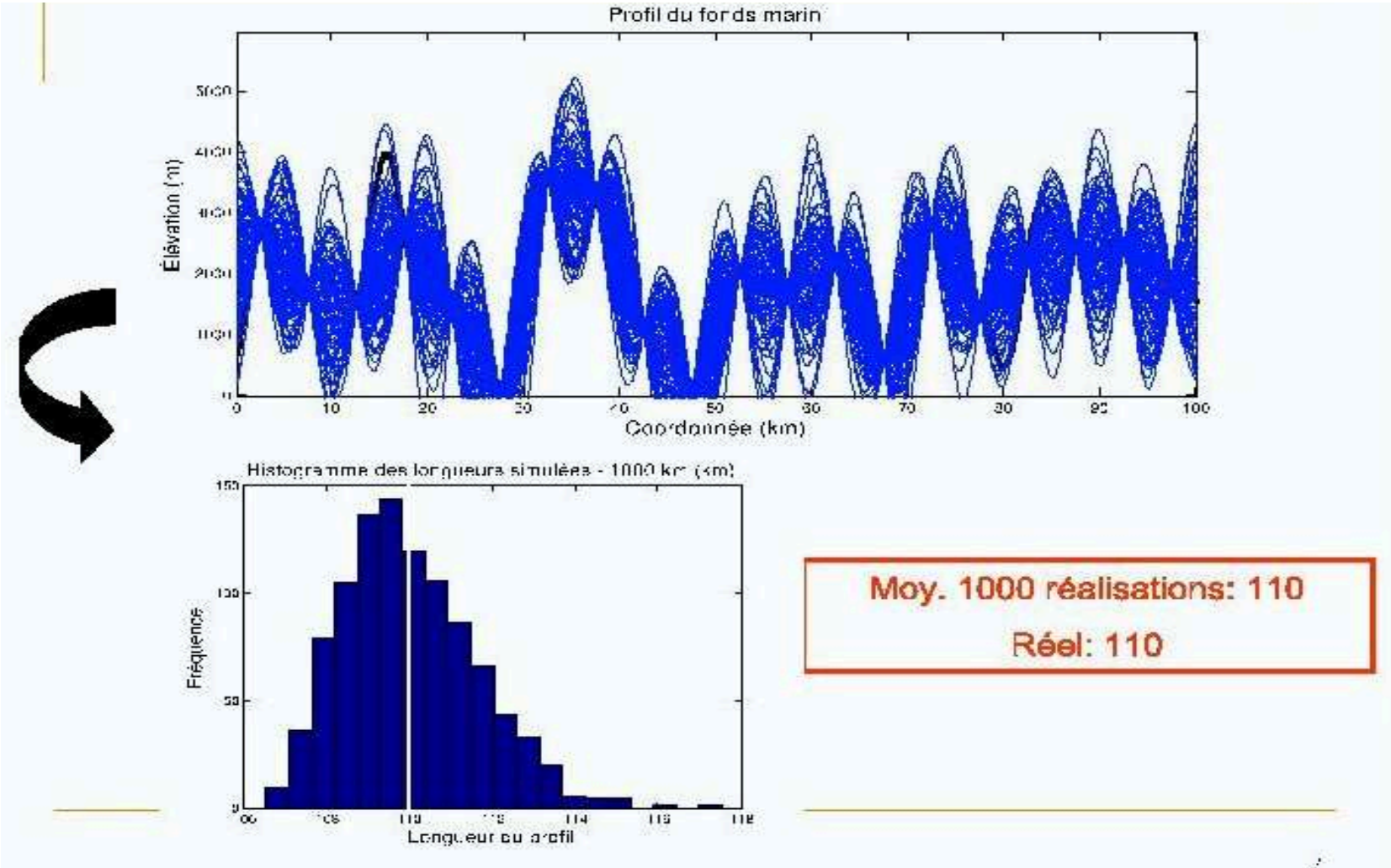

The true length is 110 km while kriging gives 104.6 km
=> some cable is missing

# Example : profile of ocean bottom (4/5)

**Another approach: the conditional simulations**

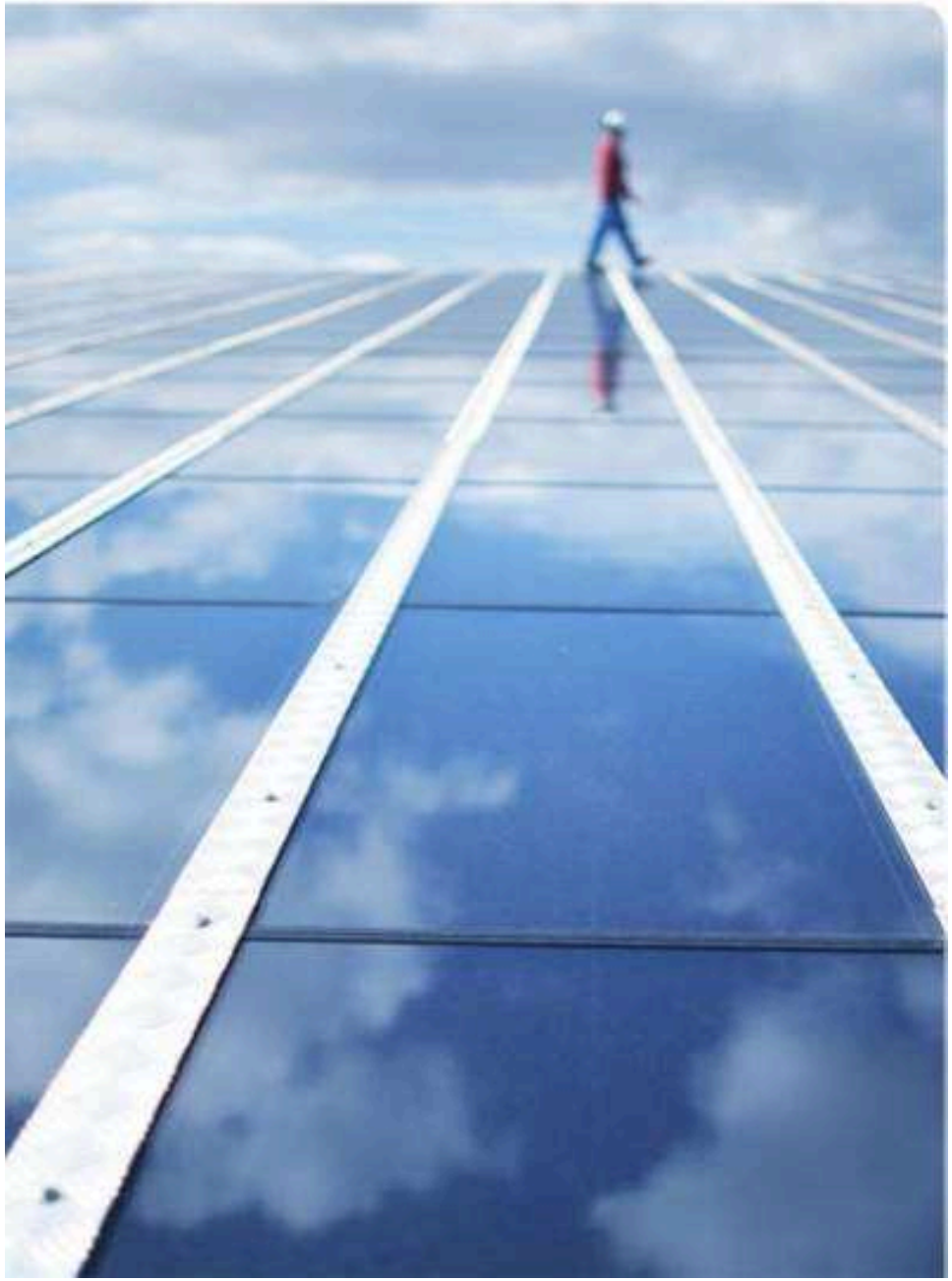


# Example : profile of ocean bottom (5/5)




**The 95%-confidence interval from conditional simulations is [108.8,113.5]**

Same problem for probability of failure estimation (non linear transfer fct)



# Gaussian process metamodel

# Gaussian process metamodel (1/2)

- Idea: Computer code results are interpolated with the kriging technique
- Necessary hypothesis: Gaussian process

- Definition:

$$Y(x) = \beta F(x) + Z(x)$$

**Regression** **stochastic part**

Stochastic process Z with :

$E[Z(x)] = 0$

$Cov(Z(x), Z(u)) = \sigma^2 R(x, u)$

where $\sigma^2$ is the variance

and $R$ the correlation function

$Z \sim N(0, \sigma^2 R)$

- Parametric choices:
  - F : polynomial of degree 1 $\beta F(\mathrm{x}) = \beta_0 + \sum_{i=1}^{p} \beta_i x_i$
  - R : stationary => covariance function

Example: Gaussian covariance $\mathrm{R}(\mathrm{x}, \mathrm{u}) = \mathrm{R}(\mathrm{x} - \mathrm{u}) = \exp\left( -\sum_{i=1}^{p} \theta_i \left| x_i - u_i \right|^2 \right)$

**Anisotropy:** $\theta_i$s are not equal (correlation length of each input variable)

# Gaussian process metamodel (2/2)

- <u>Joint distribution :</u>
  - Gaussian process (Gp) model : $Y(x) = \beta F(x) + Z(x)$, $x \in \Re^p$
  - Learning sample (LS) of $N$ simulations : $(X_{LS}, Y_{LS})$

$$X_{LS} = \left(x^{(1)}, \ldots, x^{(N)}\right), \; F_{LS} = F(X_{LS}), \; R_{LS} = \left(R\left(x^{(i)}, x^{(k)}\right)\right)_{i,k}$$
$$Y_{LS} \sim N(\beta F_{LS}, \sigma^2 R_{LS})$$

  - Conditional Gp metamodel :

$$\Rightarrow \quad Y(x)_{|X_{LS}, Y_{LS}} \sim Gp$$

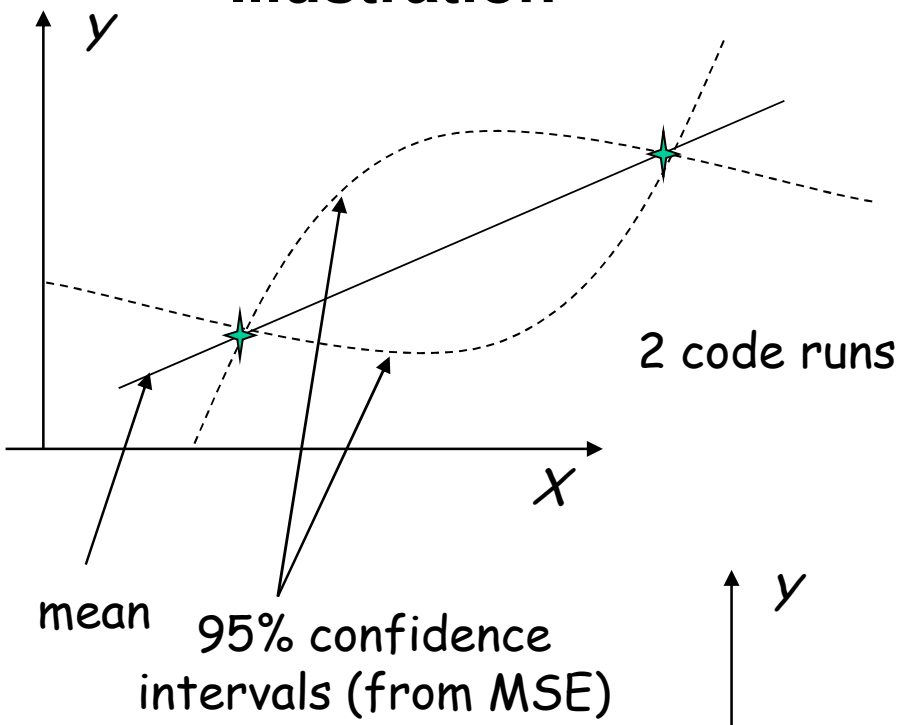
$$\text{Mean} : \hat{Y}(x) = \mathrm{E}\left[Y(x)_{|X_{LS}, Y_{LS}}\right] = \beta F(x) + r(x) R_{LS}^{-1}\left[Y_{LS} - \beta F_{LS}\right]$$

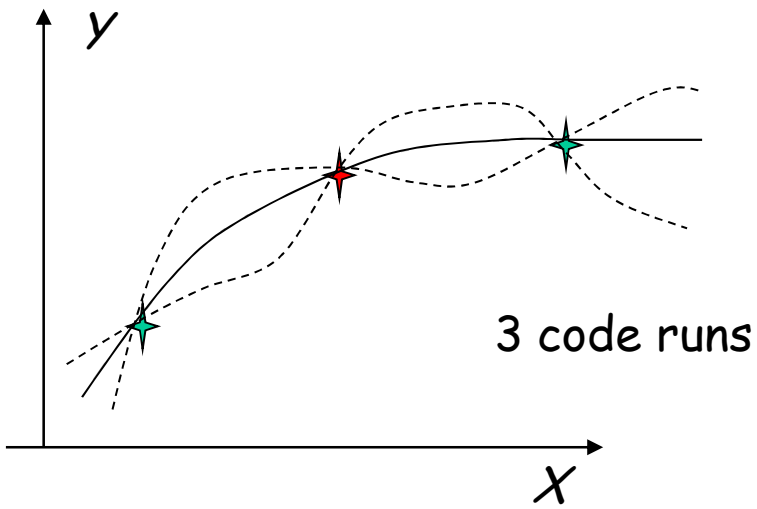
$$\text{with } r(x) = \left[R\left(x^{(1)}, x\right), \ldots, R\left(x^{(N)}, x\right)\right]$$

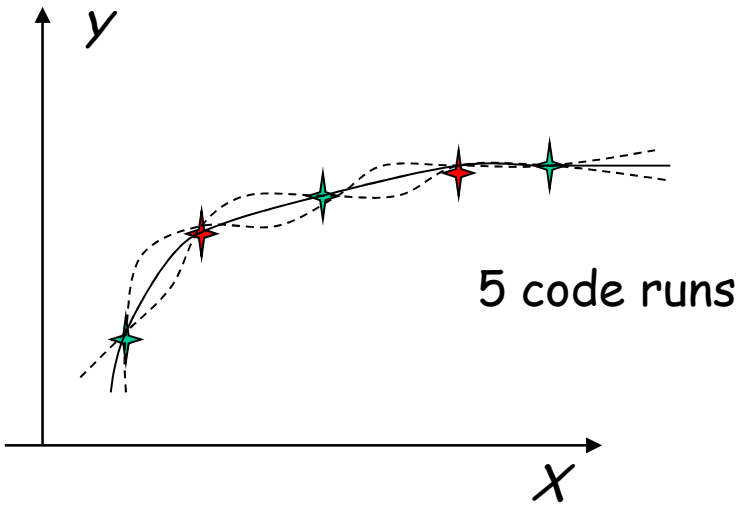
$$\text{Covariance} : \mathrm{Cov}\left(Y(u)_{|X_{LS}, Y_{LS}}, Y(v)_{|X_{LS}, Y_{LS}}\right) = \sigma^2\left(R(u,v) + {}^t r(u) R_{LS}^{-1} r(v)\right)$$

$$\Rightarrow \text{Variance} \Rightarrow \text{Mean Square Error (MSE)}$$

# Illustration




**Conclusion:** given a sufficient number of points, we obtain an accurate metamodel

# Hyperparameters estimation

- **Maximum likelihood method**

  - Likelihood maximisation on the learning basis ($X_s$,$Y_s$):

$$\left(\beta^*,\theta^*,\sigma^*\right)=\underset{(\beta,\theta,\sigma)}{\text{Argmax}}\ \ln L\left(Y_{LS},\beta,\theta,\sigma\right)$$

  - with

$$\ln L\left(Y_{LS},\beta,\theta,\sigma\right)=-\frac{N}{2}\ln\left(2\pi\sigma^2\right)-\frac{1}{2}\ln\left(\det R_{LS}\right)-\frac{1}{2}\sigma^2\,{}^t\left[Y_{LS}-\beta F_{LS}\right]R_{LS}^{-1}\left[Y_{LS}-\beta F_{LS}\right]$$

  - Joint estimation of β and σ :

$$\begin{cases}\beta^*=\left[{}^tF_{LS}R_{LS}^{-1}F_{LS}\right]^{-1}{}^tF_{LS}R_{LS}^{-1}Y_{LS}\\ \sigma^{2*}=\dfrac{1}{N}\,{}^t\left[Y_{LS}-\beta^*F_{LS}\right]R_{LS}^{-1}\left[Y_{LS}-\beta^*F_{LS}\right]\end{cases}$$

  - Estimation of correlation parameters θ :

$$\left(\theta^*\right)=\underset{\theta}{\text{Argmin}}\ \psi(\theta)\quad\text{with}\quad\psi(\theta)=\left|R_{LS}\right|^{-1/N}\sigma^{2*}$$

# Estimation and validation

$$\mathrm{R}(\mathbf{u},\mathbf{v}) = \mathrm{R}(\mathbf{u}-\mathbf{v}) = \exp\left(-\sum_{i=1}^{p}\theta_i\left|u_i - v_i\right|^2\right)$$

- **Hyperparameters $(\theta_i)_{i=1\ldots p}$ estimated by likelihood maximization**

Simplex method, **stochastic algorithms**

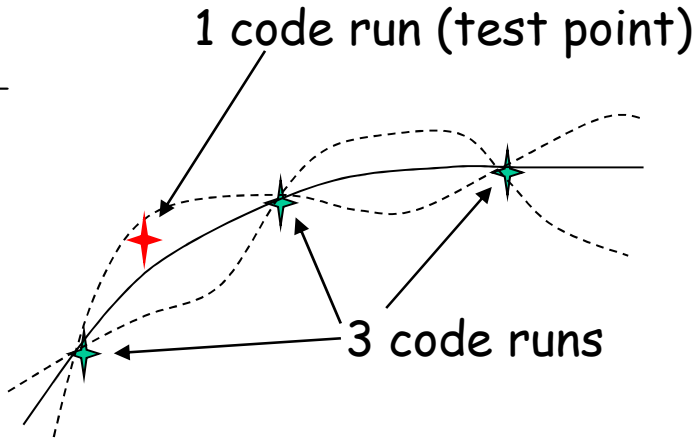
Problems in high dimensional context ( $p$ > 10), can be solved by sequential algorithms *[ Marrel et al. 2008 ]*

- **Predictor validation:**

Predictivity coefficient

$$Q_2(Y,\hat{Y}) = 1 - \frac{\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2}{\sum_{i=1}^{n}\left(\overline{Y} - Y_i\right)^2}$$

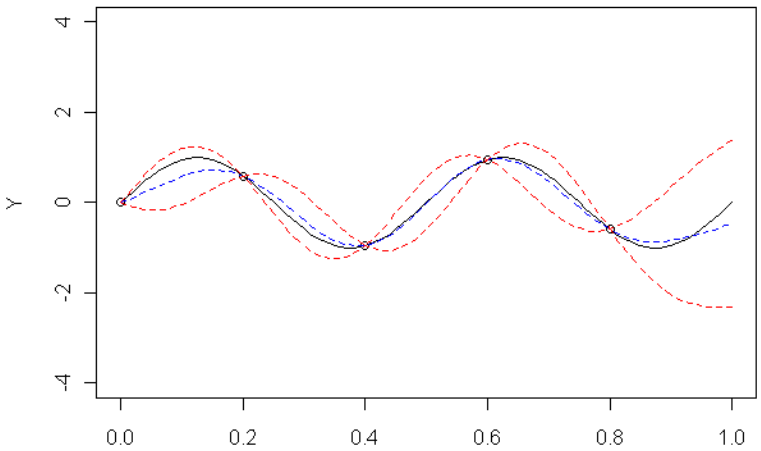
- Test sample
- or leave-one-out
- or *k*-fold cross validation



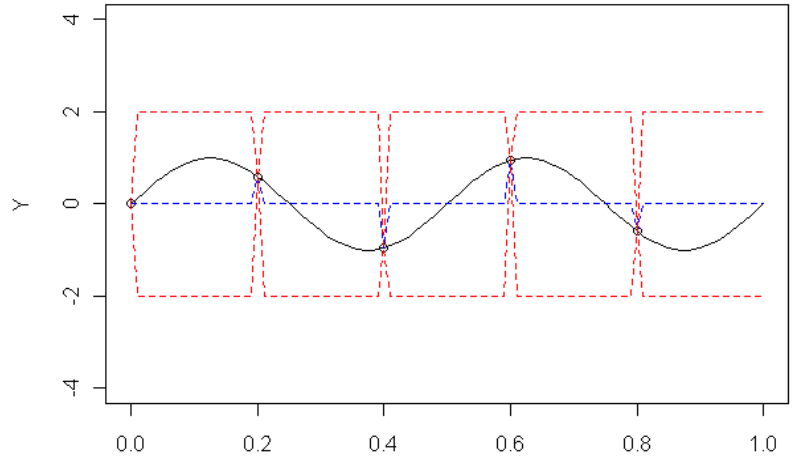

- **MSE validation:** Percentage of predicted values inside confidence bounds

# Effects of the hyperparameters $\theta$ and $\sigma$

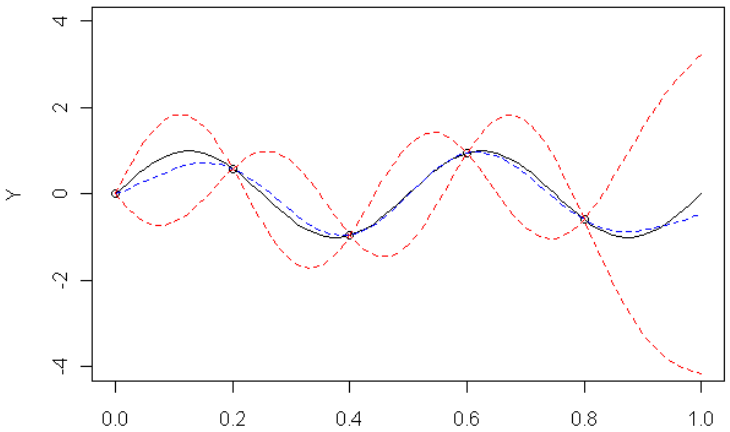
$$f(x) = \sin(4\pi x)$$



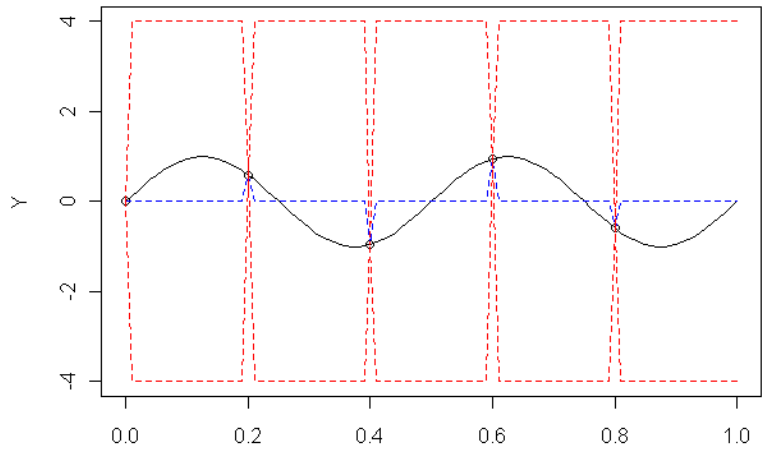

$$\sigma^2 = 1; \theta = 0.2$$




$$\sigma^2 = 1; \theta = 10^{-4}$$



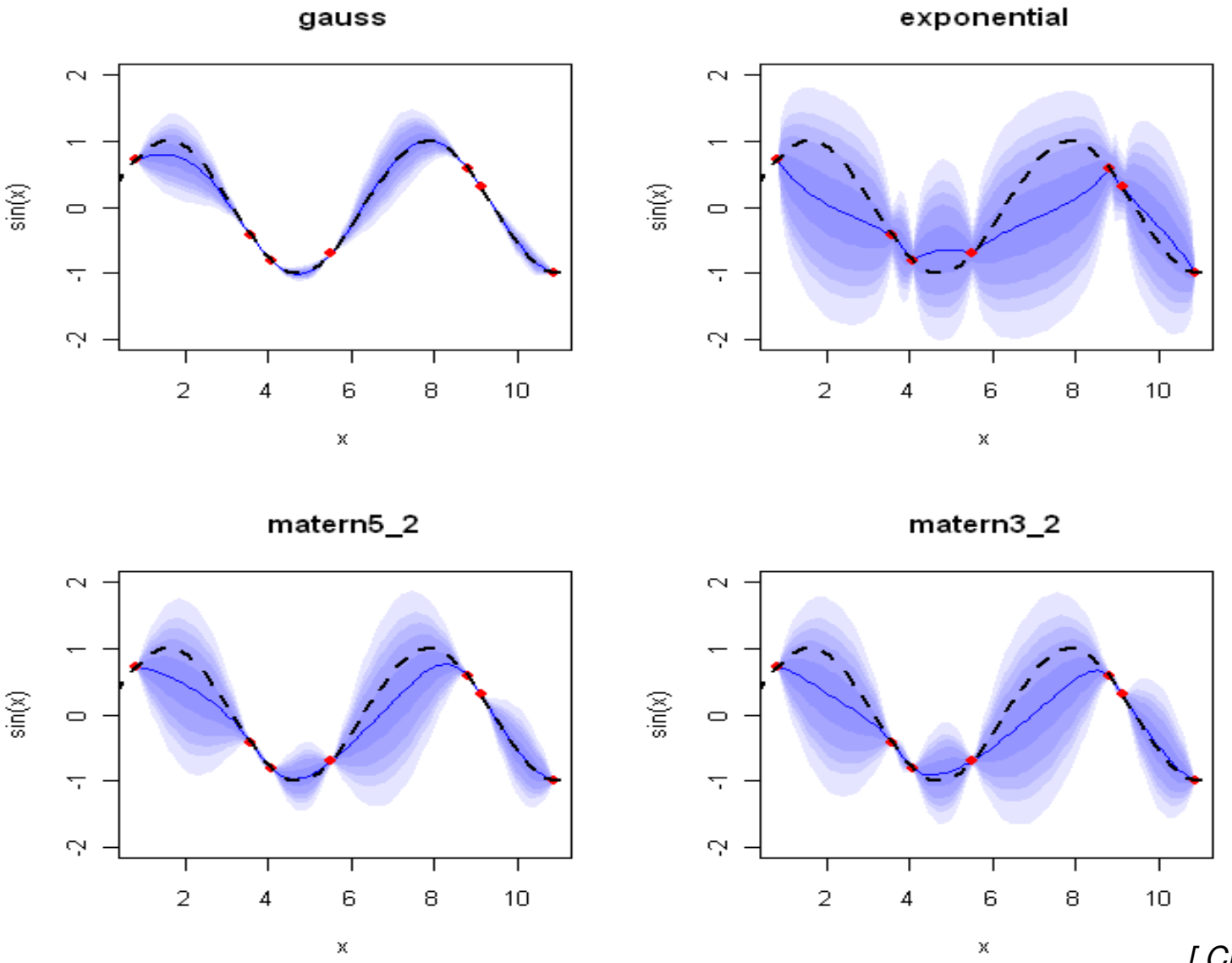

$$\sigma^2 = 4; \theta = 0.2$$




$$\sigma^2 = 4; \theta = 10^{-4}$$

*[ Le Gratiet, 2011 ]*

# Effects of the covariance structure




*[ Chevalier, 2011 ]*

# Adaptive designs using Gaussian process metamodel

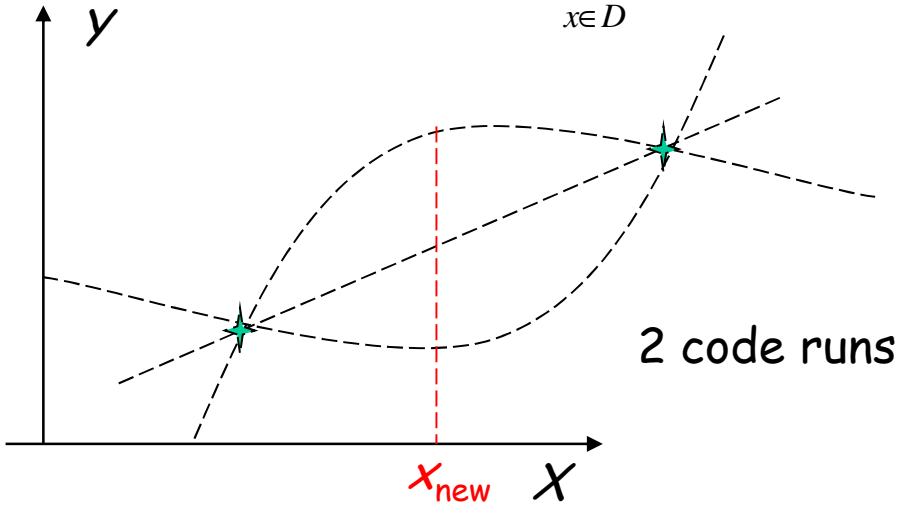
# The best way to build Gp: model-based adaptive designs

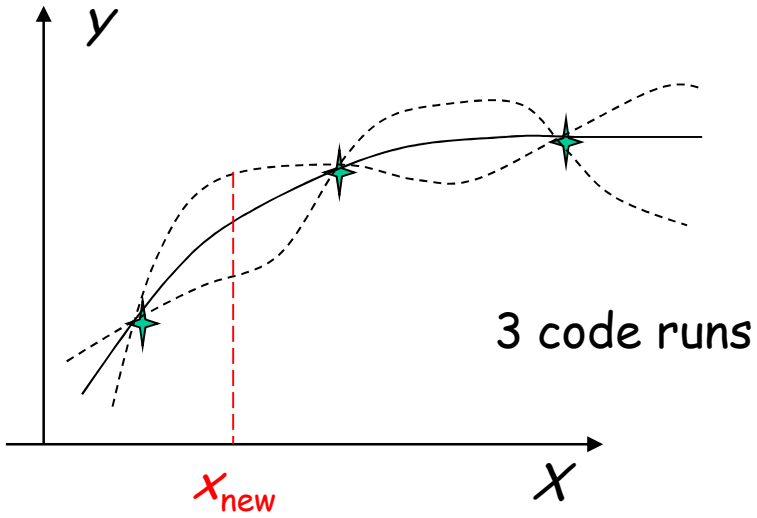
Example: criterion of the Gaussian process MSE (Mean Square Error)

$$MSE(x) = \sigma^2 + {}^t r(x) R_{LS}^{-1} r(x) + u(x)({}^t(\beta F_{LS}) R_{LS}^{-1} \beta F_{LS})^t u(x)$$

$$u(x) = \beta F(x) - {}^t k(x) R_{LS}^{-1} \beta F_{LS}$$

$$x_{\text{new}} = \arg\max_{x \in D} MSE(x)$$




<u>Remark:</u> other criteria are possible (e.g. focusing to active variables)

**<u>Conclusion:</u>** Model-based adaptive designs are the most efficient ones,
but are not always applicable
In practice, we need to initiate the process with a space-filling design

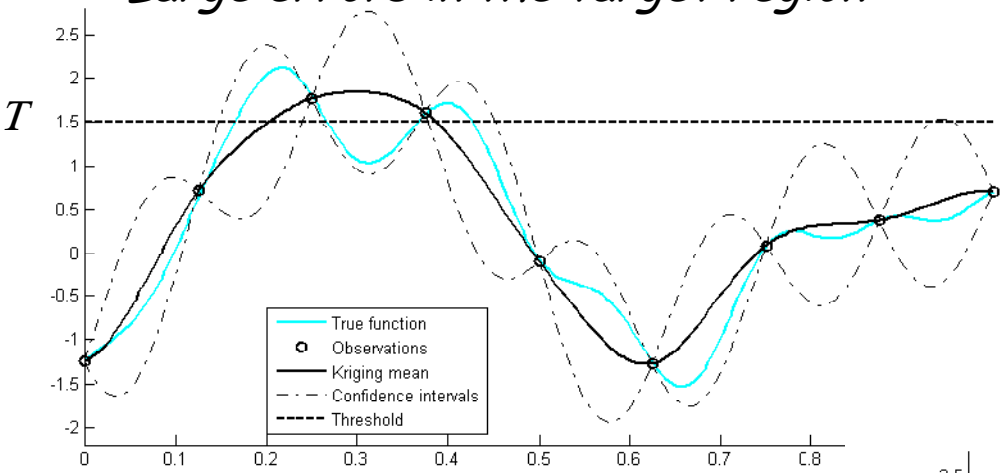
# Estimation of rare events probability using kriging

*[ Bect et al. 2012 ]*

**Industrial problems: safety analysis with computer code** (nuclear, transport, …)

<u>Problem:</u> find $P_f$ = Prob [ $f(X) > T$ ] with $X$ = random inputs ; $T$ = treshold

*Reasonable variance everywhere*
*Large errors in the target region*



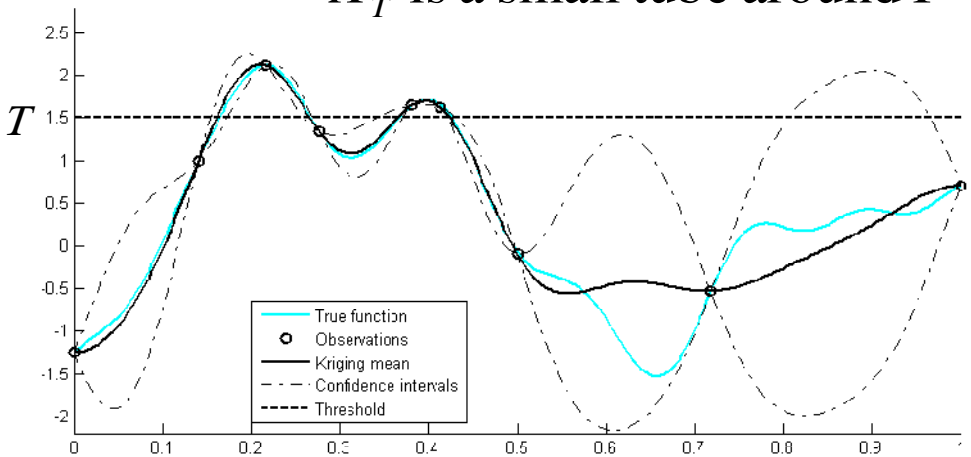

*[ from: Picheny et al. 2010 ]*

☺ **New adaptive design**

$$X^* = \arg\min_X (IMSE_T)$$

$$IMSE_T = \int MSE(x) 1_{X_T}(x) dx$$

$X_T$ is a small tube around $T$




*Large variance in non-target region*
*Good accuracy in target region*

# Optimisation of a model output using kriging

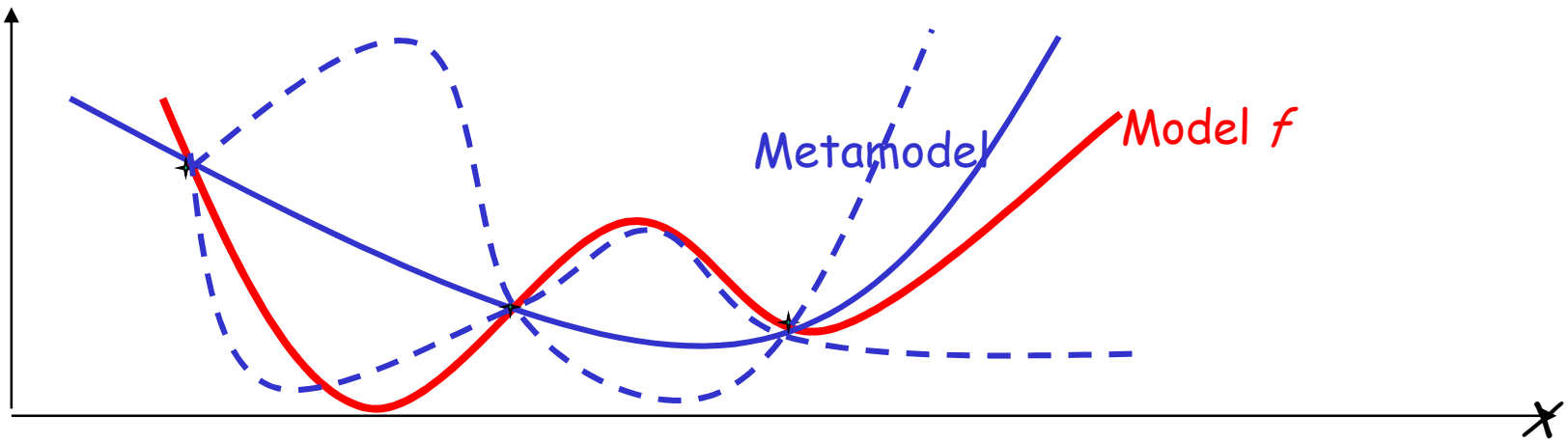
**Industrial problems: conception with costly computer code** (automobile, nuclear, aeronautics, …)

<u>Problem:</u> find the values of X which minimize the model output

$$X^* = \arg\min_{X \in D} f(X)$$

☠ **If *f* is costly, a natural solution would be to optimize a metamodel of *f*** : dangerous idea because the metamodel tends to smooth the true model

☺ Gp metamodel allows to take into account the metamodel error, and to define the expected improvement EI*(X)* for each $X \in D$

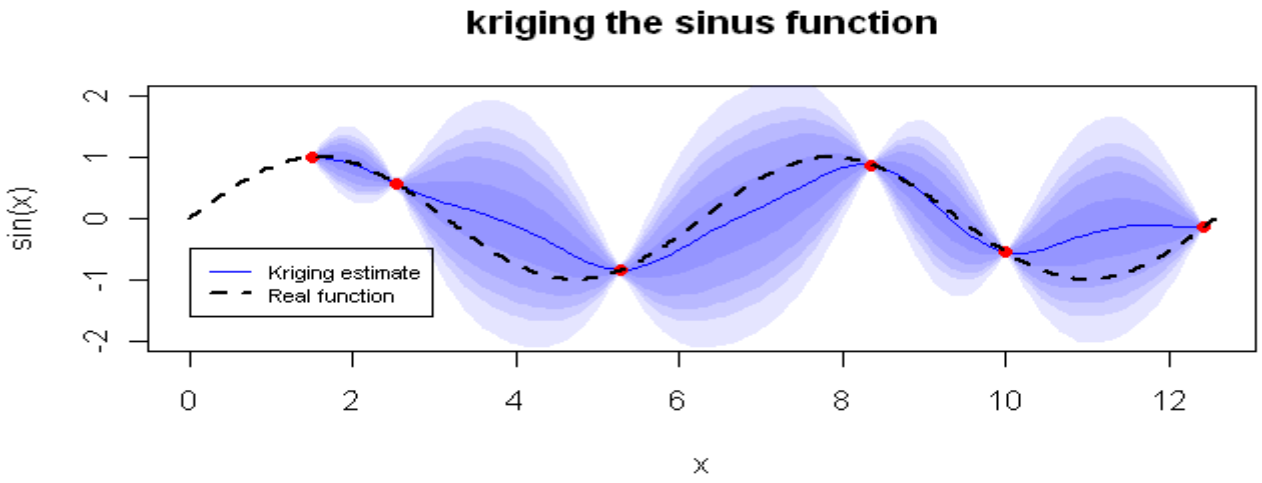



**EI(x) = E[ max( 0 , observed minimum – f(x) ) ]**

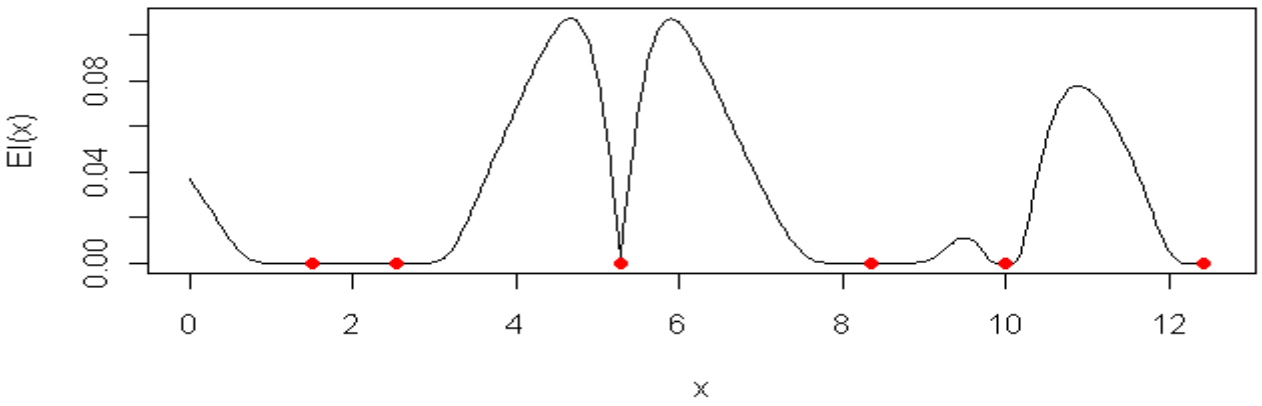
# Adaptive design for optimization: EGO algorithm

*[ Jones et al. 1998 ]*

**EGO: step 0**

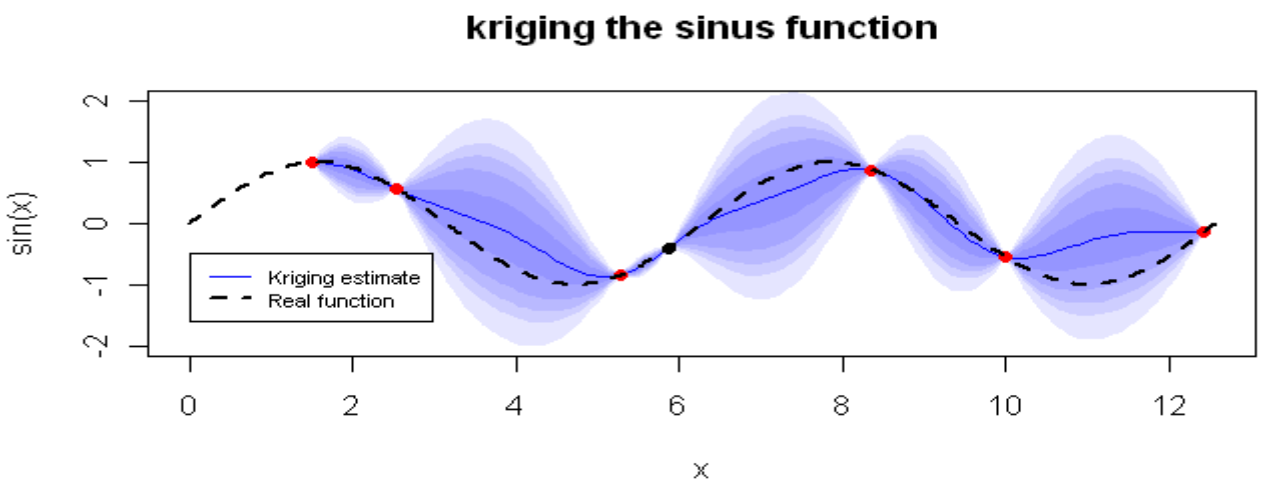



*[ Chevalier, 2011 ]*

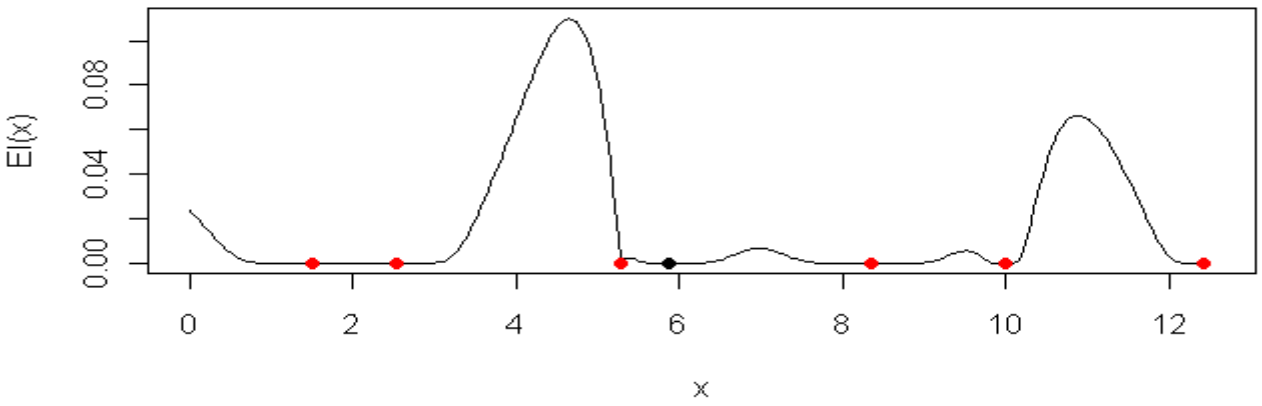


# Adaptive design for optimization: EGO algorithm

**EGO: step 1**

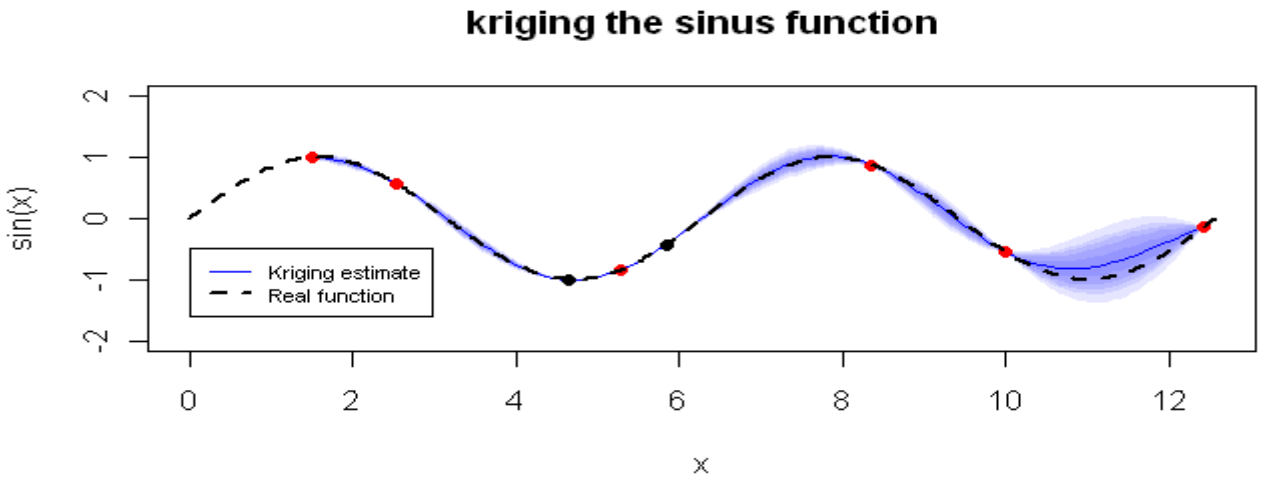



*[ Chevalier, 2011 ]*

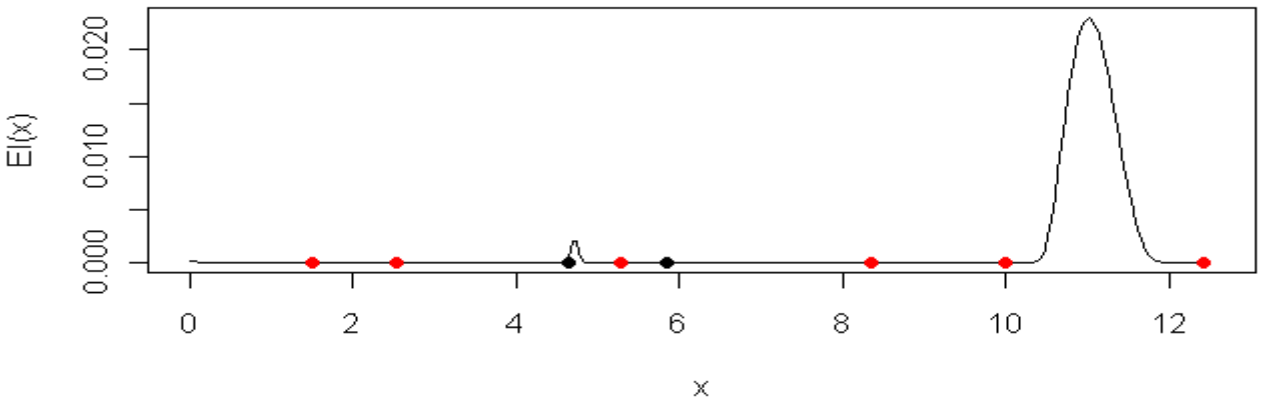


# Adaptive design for optimization: EGO algorithm

**EGO: step 2**

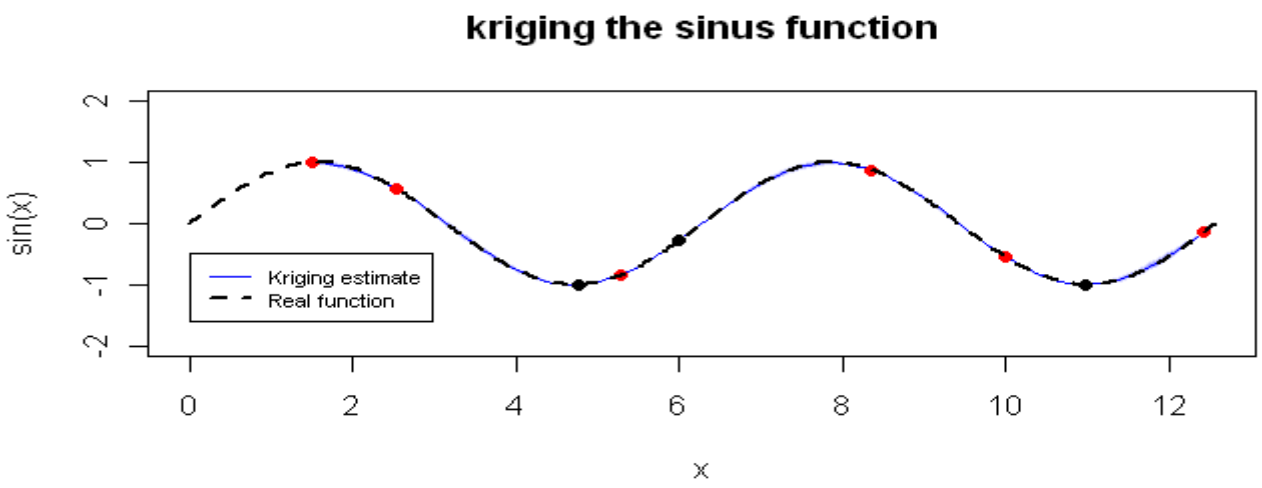



*[ Chevalier, 2011 ]*

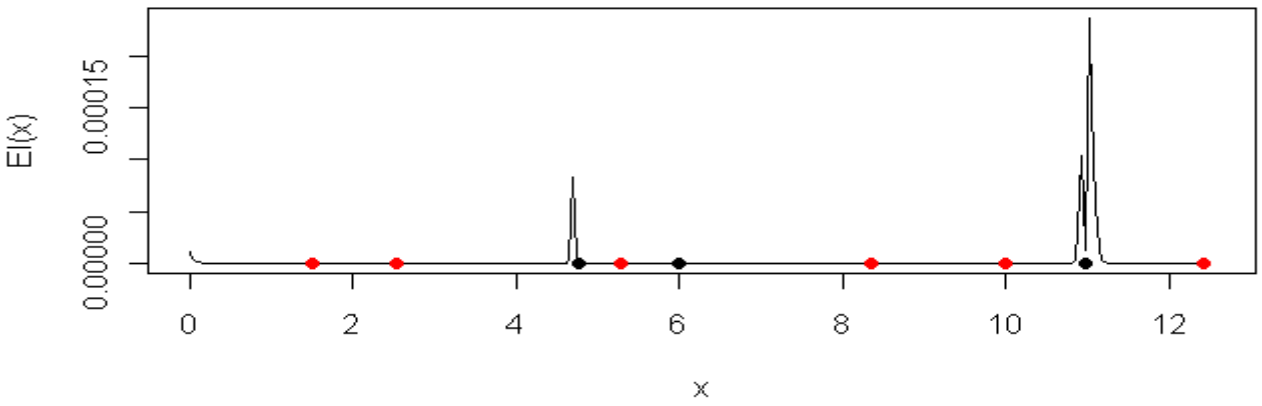


# Adaptive design for optimization: EGO algorithm

**EGO: step 3**




*[ Chevalier, 2011 ]*



# Conclusions on the Gaussian process metamodel

- Gp model construction is possible even in high dimensional case

- Main advantage of Gp: probabilistic metamodel which gives confidence bands in addition to a predictor

- Fitting quality is dependent of the initial design
  Gp model is well adapted to sequential and adaptative designs

- Caveats : it can require a large amount of effort during the fitting process and cases with more than 1000 points begin to be difficult (matrix inversion)

- Designs for specific objectives (optimization, quantile, probability, etc.)

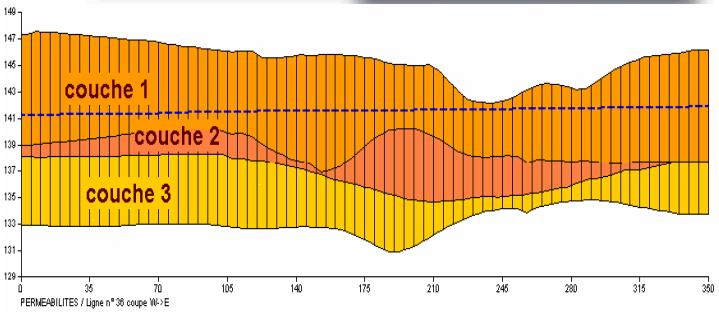
# Application

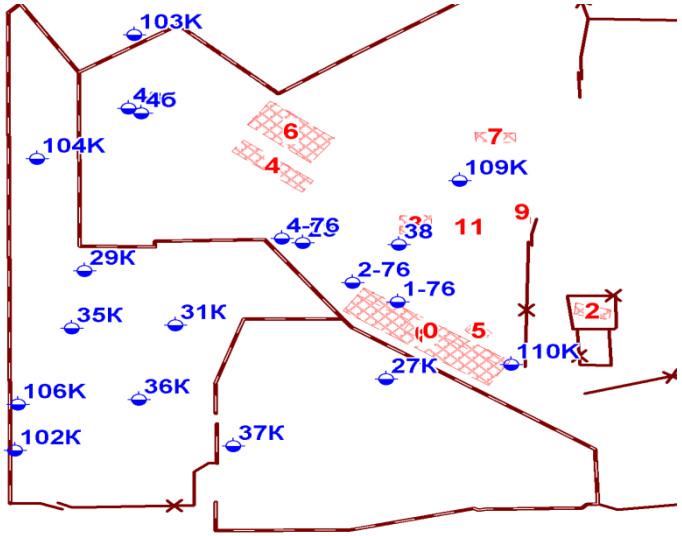
# Motivating example: hydrogeological modeling

Collaboration Kurchatov Institute/CEA

*[ Volkova et al. 2008 ]*

- Site (2 ha) near Moscow
- From 1943 to 1974 : radioactive waste repositories
- 1990 : site recognition with 20 piezometers
- Upper aquifer contamination in $^{90}$Sr




**Questions:**

**- impact assessment of the contamination on the environment**

**- degree of rehabilitation of the site**

# Uncertainty management in hydrogeological modeling

- Computation of the spatio-temporal evolution of $^{90}Sr$ concentration in an ancient radwaste disposal site between 2002 and 2010

- Goal: Estimate the contamination impact on the environment
  **Identify the influent inputs on predicted outputs**

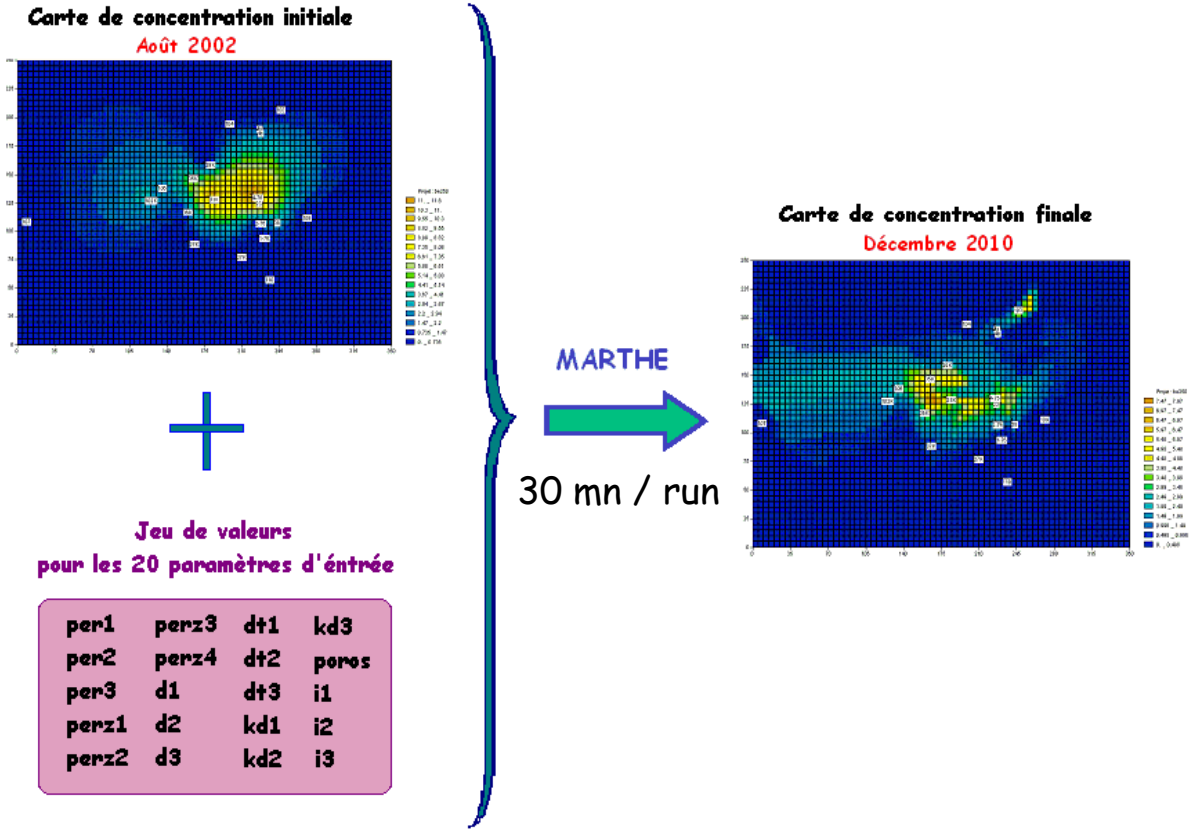
## Step A

**Numerical modeling:**
Hydrogeological transport (Darcy's law) scenario of $^{90}Sr$ with the MARTHE software

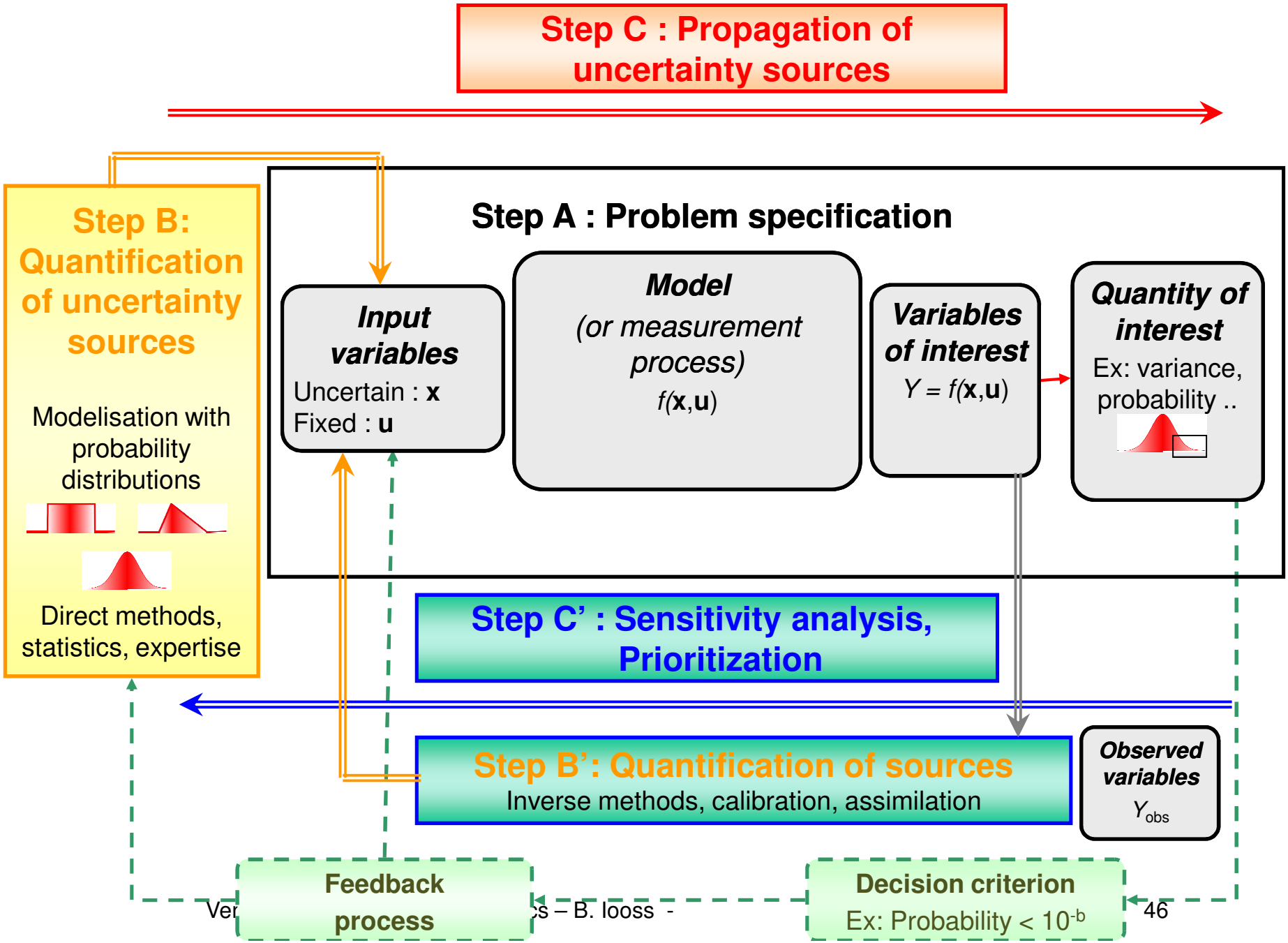
***p* = 20 uncertain inputs X:**
Permeability, dispersivity, Kd, infiltration intensity, …

**Output of interest:**
Concentration values Y

**Quantity of interest :**
Distribution, variance



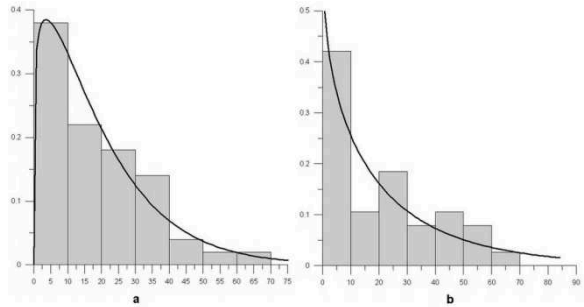
# Uncertainty management - The generic methodology



# Step B: Quantification of uncertainty sources

**Statistical modeling of the uncertainty of each input**

Different cases:




1. A lot of data
   - Fitting of probability distributions
   - Statistical hypothesis test

   MARTHE case : hydraulic conductivity (lognormal distribution)

2. Few data ($n < 10$)
   - Bayesian inference

3. No data
   - Bibliography
   - Expert judgment techniques

   MARTHE case : dispersivity, permeability, … (uniform distributions)

# Step B: Quantification of uncertainty sources

- **Input variables of the model**

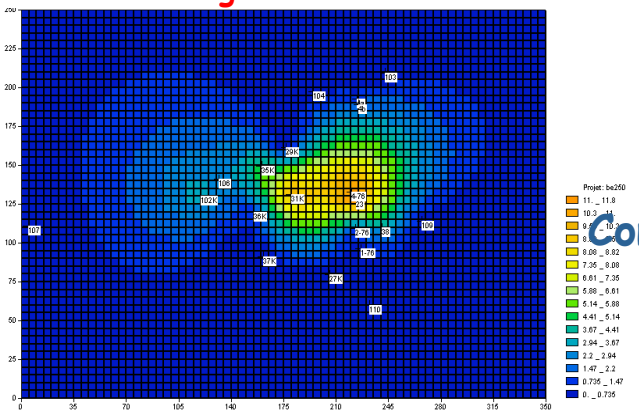
→ nominal value, type of distribution and parameters

| | Paramètres | Indicateur | Valeur du modèle | Type de distribution | Intervalle ou paramètres de distribution |
|---|---|---|---|---|---|
| 1 | Perméabilité couche 1 | per1 | 8 | Uniforme | 1 - 15 |
| 2 | Perméabilité couche 2 | per2 | 15 | Uniforme | 5 - 20 |
| 3 | Perméabilité couche 3 | per3 | 8 | Uniforme | 1 - 15 |
| 4 | Perméabilité zone 1 | perz1 | 8 | Uniforme | 1 - 15 |
| 5 | Perméabilité zone 2 | perz2 | 8 | Uniforme | 1 - 15 |
| 6 | Perméabilité zone 3 | perz3 | 8 | Uniforme | 1 - 15 |
| 7 | Perméabilité zone 4 | perz4 | 8 | Uniforme | 1 - 15 |
| 8 | Dispersivité longitudinale couche 1 | d1 | 0,8 | Uniforme | 0,05 - 2 |
| 9 | Dispersivité longitudinale couche 2 | d2 | 0,8 | Uniforme | 0,05 - 2 |
| 10 | Dispersivité longitudinale couche 3 | d3 | 0,8 | Uniforme | 0,05 - 2 |
| 11 | Dispersivité transversale couche 1 | dt1 | 0,08 | Uniforme | 0,01*d1 - 0,1*d1 |
| 12 | Dispersivité transversale couche 2 | dt2 | 0,08 | Uniforme | 0,01*d2 - 0,1*d2 |
| 13 | Dispersivité transversale couche 3 | dt3 | 0,08 | Uniforme | 0,01*d3 - 0,1*d3 |
| 14 | Coefficient de partage volumique c. 1 | kd1 | 5,1 | Weibull | 1.1597, 19.9875 |
| 15 | Coefficient de partage volumique c. 2 | kd2 | 0,34 | Weibull | 0.891597, 24.4455 |
| 16 | Coefficient de partage volumique c. 3 | kd3 | 5,1 | Weibull | 1.27363, 22.4986 |
| 17 | Porosité tous les couches | poros | 0,3 | Uniforme | 0,3 - 0,37 |
| 18 | Infiltration type 1 | i1 | 0,0001 | Uniforme | 0 - 0,0001 |
| 19 | Infiltration type 2 | i2 | 0,004 | Uniforme | i1 - 0,01 |
| 20 | Infiltration type 3 | i3 | 0,02 | Uniforme | i2 - 0,1 |

# Step C: Uncertainty propagation

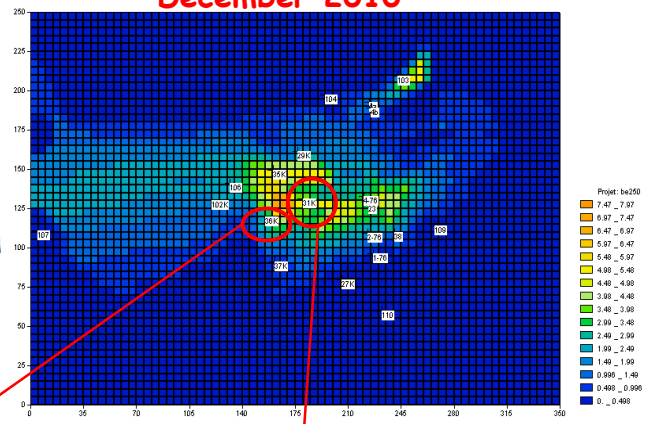
Initial concentration

August 2002



Concentration maps

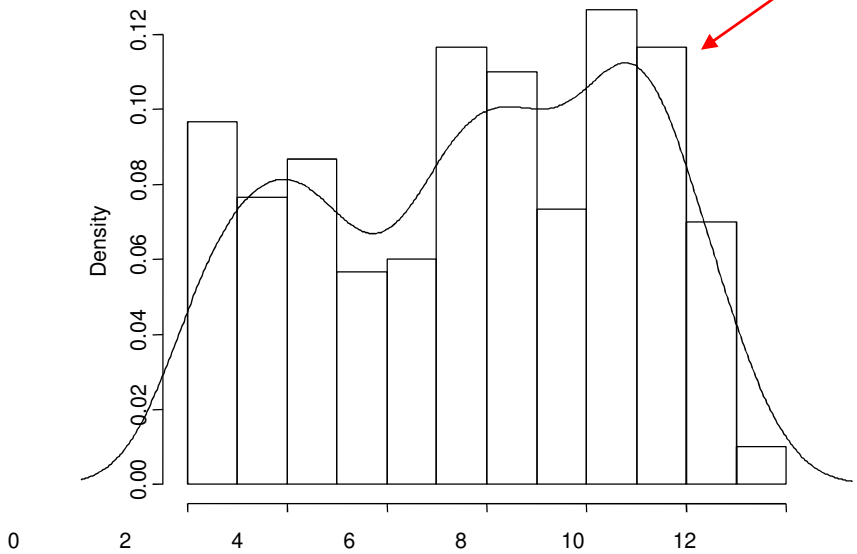
December 2010



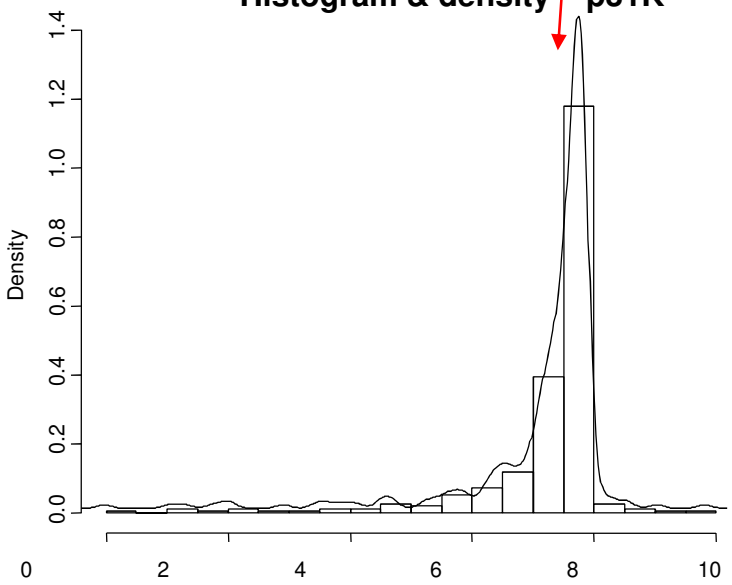
*N* = 300 runs from Latin Hypercube Sample

concentration distributions at the 20 piezometers (Bq/l)

Histogram & density - p23

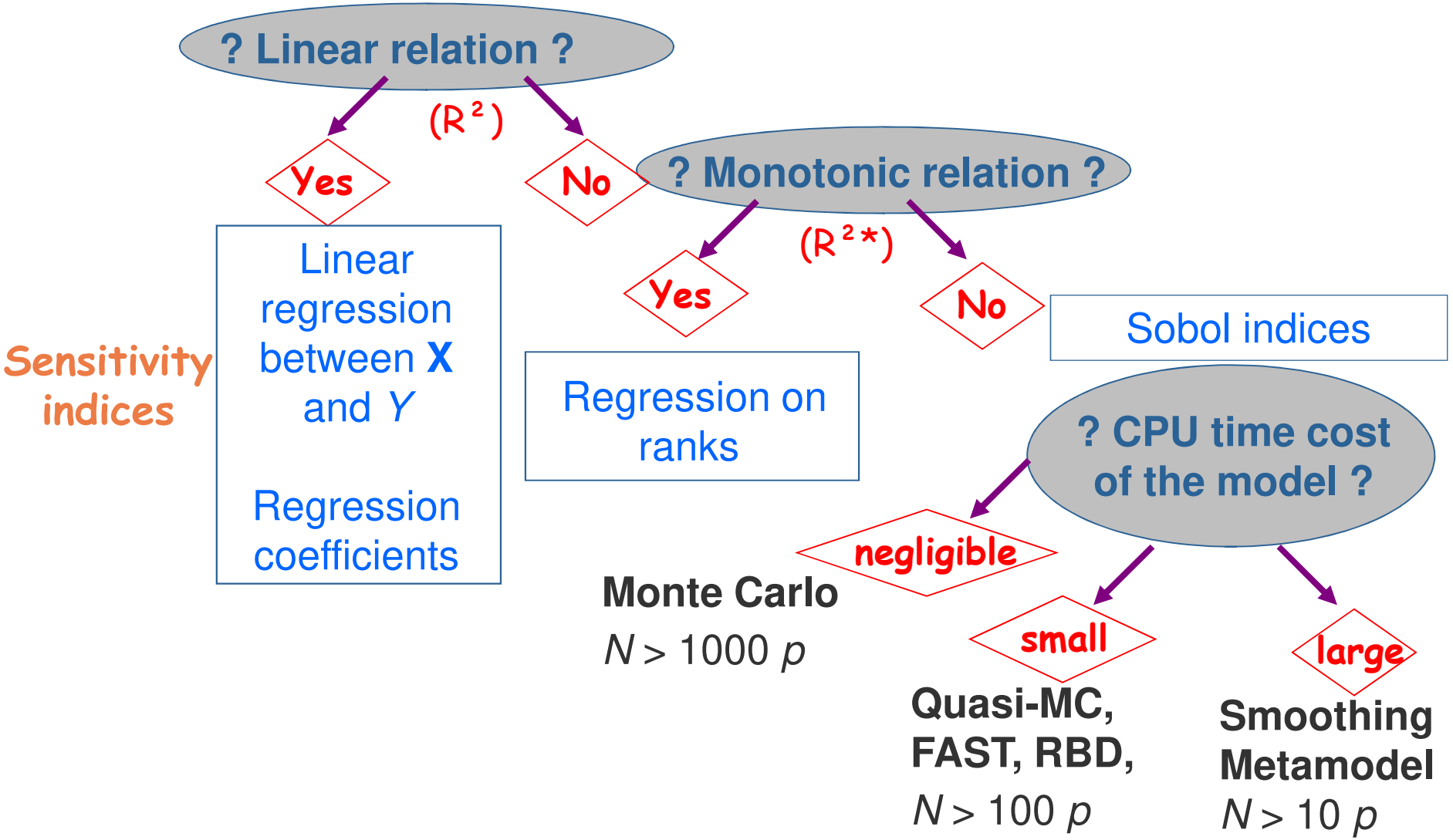



Histogram & density – p31K



# Step C': Sensitivity analysis - Sampling-based approaches

Sample ( $\mathbf{X} \in \Re^p$, $Y(\mathbf{X}) \in \Re$ ) of size $N > p$



# Step C': Regression-based approach

- **Outputs with larger $R^2$** **(linear relation )**

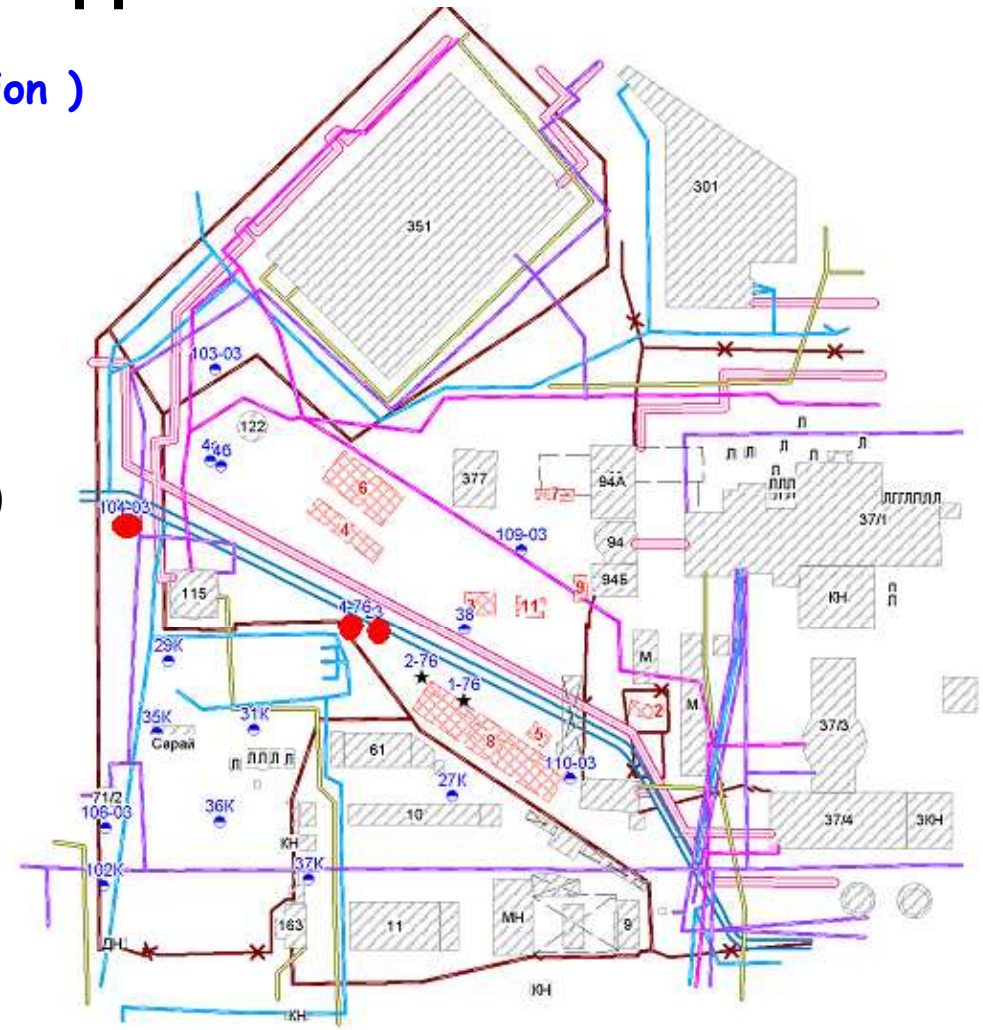
- p23 ($R^2$ = 0,78) p104 ($R^2$=0,68)
- p4-76 ($R^2$ = 0,71)

- **Outputs with larger $R^{2*}$** **(monotonic relation)**

- p4-76 ($R^{2*}$ = 0,95) p102K ($R^{2*}$ = 0,90)
- p107 ($R^{2*}$ = 0,92) p23 ($R^{2*}$ = 0,90)
- p104 ($R^{2*}$ = 0,91) p29K ($R^{2*}$ = 0,83)

- **Most influent inputs**

- Distribution coefficient, layer 2
- Distribution coefficient, layer 1
- Infiltration intensity
- permeability, layer 2




PROBLEM: 14 outputs are non monotonic and we have only 300 simulation runs

# Sensitivity analysis results for one scalar output « p104 »

Gaussian process (Gp) metamodel :

Predictivity coefficient: $Q_2$ = 93% - Linear regression : $Q_2$ = 68%

Sobol indices estimation + confidence intervals

| (en %) | $SRC_i^2$ (linear regression) | $\mu_i = E_\Omega[\tilde{S}_i]$ Gaussian process | IC- 90% $(\tilde{S}_i)$ Gaussian process |
|---|---|---|---|
| **per1** | 2 | 8 | [ 5 ; 11 ] |
| **kd1** | 52 | 69 | [ 56 ; 83 ] |
| **i3** | 13 | 13 | [ 10 ; 17 ] |

*This can be done for several outputs …*

# Step C': sensitivity analysis for 20 scalar outputs

## Main influent inputs

- **Group 1 : kd1**

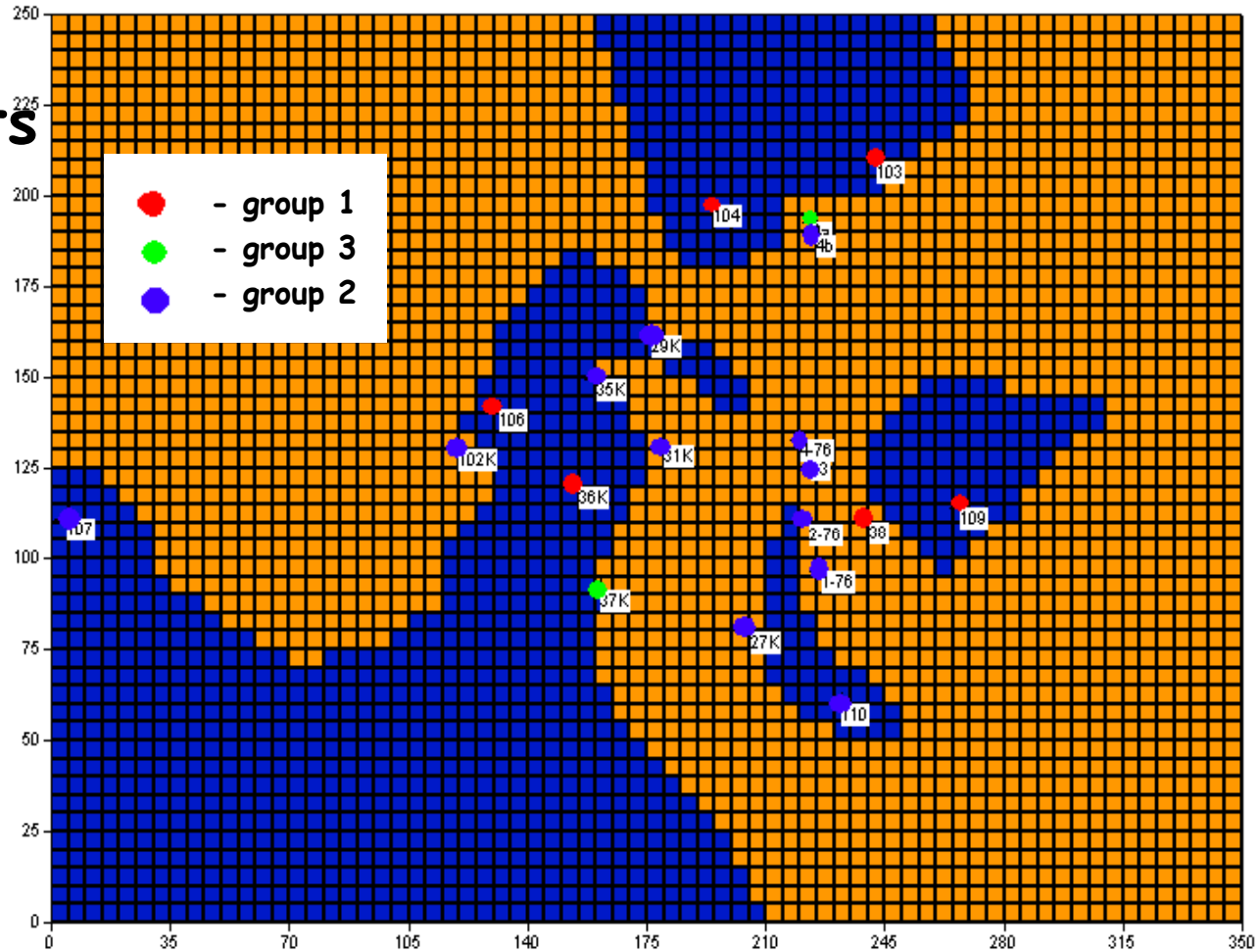
(distribution coef. of layer 1)

- **Group 2 : kd2**

(distribution coef. of layer 2)

- **Group 3 : i3**

(infiltration intensity)




Spatial location map

**… but the results are difficult to synthesize, then to interpret**

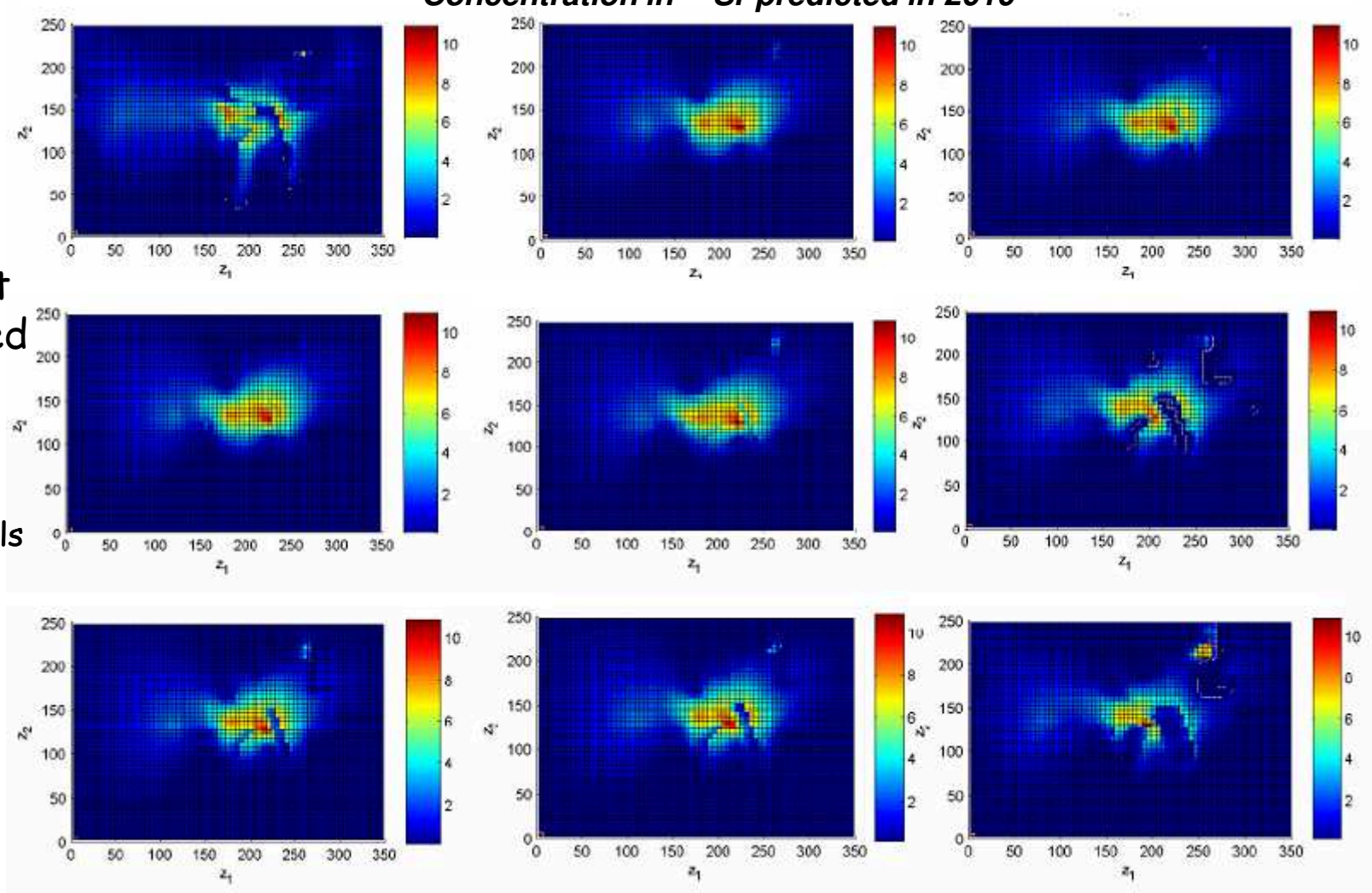
# Considering functional (spatial) output

We have simulated $N$ = 300 maps (Monte Carlo runs) with $p$ = 20 random inputs

***Concentration in $^{90}$Sr predicted in 2010***

9 output simulated maps

4096 pixels



Discretized spatial output can be considered as a functional 2D output

# Sensitivity analysis when model ouputs are functions

**Elementary cases** (sensitivity analysis on each scalar output):

- Very small CPU time consuming model
- Linear or monotonic model

**Difficult cases:**

- Complex/Non linear model ⇒ need of Sobol indices
- CPU time expensive model ⇒ need of metamodel

# Sensitivity analysis for spatial outputs: methodology

*[ Marrel et al. 2011 ]*

- Computer code $f(.)$ :

  Input: $\mathbf{X} = (X_1, \dots, X_p)$ random vector

  Output for input $\mathbf{x}^*$ : $y = f(\mathbf{x}^*, \mathbf{z})$ , $\mathbf{z} \in D_z \subset R^2$

In practice, $D_z$ is discretized in $n_z$ points (here: 64 x 64 = 4096 points)

$(\mathbf{X}, Y(\mathbf{X},\mathbf{z}))$ = input-output sample of size $N$

- **Decomposition of $Y(\mathbf{z})$ on an orthogonal function basis** (fixed basis)

For example, a wavelet basis is well-suited if there are discontinuities

- **Modeling of the decomposition coefficients by a Gp metamodel**

  Selection procedure of the most important coefficients

- **Prediction: $\mathbf{x}^*$** => prediction of coeff. => spatial output map reconstruction

Functional metamodel

**Sensitivity analysis :**

Spatial maps of sensitivity indices

# Metamodel fitting: methodology for spatial output

- **Step 1 : Wavelet decomposition of each map (300 maps)**

- **Step 2 : Kriging metamodeling of the main wavelet coefficients (the most variables) in fonction of X ; constant for the other coef.**

- **Step 3 : Prediction for a new input x***
  x*=> prediction of the coefficients => spatial output map reconstruction

- **Example of use: Sensitivity analysis (spatial map of sensitivity indices)**

**Sensitivity indices (Sobol indices,** based on functional ANOVA):

$$S_i = \frac{Var_{X_i}[E(Y|X_i)]}{Var(Y)} \quad ; \quad S_{ij} \quad ; \quad \ldots \quad ; \quad S_{Ti} = S_i + \sum_j S_{ij} + \sum_{j,k} S_{ijk} + \ldots$$

1st order — 2nd order — Total indices

The estimation of Sobol indices require a large number of simulations

⇒ computation of the Sobol indices by the way of the metamodel

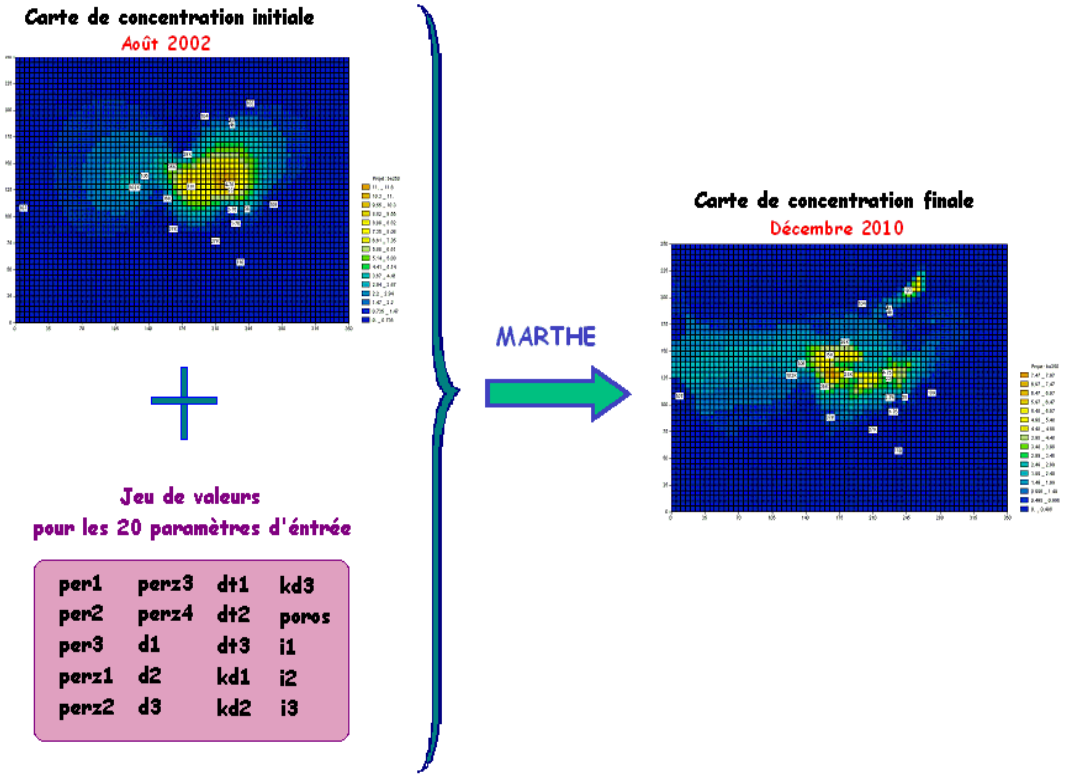
# Application on our test case (hydrogeological pollution)

$N$ = 300 simulations

$p$ = 20 random input variables

$K$ = 4096 pixels

$k$ = 100 wavelet coefficients
modeled by Gaussian process




Mean predictivity (functional metamodel): $Q_2$ = 72%

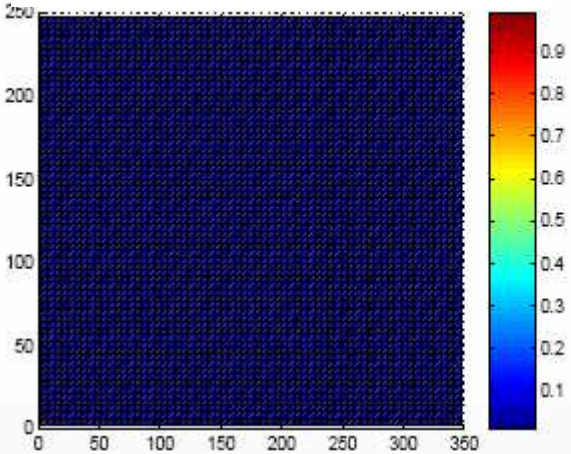
Estimation of first order and total Sobol' indices maps by Monte Carlo
(22000 runs with the fonctional metamodel)

→ 20 maps of sensitivity indices

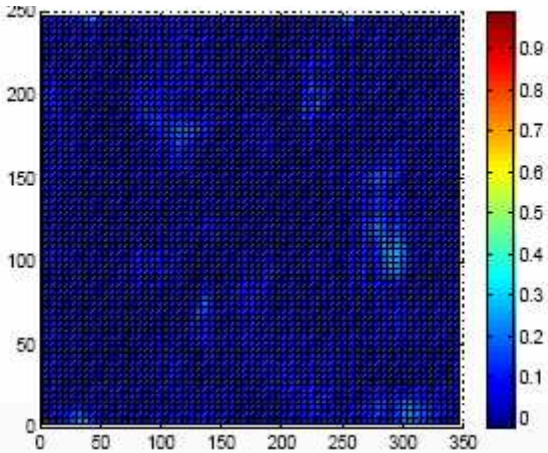
# Spatial output: results of sensitivity analysis

## Spatial maps of Sobol sensitivity indices of first order, for 6 inputs

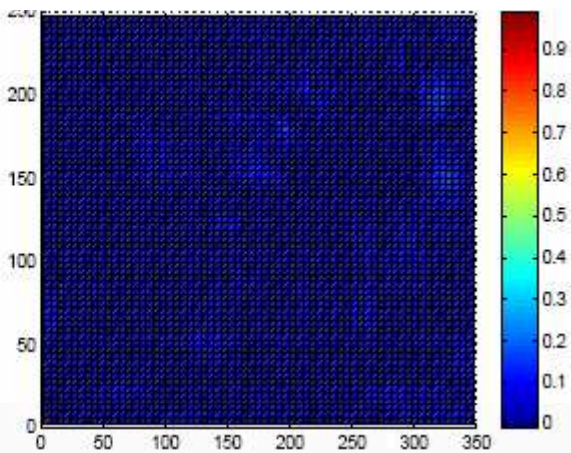
**Permeability layer 1**



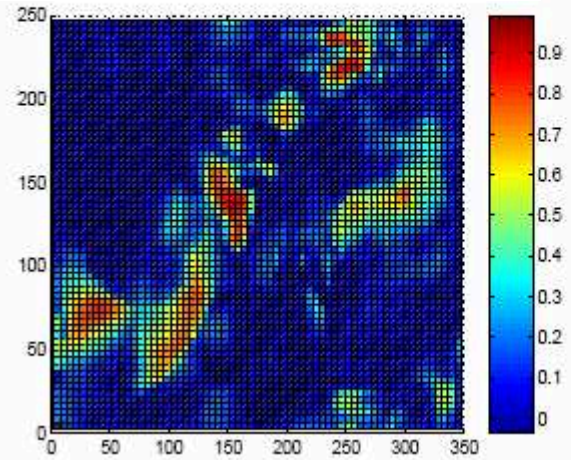

**Permeability layer 2**



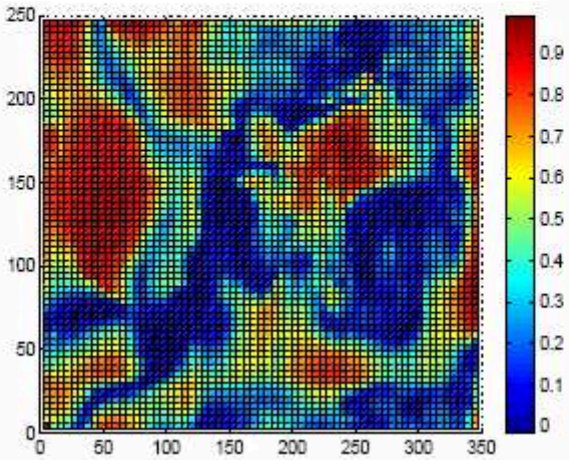

**Permeability layer 3**



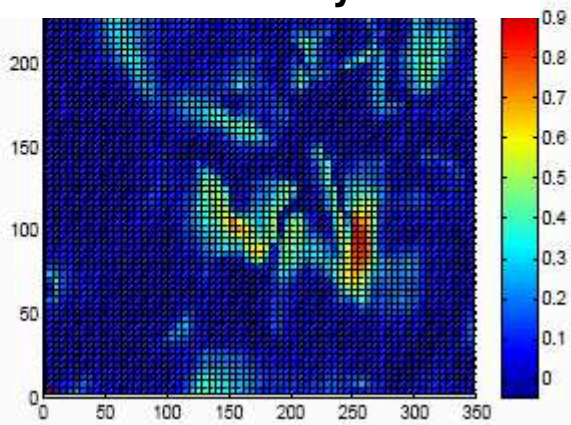

**Kd layer 1**




**Kd layer 2**




**Strong infiltration intensity**



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