Uncertainties Propagation with URANIE

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Workshop $P(ND)^2 - 2$

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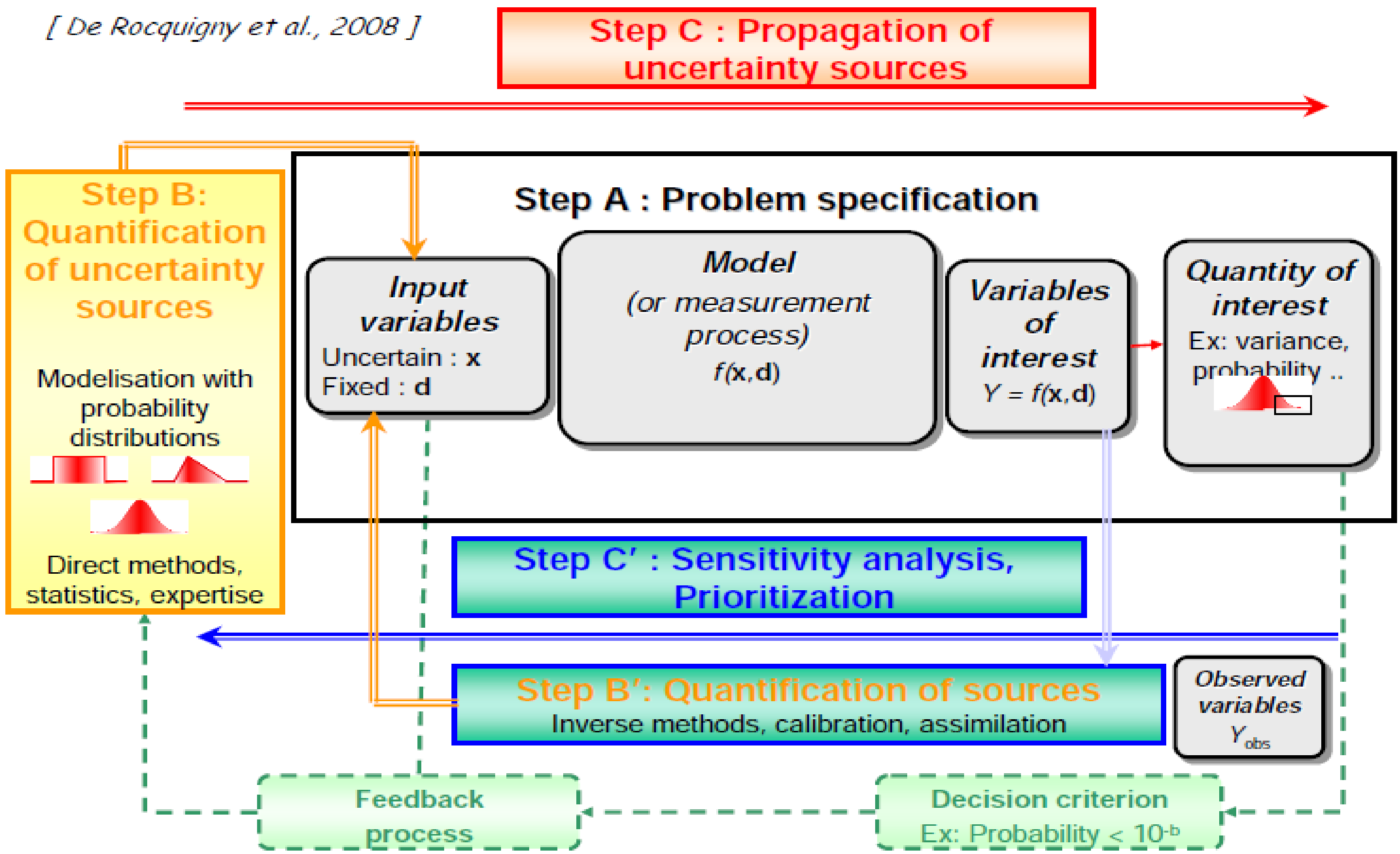
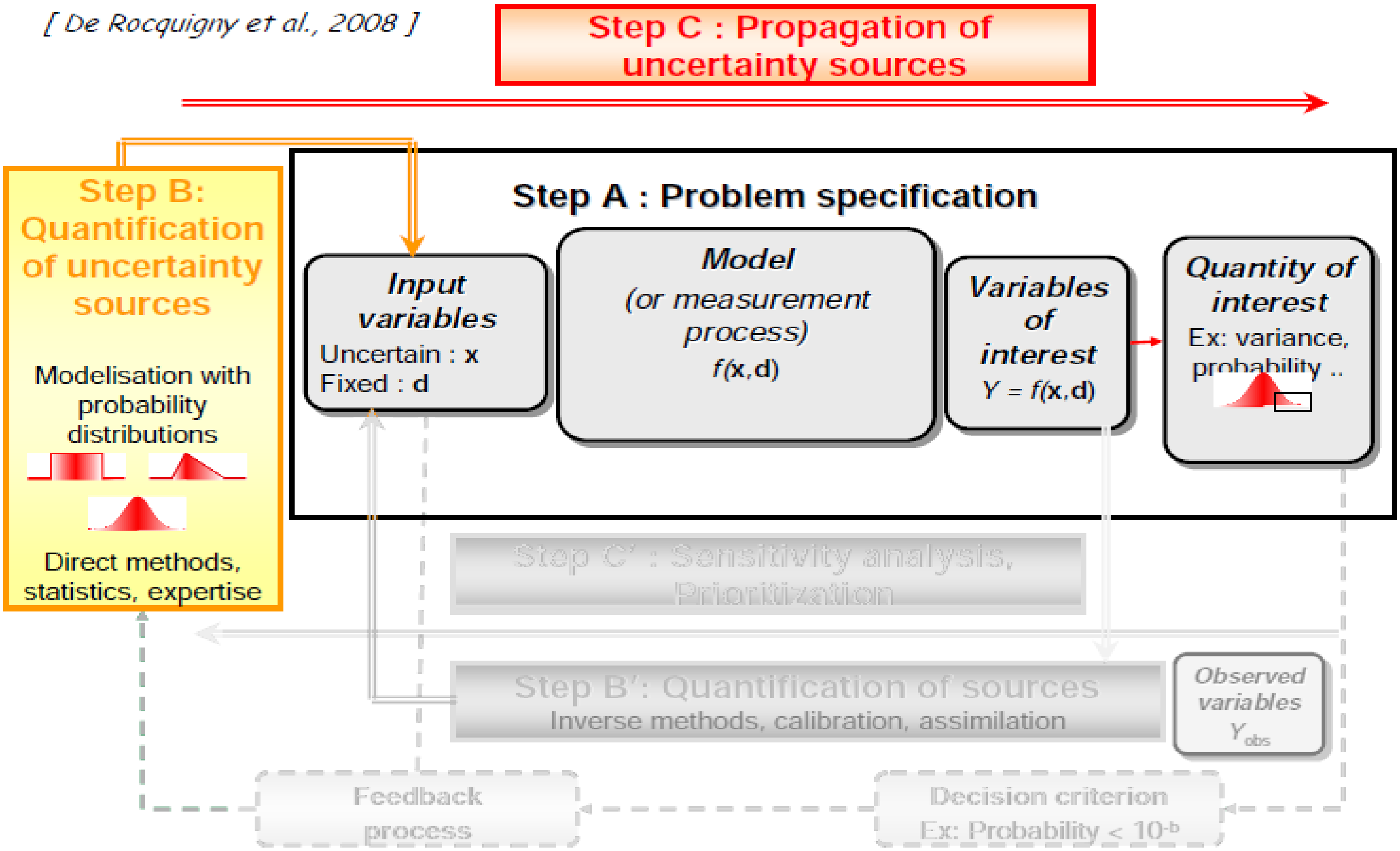
Outline

- Uncertainties Propagation
  - Input modelisation
  - Distribution of the computation code
  - Output analysis
- the Uranie platform
- Example of Uncertainties Propagation

General Flowchart of Sensitivity Methods

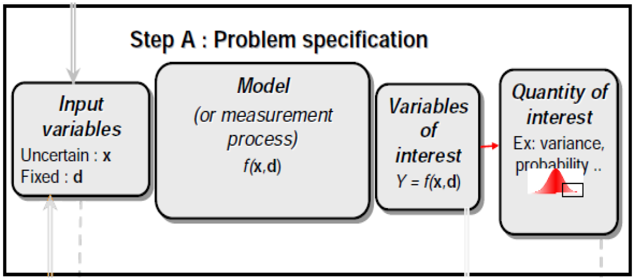


Focus on the Uncertainties Propagation

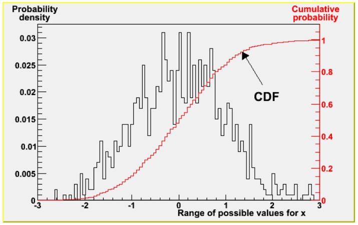


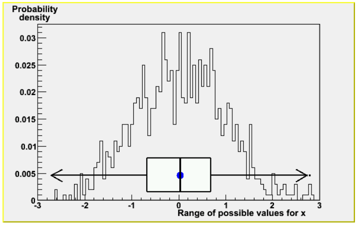
Step A : Problem Specification

- Computer code f
- Two types of input parameters (x, d)
  - Fixed parameters d
  - Uncertain parameters x

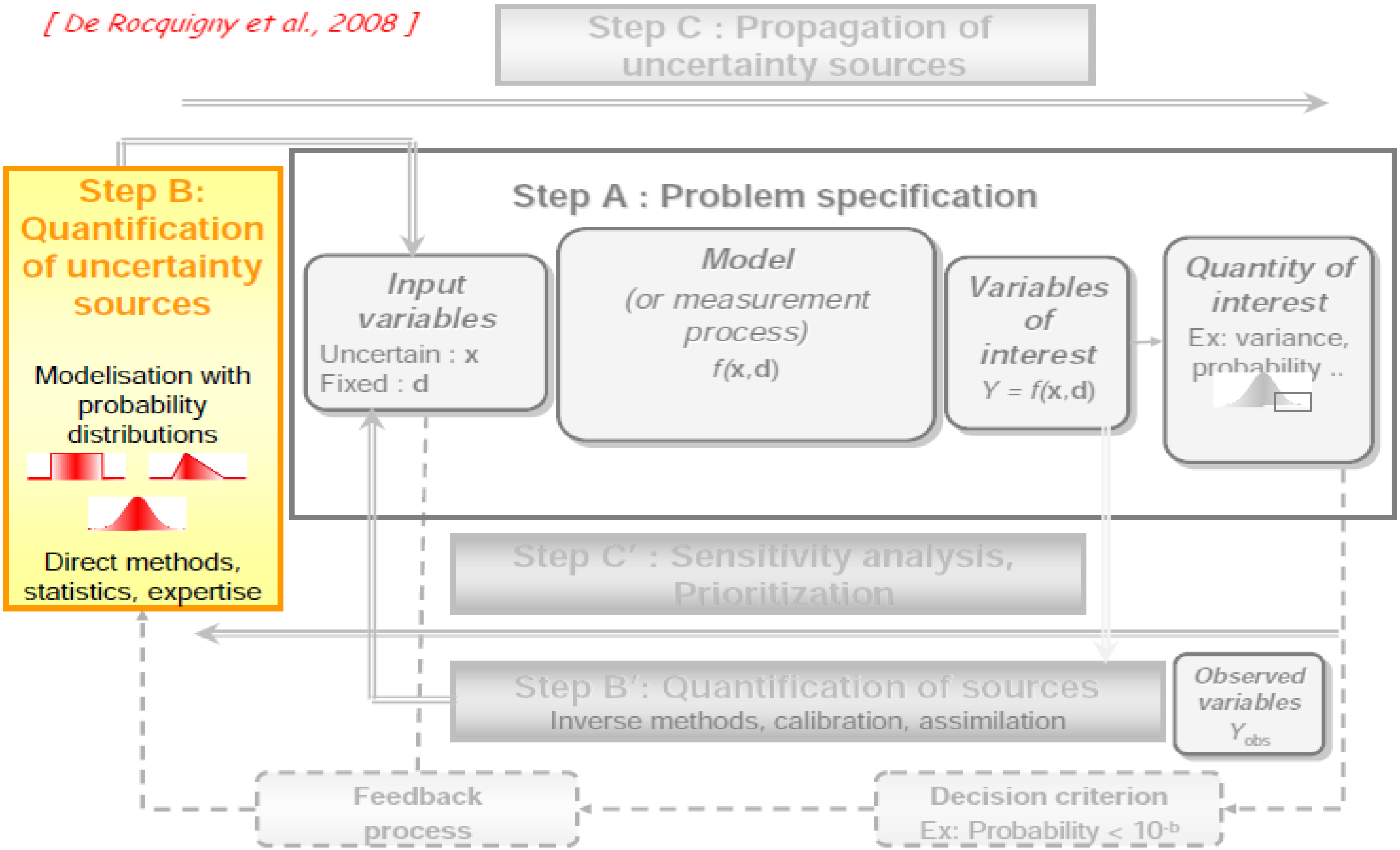


- Outputs of interest $y = f(x, d)$
- Quantity of interest on the Uncertainties Propagation
  - *Location* : Mean μ, Min, Max, Mode, Median, Quantile q_α
  - *Dispersion* : Standard-deviation σ , Variance σ^2, Range $(Max - Min)$, Coefficient of Variation $(\delta = \sigma/\mu)$
  - Probability Density Function (PDF), Cumulative Density Function (CDF)





Step B : Quantification of uncertainty sources

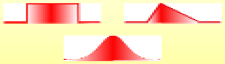


Quantification of uncertainty with PDF

- Expert judgment
- With *"large"* dataset : Fitting the parameters of the PDF
  - Parametric methods
  - Non-parametric methods
  - Statistical Tests
- With small dataset :
  - Bayesian methods
  - Bootstrap methods (resampling)

Step B: Quantification of uncertainty sources

Modelisation with probability distributions



Direct methods, statistics, expertise

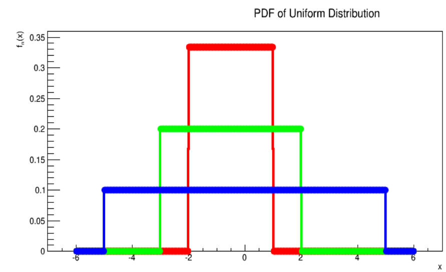
Continuous			Discrete
Bounded	**positive**	**Umbounded**	
Uniform	Exponential	Normal	Binomial
Beta	LogNormal	Cauchy	Multinomial
Triangular	Weibull	Gumbel	Poisson
Trapezium	Gamma	...	...
Uniform by parts	Khi-two		
LogUniform	Pareto		
LogTriangular	...		
...			

1. **Uniform Distribution**

– The values in the interval $[a, b]$ are equally probable

– 2 parameters a (*"Minimum"*) and b (*"Maximum"*)

$$f(x) \quad = \quad \frac{1}{b-a}\, \mathbb{1}_{[a,b]}(x)$$



– Mean : $\mu = \frac{b-a}{2}$ (*Median*)

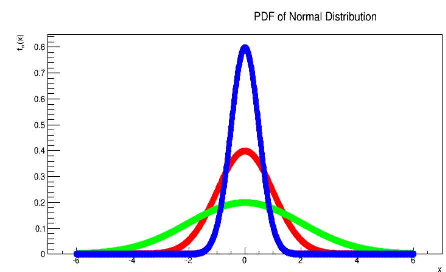
– Mode : any value in $[a, b]$

– Variance : $\sigma^2 = \frac{(b-a)^2}{12}$

2. **Normal Distribution**

– 2 parameters μ (*"Mean"*) and σ (*"Standard-Deviation"*)

$$f(x) \quad = \quad \frac{1}{\sigma\sqrt{2\pi}} \exp^{-\frac{(x-\mu)^2}{2\,\sigma^2}}$$



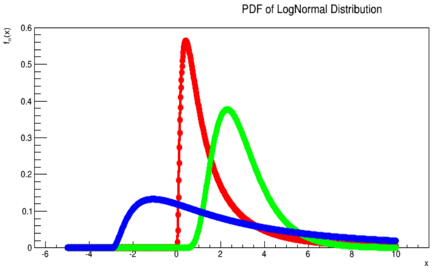
– Mean : μ (*Mode, Median*)

– Variance : σ^2

3. **LogNormal Distribution**

- A **positive** random variable x is said to follow a *LogNormal* law when $\ln x \sim \mathcal{N}$
- 3 parameters x_0 (lower bound) and (μ, σ) when $ln(X) \sim \mathcal{N}(\mu, \sigma)$

$$f(x) = \frac{1}{(x - x_0)\sigma\sqrt{2\pi}} \exp^{\frac{-(\ln(x - x_0) - \mu)^2}{2\sigma^2}} \quad \forall x > x_0$$



- Mean : $\mu_X = \exp^{(\mu + \frac{\sigma^2}{2})}$
- Median : $\exp^{(\mu)}$
- Mode : $\exp^{(\mu - \sigma^2)}$
- Variance : $\mu^2 \times (\exp^{\sigma^2} - 1.)$

4. **Beta Distribution**

– 4 parameters α, β (shapes) & $x_0 < x_1$ (bounds)

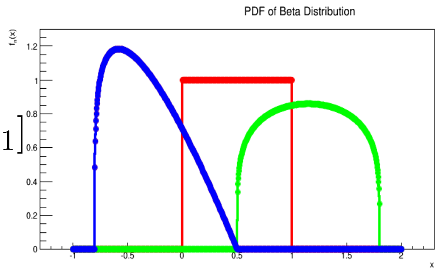
$$f(x) = \frac{u^{\alpha-1} * (1-u)^{\beta-1}}{\mathrm{B}(\alpha,\beta)} \quad \forall x \in [x_0, x_1]$$

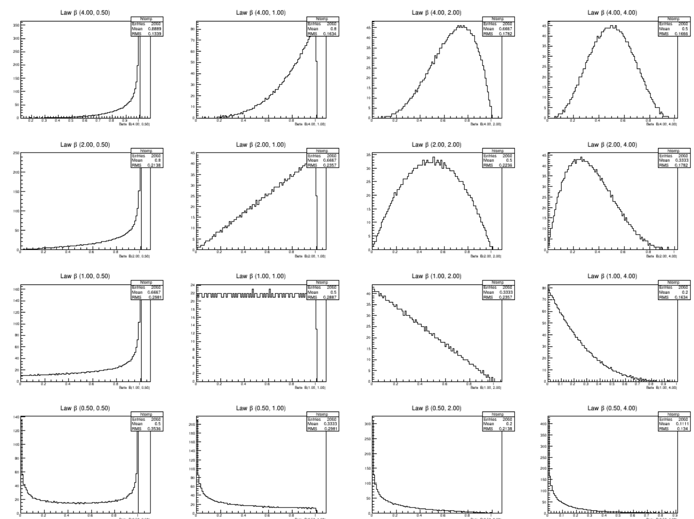
with $u = \frac{x-x_0}{x_1-x_0}$

– Mean : $x_0 + (x_1 - x_0)\frac{\alpha}{\alpha+\beta}$

– Mode : depends on (α, β)

– Variance : $(x_1 - x_0)^2 \frac{\alpha\beta}{\alpha+\beta+1}$





Parametric Estimation

- Let $(x_1, x_2, \cdots, x_n)$ an *i.i.d* sample of a PDF $f(x, \theta)$ where $\theta \in \Theta$ is a vector of parameters for this family. The true value of the parameter $\theta^\star$ is unknown
- Build an estimator $\hat{\theta}$ which would be as close to the true value $\theta^\star$ as possible

1. **Maximum Likelihood (*MLE*)**

   The method of maximum likelihood selects the set of values of the model parameters that maximizes the *likelihood* function. This function measures the *"agreement"* of the selected model with the observed data.

$$\hat{\theta}_{MLE} \quad = \quad \arg\max_{\theta \in \Theta} \quad \frac{1}{n} \ln\left(\prod_{i=1}^{n} f(x_i|\theta)\right) \quad \text{... if any maximum exists}$$

2. **Moments Method (*MM*)**

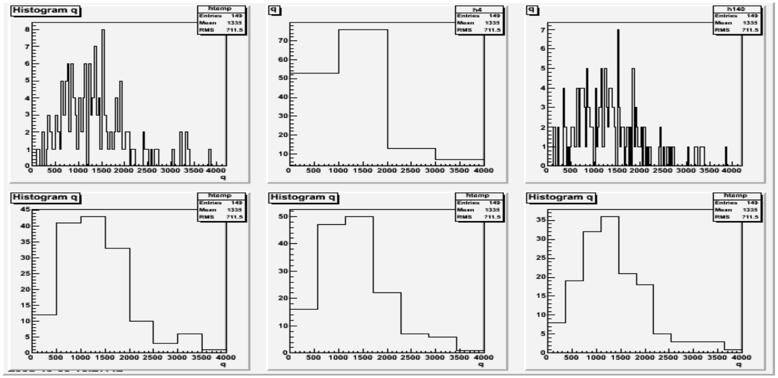
   - One starts with deriving equations that relate the population moments to the parameters θ
   - The moments are estimated from the given sample
   - The equations are then solved for the parameters θ, using the sample moments in place of the (unknown) population moments

$$g_k(\theta_1, \theta_2, \cdots, \theta_k) = \mathbb{E}[X]^k = \mu_k \quad \text{and} \quad \widehat{\mu_k} = \frac{1}{n}\sum_{i=1}^{n} x_i^k = g_k(\widehat{\theta_1}, \widehat{\theta_2}, \cdots, \widehat{\theta_k})$$

Non-parametric methods : Histogram

- The **histograms** are classical density estimation
- The followings steps are needed to build the histogram:
  - Arrange the sample in increasing order;
  - Subdivide the range of the sample into several equal intervals, and count the number of observations in each intervals;
  - plot the number of observations in each interval versus the random variable
- but the form depends on the number of bins

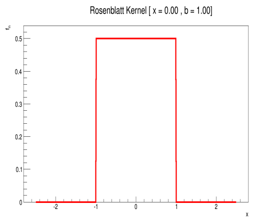
1. **Sturges** $N_{bin} = log_2(n) + 1$
2. **Scott** $N_{bin} = (x_{max} - x_{min}) * \sqrt[3]{n}/3.5\hat{\sigma}_x$
3. **Freedman & Diaconis** $N_{bin} = (x_{max} - x_{min}) * \sqrt[3]{n}/2 * (Q_x^{0.75} - Q_x^{0.25})$



Non-parametric methods : Kernel Methods

- A function $K : I\!R \to I\!R$ is said a **Kernel** if

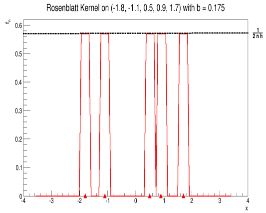
$$\int K(u)\,\mathrm{du} \quad = \quad 1.$$



- Often, but not necessarily,
  - K is symmetric around the origin: $\quad K(-u) = K(u) \quad \forall u$
  - K is positive: $\quad K(u) > 0 \quad \forall u$

- $\forall h > 0$,

$$\hat{f}_{n,h}(x) \quad = \quad \frac{1}{n}\sum_{i=1}^{n}\frac{1}{h}K(\frac{X_i - x}{h})$$



  is a ***kernel estimator*** of the density f $\;(\int \hat{f}_{n,h}(x)\,\mathrm{d}x = 1\;)$

- Kernel approach is a histogram which, for estimating the density of $f(x)$, has been shifted so that x, say, lies at the center of a mesh interval. And For evaluating the density at another point, say y, the mesh is shifted again, so that y is at the center of a mesh interval.

- The parameter h is a *smoothing* parameter called ***bandwidth***.
  More greater h is, more the estimation $\hat{f}_{n,h}$ is smooth.

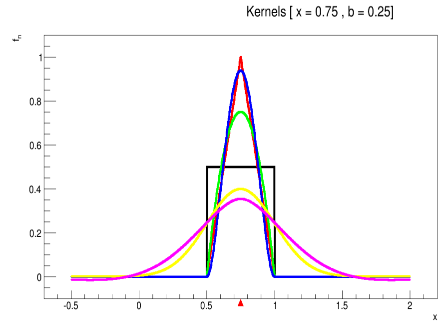
Non-parametric methods : Kernel Methods

- Optimal bandwidth with the Silverman Rule (1996)

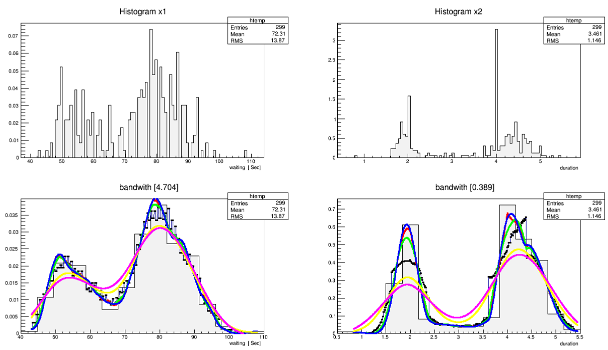
$$h_n = 1.364 \times \alpha_K \times \textsc{Min}\{\hat{\sigma}, \frac{\textsc{Iqr}}{1.349}\} \times \mathrm{n}^{-1/5}$$

with

1. $\hat{\sigma}$ is the sample standard deviation
2. $\textsc{Iqr}$ is the "*I*nter*Q*uartile *R*ange" ($\textsc{Iqr} = q_{0.75} - q_{0.25}$)
3. α_K is a constant that only depends on the used kernel



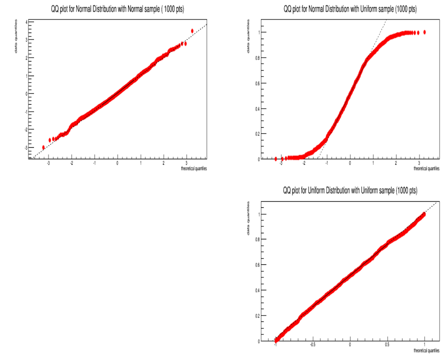
Kernel	$K(x)$	α_K
Rectangular	$1/2 \ , \ \lvert x\rvert < 1$	1.3510
Triangular	$1 - \lvert x\rvert \ , \ \lvert x\rvert < 1$	1.8882
Epanechnikov	$\frac{3}{4}(1 - x^2) \ , \ \lvert x\rvert < 1$	1.7188
Biweight	$\frac{15}{16}(1 - x^2)^2 \ , \ \lvert x\rvert < 1$	2.0362
Gaussian	$\frac{\exp^{-x^2/2}}{\sqrt{2\pi}}$	0.7764



Geyser database for Gaussian Kernel (*left*) waiting b = 4.70, (*right*) duration b = 0.39

Goodness-of-Fits techniques

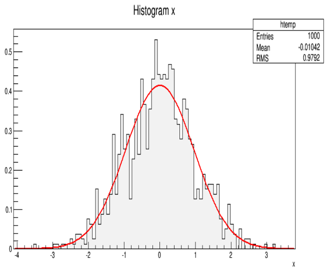
- **QQPlot** (Graphical methods)
  - a **QQ-plot** (*"Q" stands for Quantile*) is a probability plot to compare two probability distributions by plotting their quantiles against each other
  - A point (x, y) on the plot corresponds to one of the quantiles of the second distribution (y-coordinate) plotted against the same quantile of the first distribution (x-coordinate).



  - If the two distributions being compared are similar, the points in the QQ-plot will approximately lie on the line $y = x$
  - If the distributions are linearly related, the points in the QQ-plot will approximately lie on a line, but not necessarily on the line y = x.
  - Select one axe for the theoretical distribution for Goodness-of-Fit test

Goodness-of-Fits techniques

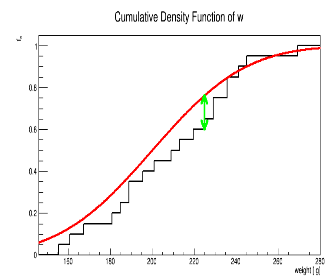
- Statistical Tests
  - **Chi-Squared** : The basic idea is to partitioned the range of the sample into k cells, and compare the observed frequency O_i with the expected frequency E_i in each cell i



$$\chi^2 = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i}$$

which follows a χ^2 distribution with $(k-1-t)$ degrees of freedom, where t is the number of parameters of the distribution to estimate

  - **Tests based on EDF Statistics** (*"Empirical Distribution Function"*)
    - ⋆ Measures the discrepancy between the empirical and the theoretical CDFs (based on the differences between $F_n(x)$ and $F(x)$)
    - ⋆ Two classes : the **supremum** and the **quadratic**



$$D = \sup_x |F_n(x) - F(x)|$$

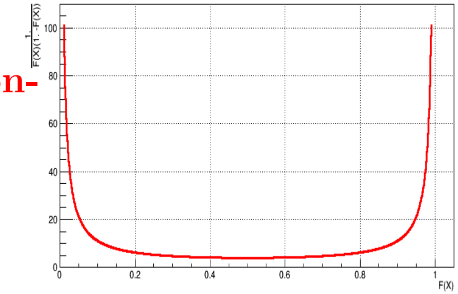
$$Q = n\int_{-\infty}^{+\infty} (F_n(x) - F(x))^2 \psi(x) \mathrm{d}x$$ where ψ is a *weight* function

– For $\psi(x) = 1$ we obtain the **Cramer-von Mises** Tests, denoted as W^2:

$$W^2 = n \int_{-\infty}^{+\infty} (F_n(x) - F(x))^2 \mathrm{d}x$$

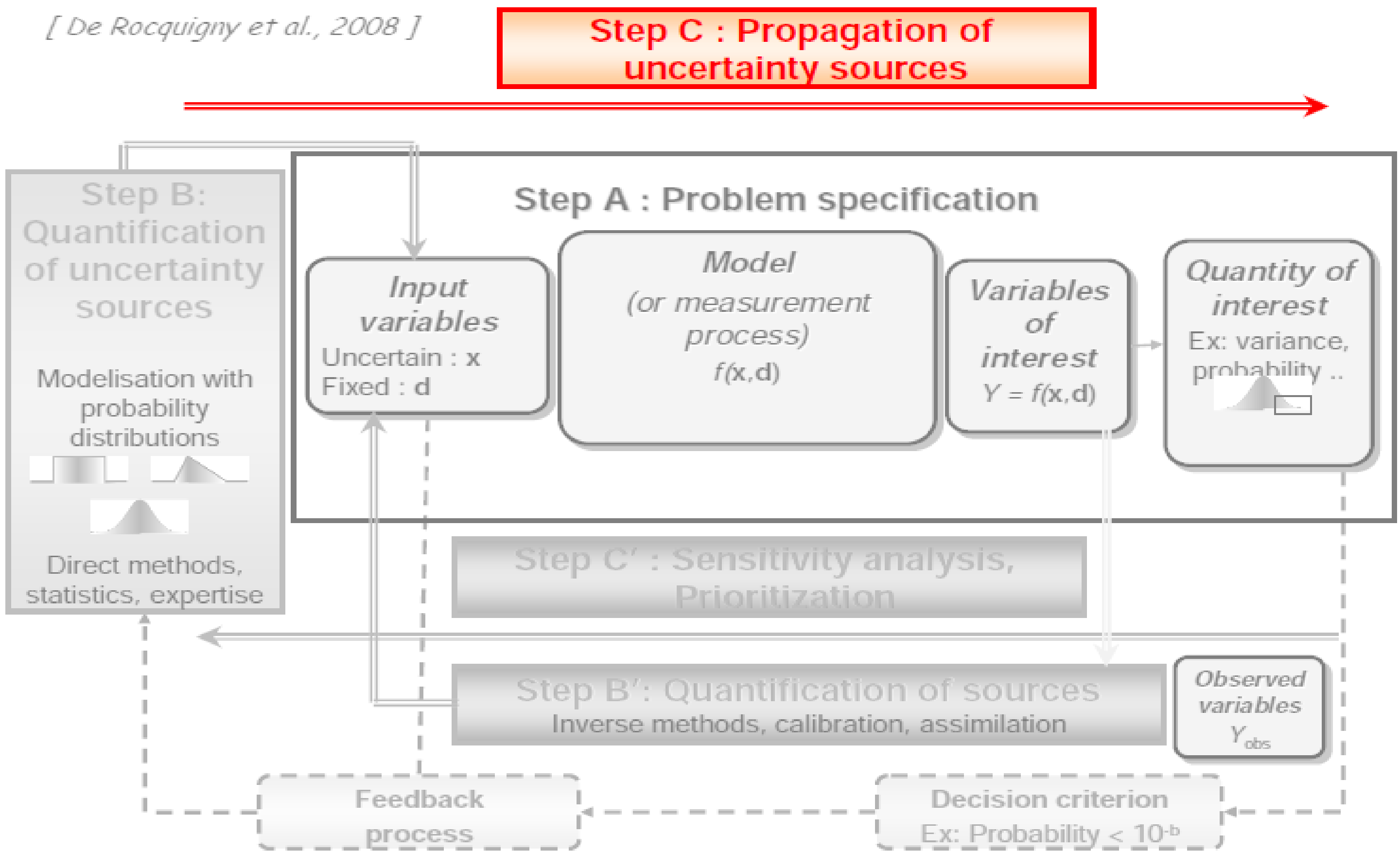
– For $\psi(x) = \frac{1.}{F(x)(1.0 - F(x))}$ we obtain the **Anderson-Darling** test, denoted A^2:

$$A^2 = n \int_{-\infty}^{+\infty} \frac{(F_n(x) - F(x))^2}{F(x)(1.0 - F(x))} \mathrm{d}x$$



- The χ^2 statistic is the lower powerful for continuous PDF
- EDF statistics are usually much more powerful than the χ^2 statistic (where data must be grouped, then loss of information)
- the **Kolmogorov-Smirnov** D statistic is the most well-known of the EDF statistics, but it is often much less powerful than the quadratic statistics W^2 and A^2
- A^2 and W^2 give often similarly values, but A^2 is on the whole more powerful when the distribution F departs from the true distribution in the tails (weight function)

Step C : Propagation of uncertainty sources



Steps of Uncertainties Propagation

- Generate Design of Experiments *("DoE")*
  - Monte-Carlo Sampling ("SRS"), Latin HyperCube Sampling ("LHS")
  - quasi Monte-Carlo Sampling ("qMC")
  - Low Discrepancy Sequences (*"Space-Filling Design"*)

  Take into account correlations between variables

- Evaluate the code for each points of the DoE (sequential on a PC, or parallel on MultiCore PC/Cluster)
  - Substitute the values on the current point into the input files of the code
  - Launch the code with the new input files
  - Catch the output values of the variables of interests

  Using *"Surrogate Model"* (linear, polynomial, Artificial Neural Network, Kriging) to reduce the computational times of the code evaluation

- Analyze the *Quantity of interest* by statistics
  - Univariate attribute
  - Data Modelisation with ***PDF*** or ***Kernel*** (*as Step B*)
  - Goodness-of-Fit Techniques (*as Step B*)

The effect of the "location" parameter is to translate the graph relative to the standard distribution

- **Mean μ** :

$$\mu = \frac{1}{nS} \sum_{i=1}^{nS} x_i$$

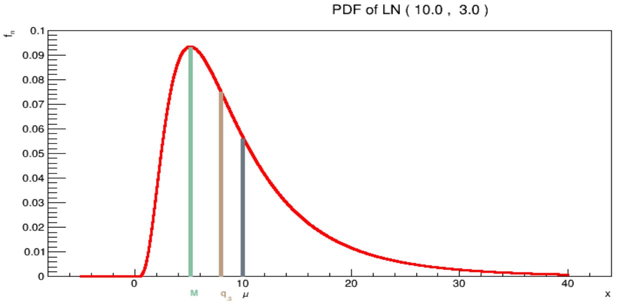
- **Mode M** : Value where the probability is the greatest value
- **Median $q_{0.5}$** : it is the 0.5-quantile

$$q_{0.5} \quad as \quad \mathbb{P}\left[X \leq q_{0.5}\right] = 0.5 = \mathbb{P}\left[X \geq q_{0.5}\right]$$

- **α-Quantile q_α with $\alpha \in [0,1]$** :

$$q_\alpha \quad as \quad \mathbb{P}\left[X \leq q_\alpha\right] = \alpha$$

- **Quartiles $q_{0.25}, q_{0.50}, q_{0.75}$**
- **Extremes values min, max**



Univariate Case : "Dispersion" parameters

The effect of a "dispersion" parameter is to stretch|shrink the standard distribution

- **Variance** $Var[X]$: measure of spread in the data about the mean $Var[X] = \mathbb{E}[(X - \mathbb{E}[X])^2]$, and can be estimated by :

$$Var[X] = \frac{1}{nS - 1} \sum_{i=1}^{nS} (x_i - \mu)^2$$

- **Standard Deviation** σ : to have an information in the same unit as the variable

$$\sigma = \sqrt{Var[X]}$$

- **Coefficient of Variation** δ : σ does not indicate **the degree (%)** of dispersion around the mean value μ, a **nondimensional** term can be introduced :

$$\delta = \frac{\sigma}{\mu}$$

- **Range** R :

$$R = Max - Min$$

- **InterQuartile Range** IQR :

$$\text{IQR} = q_{0.75} - q_{0.25}$$

Univariate Case : "Shape" parameters

A "shape" parameter is any parameter of a PDF that is neither a location parameter nor a scale parameter. Such a parameter must affect the shape of a distribution rather than simply shifting it (location parameter) or stretching/shrinking it (dispersion parameter).

- **Moment order p : μ_p** $:= \mathbb{E}[(X - \mathbb{E}[X])^p]$

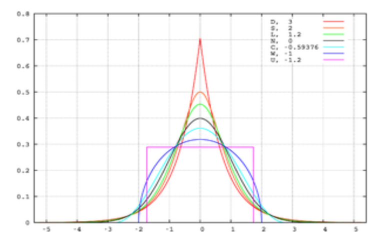
$$\mu_p = \frac{1}{nS}\sum_{i=1}^{nS}(x_i - \mu)^p$$

- **Skewness : γ_1** is a measure of the asymmetry of the PDF about its mean. The skewness value can be positive or negative, or even undefined.

$$\gamma_1 := \mathbb{E}\left[\left(\frac{X-\mu}{\sigma}\right)^3\right] = \frac{\mu_3}{\sigma^3} = \frac{\mathbb{E}[X^3] - 3\mu\sigma^2 - \mu^3}{\sigma^3}$$

- **Kurtosis : γ_2** is a measure of the "peakedness/flatness" of the PDF

$$\gamma_2 = \frac{\mu_4}{\sigma^4} - 3.0$$

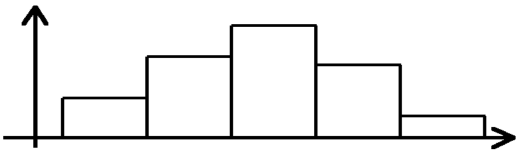


from Wikipedia

Univariate Case : Graphical Representations

- **Histogram**

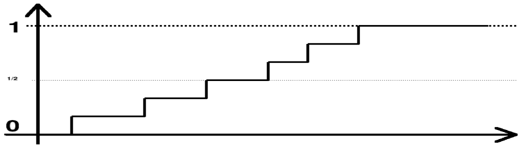
$$H(x) = \frac{1}{nS}\sum_{i=1}^{nS}\frac{\mathrm{1\!I}_{[t_i,t_{i+1}]}(x)}{(t_{i+1}-t_i)} \quad \text{when} \quad x \in [t_i, t_{i+1}]$$



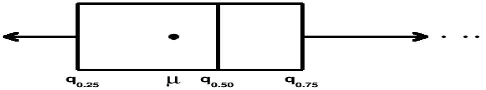
where $[a,b] = \bigcup_i [t_i, t_{i+1}]$

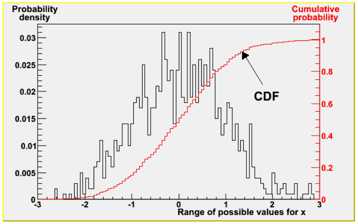
- **Empirical Cumulative Density Function** (***eCDF***)

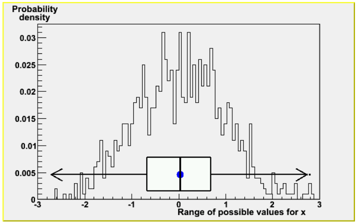
$$F_n(x) \quad = \quad \frac{1}{nS}\sum_{i=1}^{nS}\mathrm{1\!I}(X_i \leq x)$$



- **Boxplot** (**Tukey**)







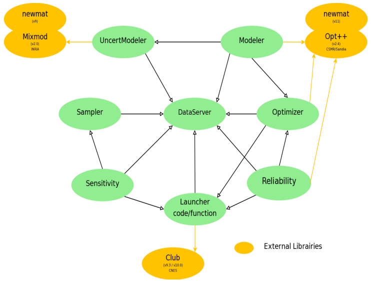
Outline

- Uncertainties Methodology
  - Input modelisation
  - Distribution of Computation
  - Output analysis
- **the Uranie platform**
- Example of Uncertainties Propagation

URANIE : CEA/DEN Uncertainty Platform

- ROOT (CERN), MIXMOD (Gaussian Mixtures - INRIA), OPT++ (Optimization - Sandia), NLOpt (Optimization - MIT)

- Data access :



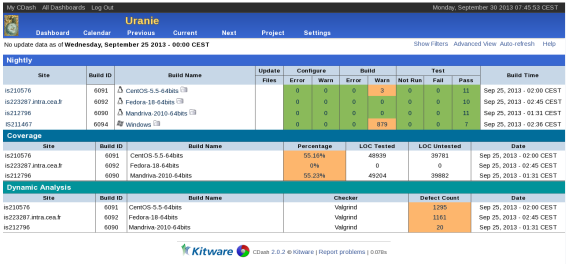
  - Flat file with header ("Salomé Table")
  - TTree (internal ROOT)
  - SQL Data base (MySQL, PostgreSQL, ...)

- Uncertainty/Sensitivity/Optimisation methods in URANIE
  - Design Of Experiments (SRS, LHS, ROA, qMC, MCMC, Copulas)
  - Clustering methods
  - Surrogate models (Polynomial, Artificial Neural Networks, Kriging, GLM)
  - Non Intrusive Spectral Projection : Generalized Polynomial Chaos
  - Inverse Quantification of Uncertainty (CIRCE)
  - Sensitivity Analysis: Local, Morris, Regressions (*Pearson, Spearmann*), Sobol, FAST & RBD
  - Optimization, Multi-Criteria (**Vizir** library : Genetic Algorithms)
  - Computing distribution (**HPC** : TGCC, CCRT)

The URANIE project : v3.5 - 2014/07

- **115 000** lines & **235** classes
- Version of ROOT :
  v5.34.13 (2013 Nov.)
  v5.32 (2011 Dec.)
  v5.34.19 (2014/07/09)
- Compilation with **cmake**
  (Linux-Makefiles/Windows-Visual Project)
- CDash reporting
  - Unitary tests with **CppUnit**
  - Coverage with **gcov**
  - Memory check with **valgrind**
- **Exceptions** (Warning, Error, Deprecated)
- Open source since 2013/05

http://sourceforge.net/projects/uranie


My CDash All Dashboards Log Out — Monday, September 30 2013 07:45:53 CEST

Uranie

Dashboard Calendar Previous Current Next Project Settings

No update data as of **Wednesday, September 25 2013 - 00:00 CEST** — Show Filters Advanced View Auto-refresh Help

Nightly

Site	Build ID	Build Name	Update Files	Configure Error	Configure Warn	Build Error	Build Warn	Test Not Run	Test Fail	Test Pass	Build Time
is210576	6091	CentOS-5.5-64bits		0	0	0	3	0	0	11	Sep 25, 2013 - 02:00 CEST
is223287.intra.cea.fr	6092	Fedora-18-64bits		0	0	0	0	0	0	10	Sep 25, 2013 - 02:45 CEST
is212796	6090	Mandriva-2010-64bits		0	0	0	0	0	0	11	Sep 25, 2013 - 01:31 CEST
IS211467	6094	Windows		0	0	0	879	0	0	7	Sep 25, 2013 - 02:36 CEST

Coverage

Site	Build ID	Build Name	Percentage	LOC Tested	LOC Untested	Date
is210576	6091	CentOS-5.5-64bits	55.16%	48939	39781	Sep 25, 2013 - 02:00 CEST
is223287.intra.cea.fr	6092	Fedora-18-64bits	0%	0	0	Sep 25, 2013 - 02:45 CEST
is212796	6090	Mandriva-2010-64bits	55.23%	49204	39882	Sep 25, 2013 - 01:31 CEST

Dynamic Analysis

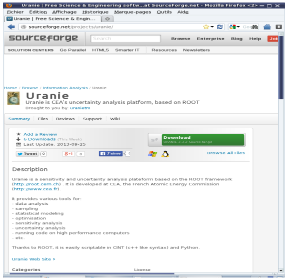
Site	Build ID	Build Name	Checker	Defect Count	Date
is210576	6091	CentOS-5.5-64bits	Valgrind	1295	Sep 25, 2013 - 02:00 CEST
is223287.intra.cea.fr	6092	Fedora-18-64bits	Valgrind	1161	Sep 25, 2013 - 02:45 CEST
is212796	6090	Mandriva-2010-64bits	Valgrind	20	Sep 25, 2013 - 01:31 CEST

Kitware CDash 2.0.2 © Kitware | Report problems | 0.078s

CDash reports

```
--- <WARNING> URANIE::MessageLogger : ==================== WARNING =======================
--- <WARNING> URANIE::MessageLogger : Deppreciated constructor since v0.3 to v0.5
--- <WARNING> URANIE::MessageLogger : Using the same constructor with a TDataServer object
--- <WARNING> URANIE::MessageLogger : ================ End Of Warning ===================
```

Deprecated message



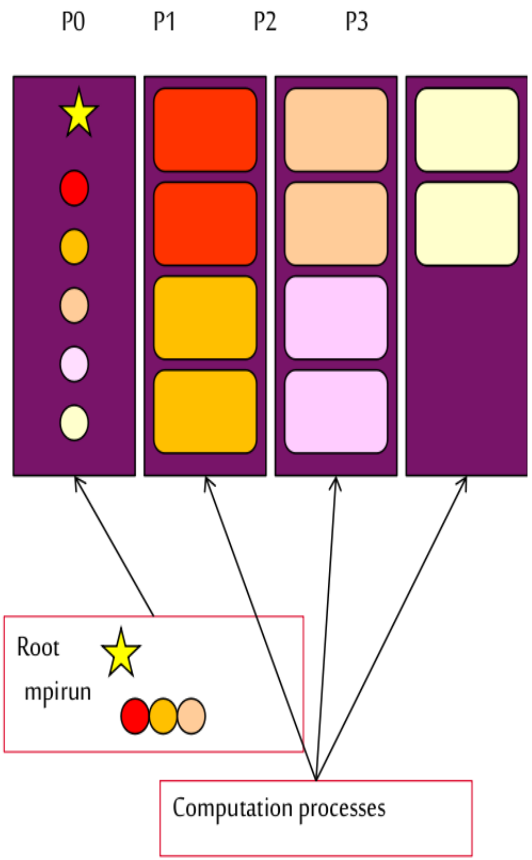
Uranie SourceForge site

Using URANIE on Supercomputers

- Distribution of computations:
  - Sequential on PCs
  - Parallel on Multicore PCs
  - Parallel on Cluster (LSF, SGE, SLURM, LoadLeveler) with
    bsub < BsubFile
- The mechanism for launching computations in URANIE is transparent for the user : the URANIE script is the same whether you run it on the local machine, a cluster or a supercomputer
- The sequence is the following:
  - The design of experiments is created (depending on the method and on the uncertainties on the input parameters)
  - URANIE analyses the machine through the environment variables and deduces the number of available processes
  - A pool of processes is managed in order to distribute computations as the processors become available

Using URANIE on Supercomputers

- Chosen strategy
  - One job in which the computations are hosted
- Aim : being able to run design of experiments
  - On serial codes
  - On MPI-based parallel codes
  - On coupled simulations (with SALOME platform or with MPI)
- Difficulty related to the fact that MPIRUN cannot call itself
- Chosen implementation
  - The master node manages the distribution of computations as processors become available
  - When a processor group becomes available, the master process is forked and runs MPIRUN
  - The end of the job execution is detected by analyzing the state of the child process



Outline

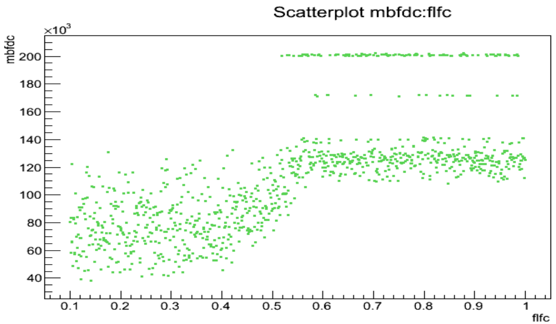
- Uncertainties Methodology
  - Input modelisation
  - Distribution of Computation
  - Output analysis
- the Uranie platform
- **Example of Uncertainties Propagation**

Example of Uncertainties Propagation - Context

- Thermal hydraulic code (study in 2009)
- CPU time for single computation :

  $\sim$ 5 minutes (approximation of the true code)
- Design of Experiments
  - nX = 32 input attributes with Uniform and Normal Distributions
  - nY = 23 output attributes
  - nS = 1500 points

The Code's developper use to see one output y_i *versus* one input x_j :



Example of Uncertainties Propagation - Context

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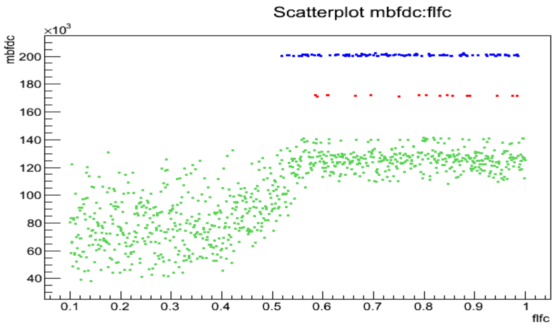
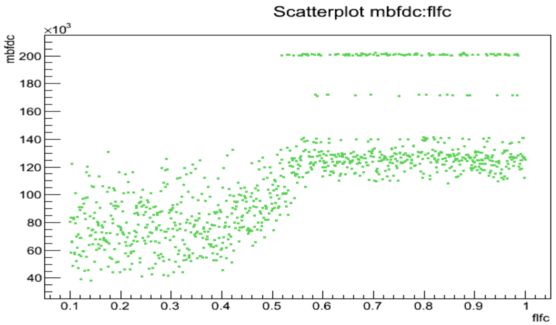
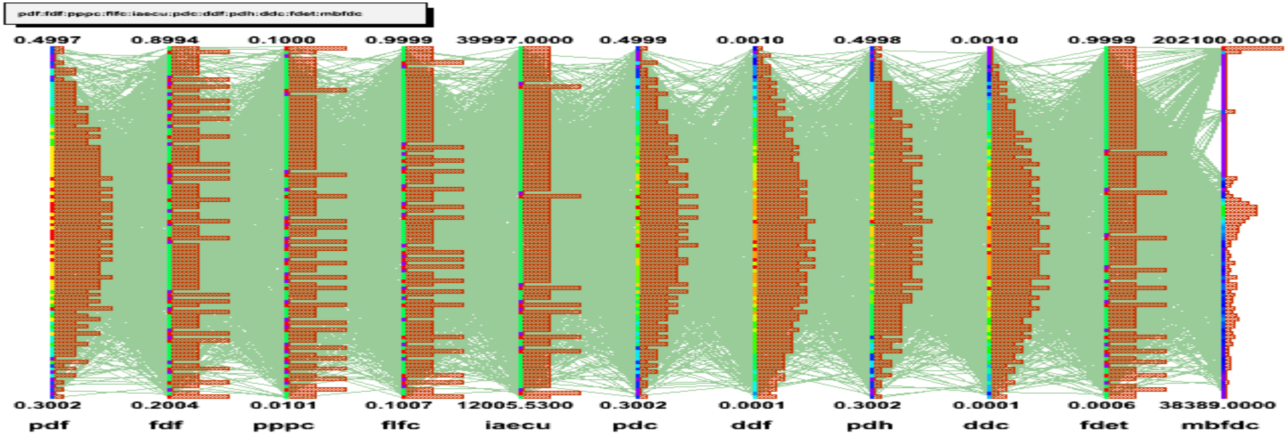


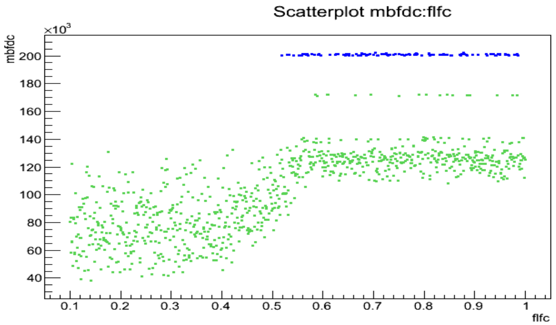
Example of Uncertainties Propagation

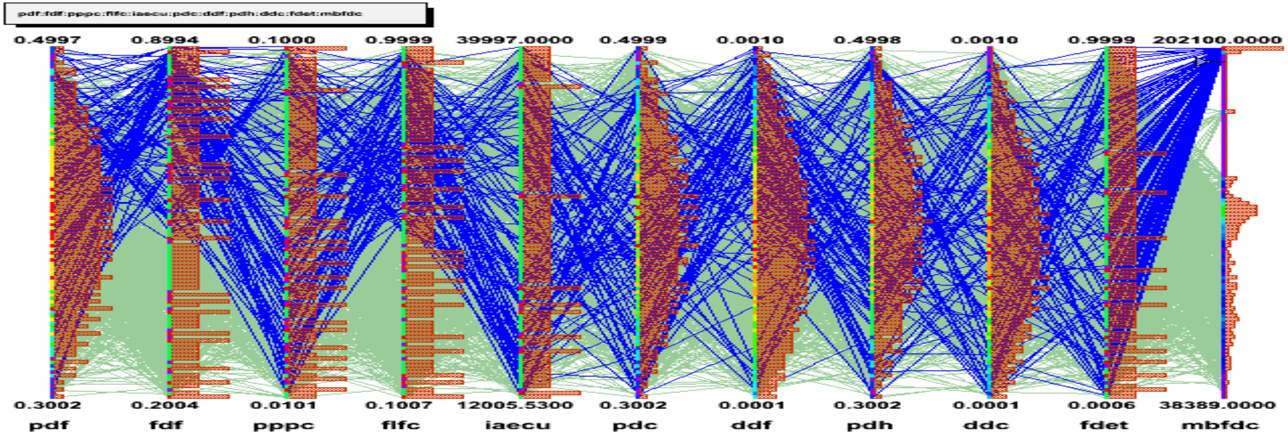




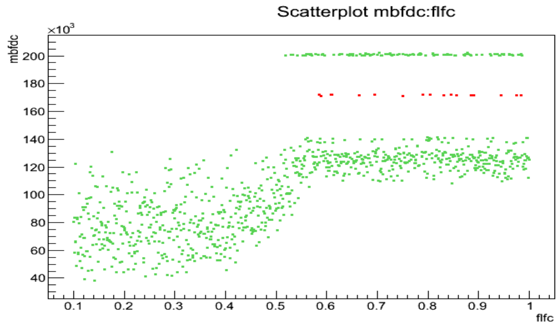

```
tds->Draw( "pdf:fdf:pppc:flfc:iaecu:pdc:ddf:pdh:ddc:fdet:mbfdc","","para");
```

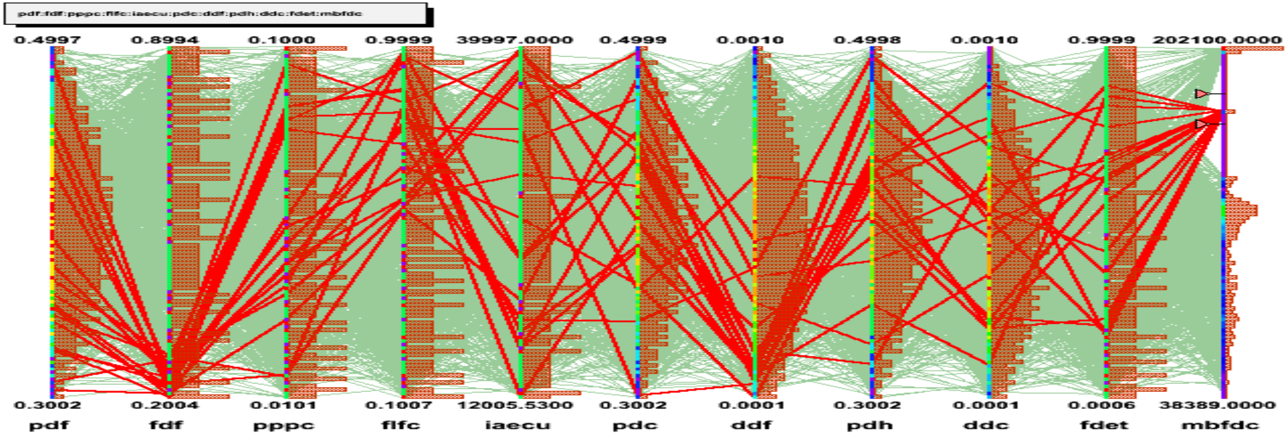
Example of Uncertainties Propagation (2/6)



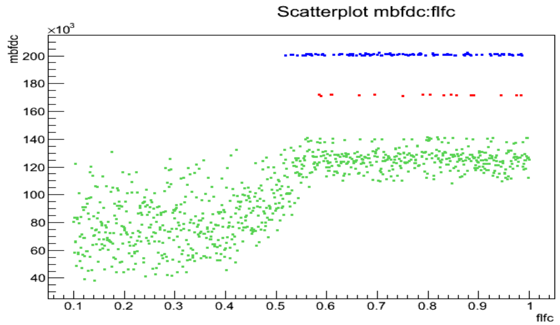


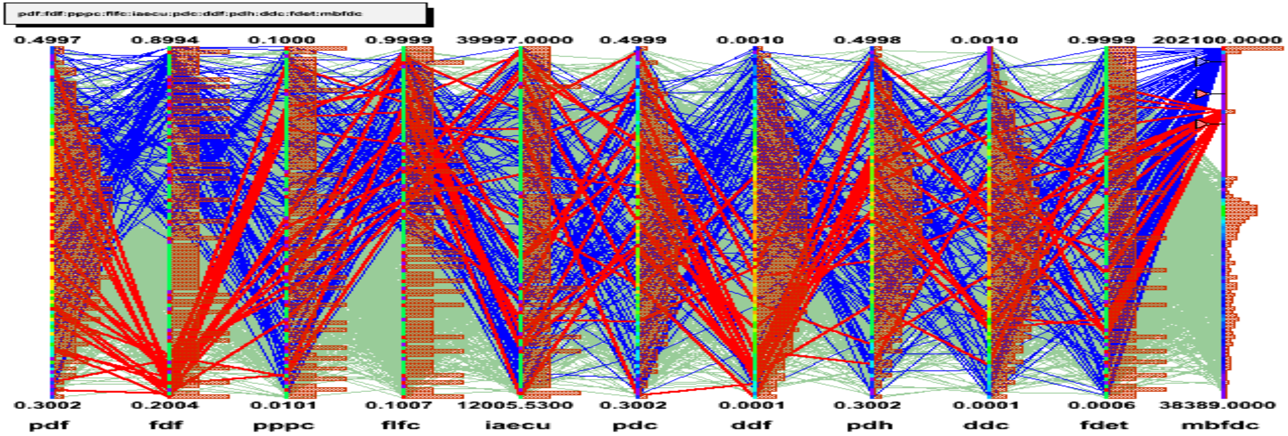
Example of Uncertainties Propagation (3/6)



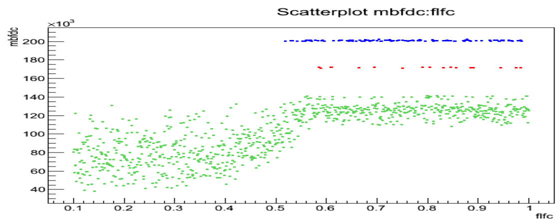


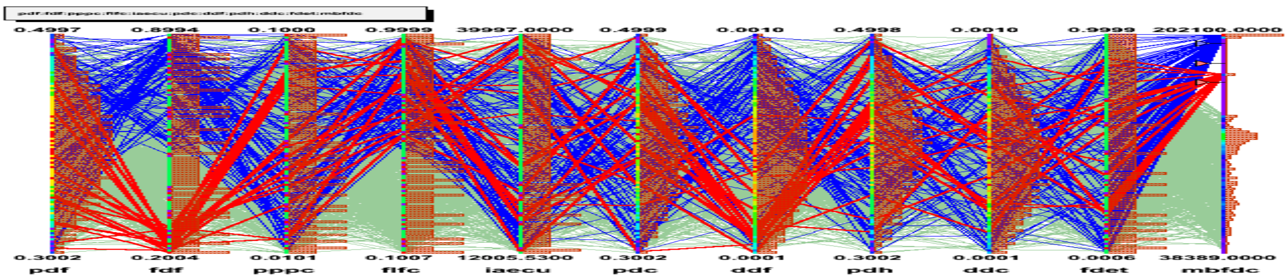
Example of Uncertainties Propagation (4/6)

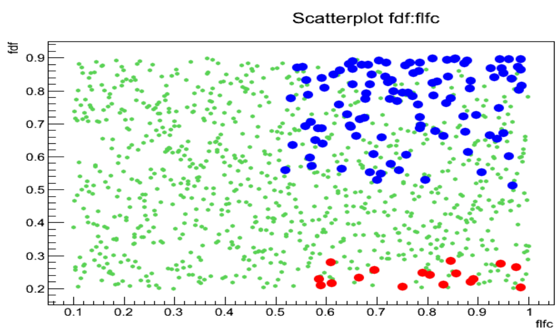




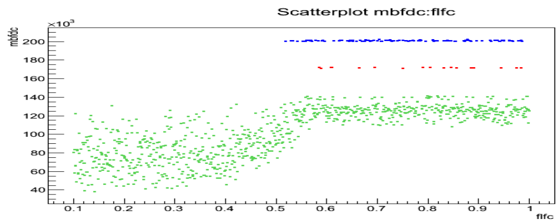
Example of Uncertainties Propagation (5/6)

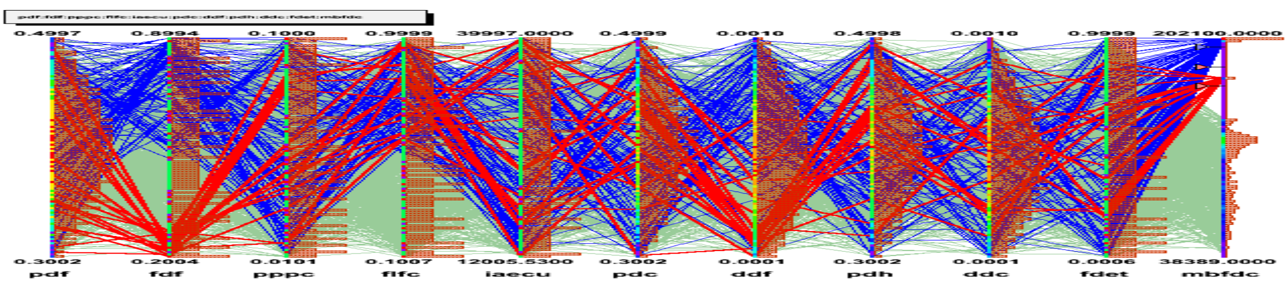


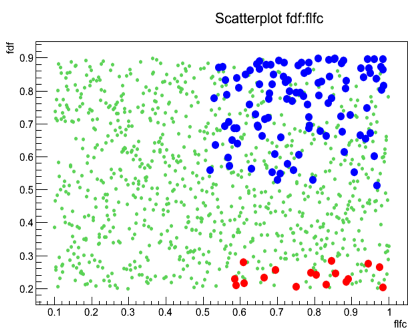


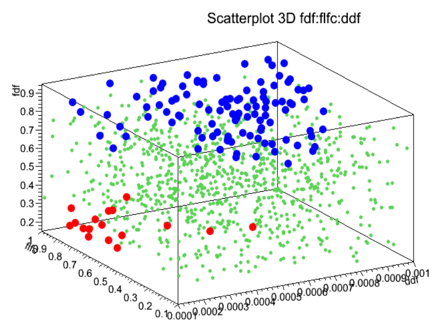


Example of Uncertainties Propagation (6/6)









Conclusions

- The Uncertainties Propagation procedure
- A presentation of the Uranie Platform
- UQ example (*"powerful"* **CobWeb/Parallel Coordinates** graphic)

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 D'Agostini, *R.* and Stephens, *M.* (1986). *Goodness-of-Fit techniques*. Dekker, Statistics monographs, vol 68.

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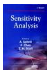
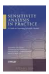
 Saltelli, A., Chan, K., and Scoot, M., editors (2000). *Sensitivity Analysis*. John Wiley and Sons.

 Saltelli, A., Tarantola, S., Campolongo, F. and Ratto, M. (2005). *Sensitivity Analysis in Practise*. John Wiley and Sons.

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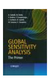
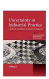
 Saltelli, and all (2008). *Global Sensitivity Analysis : the Primer*. John Wiley and Sons.

 de Rocquigny *E.*, Devictor *N.* and Tarantola *S.* (2008). *Uncertainty in Industrial Practice : A Guide to Quantitative Uncertainty Management*. John Wiley and Sons.

Thank you for your attention!

Questions?