Sensitivity and Uncertainty Analysis for computer code experiments a first tour

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18th-23th of March 2013

Agenda

The small story

Early 2000, IMT Toulouse begin to work with many Labs :

- **CEA Cadarache. N. Devictor, B. Iooss. Nuclear safety (Ph D A. Marrel-currently CEA-)**
- **ONERA-DOTA Palaiseau. G. Durand, A. Roblin. infrared profile of a plane (Ph D S. Varet)**
- **IFP Lyon. P. Duchène, F. Wahl-Univ Grenoble. A Antoniadis. Chemical cinetic problems (Ph D S. Da Veiga-Currently IFP-)**

⇒ Scientific meetings in Toulouse- Février 2006 and in Lyon en 2007 GDR CNRS borned

What are we dealing with?

Big computer codes= F **black box**

$$Y = F(X)$$

- Code inputs: X high dimension object (vectors or curves).
- Code outputs Y (scalar or vectorial).

X complex structure and/or uncertain

$\Rightarrow$ **seen as random**

STOCHASTIC APPROACH

Some questions on the general model

- **Sensitivity and uncertainty analysis= take informations on the joint distribution (X, Y)**
- **F too complicated. Design a reduced model= Estimate a response surface**
- **Optimise the run number= make an experimental design**

People working around this topic

- **GDR MASCOT NUM Annual meeting march 2012 : CEA Bruyères le Chatel** http://www.gdr-mascotnum.fr/
- **ANR project : OPUS EADS, CEA, EDF, ... (CEA)** http://www.opus-project.fr/
- **ANR project : COSTA BRAVA CEA, IFP, Univ Toulouse, Univ Grenoble** http://www.math.univ-toulouse.fr/COSTA_BRAVA/doku.php?id=index
- **SIAM conference : Uncertainty quantification 2th-5Th April 2012** http://www.siam.org/meetings/uq12

Motivation-Examples

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- **Main object : complicated computer simulation code**

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  - Example functional code CERES from CEA ▸ CERES
- Need methods to enlight.

Frame: Black box

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Today conference: vectorial input et scalar output

Y =output is a number and X =input is a vector of numbers

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Black box model

Non linear regression model

$$Y = f(X).$$

The code is modeled as an abstract complicated function f

Gains of stochastic methods

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- **Take into account random characteristic of some components of X**

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  - unknown physical constants: wave in random media.

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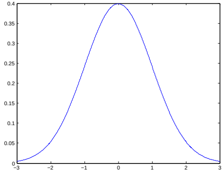
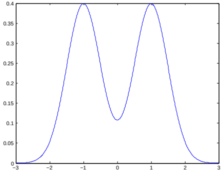
  - Allow to model multimodal distributions: double mode...





Gains of stochastic methods

- Take into account random characteristic of some components of X
  - Physical measures with error: Pressure, temperature...
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  - Allow to model multimodal distributions: double mode...
- **Parametric and non parametric estimation methods**

Presented techniques

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- **Sobol sensitivity analysis**

Presented techniques

- Sobol sensitivity analysis
  - Within the (random) components of the input (vector) X what are those having most influence on the output?
  - "influence" is quantified in terms of "variability" induced by this component.
  - Global analysis taking into account the whole distribution of the input.
- **Response surface methods (Reduced model)**

Presented techniques

- Sobol sensitivity analysis
  - Within the (random) components of the input (vector) X what are those having most influence on the output?
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  - Global analysis taking into account the whole distribution of the input.
- Response surface methods (Reduced model)
  - Replace the complicated code by a simple one easy to build from a short sample y cheap in CPU.
  - Goal: optimization, computation of a critical threshold, sensitivity analysis...
  - Discussed method: come from geostatistics (KRIGING).

Some links I

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- **Research/Developpement**

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- Research/Developpement
  - GDR CNRS MASCOT NUM http://www.gdr-mascotnum.fr/ ,
  - OPUS- ANR project big *open source* plateform including tools for codes.
  - COSTA BRAVA- ANR project functional input or output coupling random and deterministic methods.
- **Softwares**

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- Softwares
  - R package DICE (IRSN, EDF, Renault, ...). http://crocus.emse.fr/dice
  - MATLAB Kriging package: DACE http://www2.imm.dtu.dk/ hbn/dace/
  - Free software of O' Oakley and O' Hagan computation of sensitivity indices: GEM http://www.tonyohagan.co.uk/academic/GEM/index.html

Some links II

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- **Some references to begin with**

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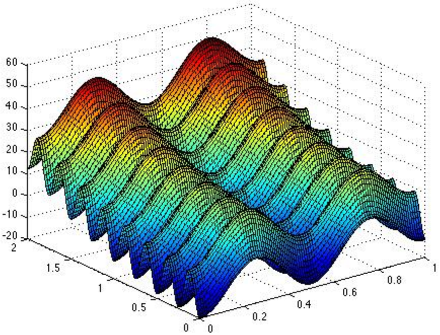
- Some references to begin with
  - Linear and non linear regression: Azais, Antoniadis et al
  - Computer code experiments : Santner et al
  - Sensitivity analysis: Tarantolla et al, pioneering papers of Sobol, Antoniadis
  - Kriging: Stein, Cressie

A toy model

Rastrigin function

$$f(x) = f(x_1, x_2) = 8\|x\|^2 - 10(\cos(4\pi x_1) + \cos(8\pi x_2))$$

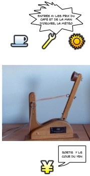


See `http://www.gdr-mascotnum.fr/doku.php?id=benchmarks`

Recall the goal

Model

$$Y = f(X).$$



- $X = (X_i)_{i=1...k}$ input vector
- Y output (real number).

Goal: Which of the components of X are more influent on Y?

Deterministic methods

Roughltly speaking are based on derivative of f:

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Effective computation of the derivative

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Effective computation of the derivative

- Finite differences

$$(\frac{\partial f}{\partial X_j})(\overline{x}) \approx h^{-1}\left[f(\overline{x}_{j,h^+}) - f(\overline{x}_{j,h^-})\right]$$

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- Adjoint methods: the derivative is directly computed by the code (PDE models).

Deterministic methods-toy model

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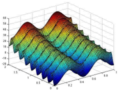

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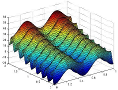
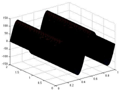
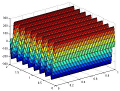


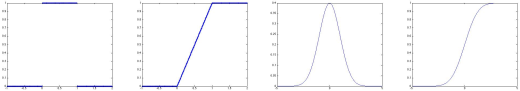


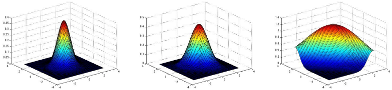


The derivative method is quite unstable.

A first insight in probability theory: Random variables

- Probability distribution
  - Z random variable on $\mathbb{R}$: most often with *density*. Repartition of Z is described by a function, ("mass function ").





  - Random vector on $\mathbb{R}^2$
  - Generalization: random vector on $\mathbb{R}^k$. Example multivariate (centered) Gaussian distribution with density

$$\frac{1}{(2\pi)^{\frac{k}{2}}\sqrt{\det \Gamma}} \exp[\frac{1}{2} z^T \Gamma^{-1} z].$$

- Independence of random variables (Z_1, Z_2): observing Z_1 give no information on the distribution of Z_2.

A first insight in probability theory: Expectation, Variance

Z a random variable having distribution F.

- Expectation of a random variable: $\mathbb{E}(Z)$
  - Gravity center
  - Constant that explains the best the random variable.
  - Projection on constant *random* variables
- Variance of a random variable: $\mathrm{Var}(Z)$
  - Inertia moment
  - Magnitud of the fluctuactions around the mean
  - Squared norm of the random variable after having taken off the mean effect

Pythagora's Theorem

$$\mathbb{E}(Z^2) = \|Z\|^2 = \|\mathbb{E}(Z)\|^2 + \|Z - \mathbb{E}(Z)\|^2 = \mathbb{E}(Z)^2 + \mathrm{Var}(Z)$$

$$\mathrm{Var}(Z) = \mathbb{E}(Z^2) - \mathbb{E}(Z)^2.$$

Distribution examples : Expectation, Variance

- The most popular: Gaussian distribution (m, σ^2)
  - density on $\mathbb{R}$

$$g(z) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(z-m)^2}{2\sigma^2}\right].$$

  - Expectation

$$\mathbb{E}(Z) = \int_{-\infty}^{+\infty} z g(z) dz = \int_{-\infty}^{+\infty} \frac{z}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(z-m)^2}{2\sigma^2}\right] dz = m.$$

  - Variance

$$\mathrm{Var}(Z) = \mathbb{E}[(Z - \mathbb{E}(Z)^2)^2] = \mathbb{E}(Z^2) - [\mathbb{E}(Z)]^2 = \sigma^2.$$

- The most random: Uniform on $[z_{\text{min}}, z_{\text{max}}]$
  - density on $\mathbb{R}$

$$g(z) = \frac{\mathbf{1}_{[z_{\text{min}}, z_{\text{max}}]}(z)}{z_{\text{max}} - z_{\text{min}}}.$$

  - Expectation

$$\mathbb{E}(Z) = \int_{z_{\text{min}}}^{z_{\text{max}}} zg(z)dx = \int_{z_{\text{min}}}^{z_{\text{max}}} zdz = \frac{z_{\text{min}} + z_{\text{max}}}{2}$$

  - Variance

$$\text{Var}(Z) = \mathbb{E}[(Z - \mathbb{E}(Z)^2)^2] = \mathbb{E}(Z^2) - [\mathbb{E}(Z)]^2 = \frac{(z_{\text{max}} - z_{\text{min}})^2}{12}.$$

A first insight in probability theory: Conditional expectation

(Z_1, Z_2) a random vector

- Conditional expectation of Z_2 knowing Z_1): $\mathbb{E}(Z_2|Z_1)$
  - $Z_1 = z_1$ has been observed how one can predict the best Z_2?
  - What is the best function of Z_1 to explain Z_2?
  - Projection of Z_2 on functions of Z_1.

  Examples
  - $\mathbb{E}(Z_2|Z_1) = \mathbb{E}(Z_2)$ when (Z_1, Z_2) are independent random variables
  - $\mathbb{E}(Z_2|Z_1) = \rho Z_1$ for a centered Gaussian vector

- Some interesting facts for $\mathbb{E}(Z_2|Z_1)$
  - $\mathbb{E}[\mathbb{E}(Z_2|Z_1)] = \mathbb{E}[Z_2]$
  - $\mathbb{E}[\psi(Z_1)Z_2|Z_1] = \psi(Z_1)\mathbb{E}(Z_2|Z_1)$
  - Pythagora's Theorem

$$\mathbb{E}[Z_2^2] = \mathbb{E}[\mathbb{E}(Z_2|Z_1)^2] + \mathbb{E}[(Z_2 - \mathbb{E}(Z_2|Z_1))^2]$$

taking off $[\mathbb{E}(Z_2)]^2$

$$\text{Var}(Z_2) = \text{Var}[\mathbb{E}(Z_2|Z_1)] + \mathbb{E}[(Z_2 - \mathbb{E}(Z_2|Z_1))^2].$$

Of course, it is possible to generalize the notion of conditional expectation for a vector (Z_1 is a random vector).

Example toy model

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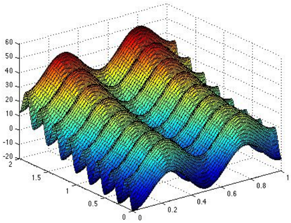
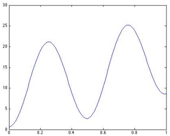


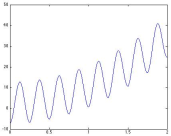
Example toy model

Assume that $X_1 \sim \mathcal{U}([0,1])$ et $X_2 \sim \mathcal{U}([0,2])$

$$\mathbb{E}(Y|X_1) = 8X_1^2 - 10\cos(4\pi X_1) + \frac{32}{3}$$



$$\mathbb{E}(Y|X_2) = 8X_2^2 - 10\cos(8\pi X_2) + \frac{8}{3}$$



An important example of vectorial conditioning

Centered Gaussian model

$$Z^T = (Z_1, Z_2)^T = (Z_1^1, \ldots Z_1^l, Z_2)$$

Gaussian vector with density

$$\frac{1}{(2\pi)^{\frac{k}{2}}\sqrt{\det \Gamma}} \exp[\frac{1}{2} z^T \Gamma^{-1} z].$$

Γ is the covariance matrix of the random vector Z (assumed to be invertible):

$$\Gamma = \begin{pmatrix} \Gamma_{Z_1} & c^T_{Z_1,Z_2} \\ c_{Z_1,Z_2} & \sigma^2_{Z_2} \end{pmatrix}$$

- Γ_{Z_1} is the covariance matrix of the random vector Z_1,
- c_{Z_1,Z_2} is the covariance vector between Z_1 and Z_2 (row vector),
- $\sigma^2_{Z_2}$ is the variance of Z_2.

Centered Gaussian model

Theorem

$$\mathbb{E}(Z_2|Z_1) = c_{Z_1,Z_2}\Gamma_{Z_1}^{-1}Z_1,$$
$$\mathbb{E}[Z_2 - \mathbb{E}(Z_2|Z_1)]^2 = \sigma_{Z_2}^2 - c_{Z_1,Z_2}\Gamma_{Z_1}^{-1}c_{Z_1,Z_2}^T.$$

- Linear prediction,
- 1-d example $\mathbb{E}(Z_2|Z_1) = \rho Z_1$,
- Kalman filter=recursive formulation of the previous theorem

Sobol method

Model

$$Y = f(X).$$

We will quantify the *stochastic* influence of each input variables using previous projections:

Definition

Sobol indices for the output Y

- *First order indice for the input X_i*

$$S_i = \frac{Var(\mathbb{E}[Y|X_i])}{Var(Y)}$$

- *2nd order indice for the inputs $X_i, X_{j)}$*

$$S_{i,j} = \frac{Var(\mathbb{E}[Y|X_i, X_j])}{Var(Y)} - S_i - S_j$$

Sobol-Antoniadis (Hoeffding) Decomposition

Generalization: third order for the input X_i, X_j, X_l

$$S_{i,j,l} = \frac{\mathrm{Var}(\mathbb{E}[Y|X_i, X_j, X_l])}{\mathrm{Var}(Y)} - \sum_{i_1 < i_2 \in \{i,j,l\}} S_{i_1,i_2} + S_i + S_j + S_l$$

$S_{i,j,l}$ joint influence of X_i, X_j et X_k (marginal effects erased).

Theorem (Sobol-Antoniadis-Hoefding)

Assume that. $X_1, X_2, \ldots, X_k$ *are independent. then*

$$1 = \sum S_{ijl\ldots}$$

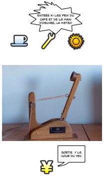
Sobol indices estimation

- Monte Carlo methods,
- Quasi Monte Carlo methods: FAST,
- Gaussian methods metamoddeling: Kriging O Oakley et al,
- Mathematical Statistics ANR COSTA BRAVA,

Recall the goal

Model

$$Y = f(X).$$



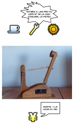
- $X = (X_i)_{i=1\dots k}$ is the input vector
- Y is the output (real number).

Goal: Build a function $\tilde{f}$ (cheap in terms of CPU) to emulate (approximate, estimate) f.

Several approaches

Model

$$Y = f(X).$$



Goal: Build a function $\tilde{f}$ (cheap in terms of CPU) to emulate (approximate, estimate) f.

- Approximation of f by a linear combination of given functions (e.g. Fourier, chaos or orthogonal polynomials,...),
- The same but non linear approximation (neural networks, non parametric statistics...),
- Discussed method: Bayesian approach using Gaussian processes (fields).

A short journey towards Gaussian fields

Gaussian vector $Z = (Z_i)_{i=1\ldots k}$: finite number of components
Random Gaussian field $Z = (Z_t)_{t \in T}$: *many* components as the elements of T ($T = \mathbb{Z}, \mathbb{R}, \mathbb{C}, \mathbb{R}^k$).
Gaussian vector: the probability density is

$$\frac{1}{(2\pi)^{\frac{k}{2}} \sqrt{\det \Gamma}} \exp[\frac{1}{2}(z - m)^T \Gamma^{-1} (z - m)].$$

The important parameters are:

- The mean (expectation) m vector of $\mathbb{R}^k$,
- The covariance matrix Γ ($\gamma_{i,j} = \text{cov}(Z_i, Z_j)$)

Random Gaussian field

Random Gaussian field: for any sample points $t_1, t_2, \dots t_p \in T$, the vector

$$Z := (Z_{t_i})_{i=1\dots p}$$

is a Gaussian vector. The important parameters are:

- The mean function $m(t) = \mathbb{E}(Z_t), \; t \in T$,
- The covariance function $\gamma(t, t') = \text{cov}(Z_t, Z_{t'}), t, t' \in T$

STATIONARY Gaussian field

STATIONARY Gaussian field: modeling an *unmoving dynamic* (in space or time) phenomena Translation on the parameters:

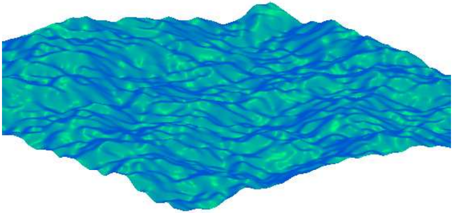
- The mean function is constant $m(t) = m, \ t \in T$,
- The covariance function only depends on $t - t'$
  $\gamma(t, t') = \text{cov}(Z_t, Z_{t'}) = r(t - t')$.

Classical frame

- Vanishing mean function $m(t) = 0, \ t \in T$,
- The covariance function $r(u)$ depends on some parameter θ. For example, assuming isotropy $r(u) = \exp(h\|u\|^\alpha) \ u \in T$. Here, the parameter is $\theta = (h, \alpha)$ $(h > 0, \alpha \geq 2)$.

Example modeling the sea

STATIONARY Gaussian process on $\mathbb{R}^2$ with an *ad hoc* covariance function (See the excellent book of Azais-Wchebor)



Kriging 0

Bayesian model in geostatistics

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$$f(x) = \alpha_\theta(x) + Z_x(\nu)(x \in T)$$

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- α_θ a simple mean function (*trend*): $\langle \theta, x \rangle$

Kriging 0

Bayesian model in geostatistics

$$f(x) = \alpha_\theta(x) + Z_x(\nu)(x \in T)$$

- θ and ν are unknown vectorial parameters
- α_θ a simple mean function (*trend*): $\langle \theta, x \rangle$
- $(Z_x)_{x \in T}$ centered stationary Gaussian field $r_\nu(x)$, $x \in T$

Kriging I

Main idea=THE COMPUTER CODE IS THE REALIZATION OF A GAUSSIAN FIELD TRAJECTORY

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The model has been played *randomly*

$$Y(x) = f(x)(x \text{ deterministic} \in T)$$

Kriging I

Main idea=THE COMPUTER CODE IS THE REALIZATION OF A GAUSSIAN FIELD TRAJECTORY

The model has been played *randomly*

$$Y(x) = f(x)(x \text{ deterministic} \in T)$$

Kriging II

Bayesian model for the black box

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- *Roughly speaking :* least square fit of the parameters with weight functions depending on the parameters

Kriging III

Bayesian approach

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- Γ_N covariance matrix between $Z^N := (Z_{x_1}, \dots, Z_{x_N})^T$.

Kriging IV

Bayesian method in a functional space

Kriging IV

Bayesian method in a functional space

- Emulation method by linear regression

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Kriging IV

Bayesian method in a functional space

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- Prediction error of Gaussian du model (if the parameter of the model are known)

$$\mathbb{E}[(Y(x) - \widehat{Y}(x))^2] = r_\nu(0) - c_x^T \Gamma_N^{-1} c_x$$

One example
from :http://www2.imm.dtu.dk/ hbn/dace/

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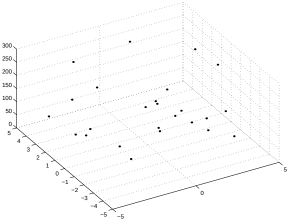
DTU

Introduction

Given $f : \mathbb{R}^n \mapsto \mathbb{R}$. May be a black-box (and "expensive") function.

Know values $y_i = f(s_i)$ at *design sites* $S = \{s_1, \ldots, s_m\}$. How does the function behave in between?



ISMP 2003 3

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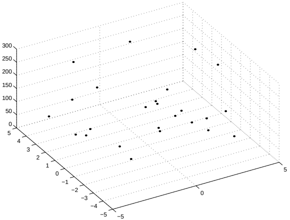
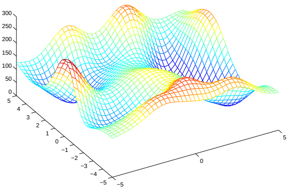


DTU

Gauss model

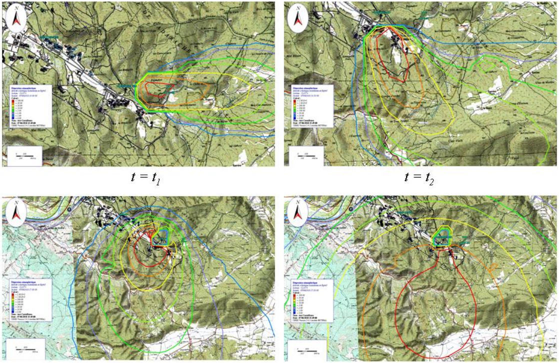


End

Gracias por su atencion
Thanks for your attention
Merci
Obrigado
Danke
Grazie

Le code CERES

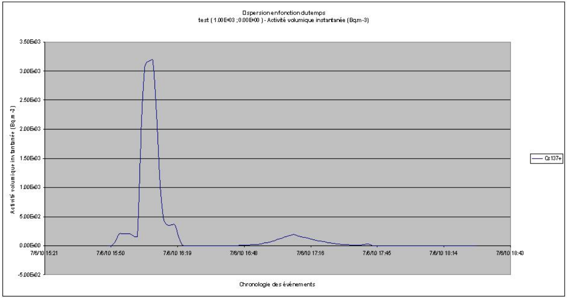
Evolution dans le temps de l'activité volumique instantanée du ^{137}Cs dans l'air



$t = t_1$ $t = t_2$ $t = t_3$ $t = t_4$

Le code CERES(bis)

Evolution dans le temps de l'activité volumique instantanée du ^{137}Cs en 1 point donné



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