Title:	OpenTURNS : An industrial software for uncertainty quantification in simulation
Name:	Michaël Baudin, Anne Dutfoy, Bertrand Iooss and Anne-Laure Popelin
Affil./Addr.:	EDF R&D
	6 quai Watier, 78401 Chatou, France
	1, avenue du General de Gaulle Clamart, France
	E-mail: michael.baudin@edf.fr, anne.dutfoy@edf.fr, bertrand.iooss@edf.fr, anne-laure.popelin@edf.fr

OpenTURNS : An industrial software for uncertainty quantification in simulation

Abstract

The needs to assess robust performances for complex systems and to answer tighter regulatory processes (security, safety, environmental control, and health impacts, etc.) have led to the emergence of a new industrial simulation challenge: to take uncertainties into account when dealing with complex numerical simulation frameworks. Therefore, a generic methodology has emerged from the joint effort of several industrial companies and academic institutions. EDF R&D, Airbus Group and Phimeca Engineering started a collaboration at the beginning of 2005, joined by IMACS in 2014, for the development of an Open Source software platform dedicated to uncertainty propagation by probabilistic methods, named OpenTURNS for Open source Treatment of Uncertainty, Risk 'N Statistics. OpenTURNS addresses the specific industrial challenges attached

to uncertainties, which are transparency, genericity, modularity and multi-accessibility. This paper focuses on OpenTURNS and presents its main features: OpenTURNS is an open source software under the LGPL license, that presents itself as a C++ library and a Python TUI, and which works under Linux and Windows environment. All the methodological tools are described in the different sections of this paper: uncertainty quantification, uncertainty propagation, sensitivity analysis and metamodeling. A section also explains the generic wrappers way to link OpenTURNS to any external code. The paper illustrates as much as possible the methodological tools on an educational example that simulates the height of a river and compares it to the height of a dyke that protects industrial facilities. At last, it gives an overview of the main developments planned for the next few years.

Key words: OpenTURNS , uncertainty, quantification, propagation, estimation, sensitivity, simulation, probability, statistics, random vectors, multivariate distribution, open source, python module, C++ library, transparency, genericity.

Introduction

The needs to assess robust performances for complex systems and to answer tighter regulatory processes (security, safety, environmental control, and health impacts, etc.) have led to the emergence of a new industrial simulation challenge: to take uncertainties into account when dealing with complex numerical simulation frameworks. Many attempts at treating uncertainty in large industrial applications have involved domain-specific approaches or standards: metrology, reliability, differential-based approaches, variance decomposition, etc. However, facing the questioning of their certification authorities in an increasing number of different domains, these domain-specific approaches are no more appropriate. Therefore, a generic methodology has emerged from the joint effort

of several industrial companies and academic institutions : [28] reviews these past developments. The specific industrial challenges attached to the recent uncertainty concerns are:

- transparency: open consensus that can be understood by outside authorities and experts,

- genericity: multi-domain issue that involves various actors along the study,

- modularity: easy integration of innovations from the open source community,

- multi-accessibility: different levels of use (simple computation, detailed quantitative results, and deep graphical analyses) and different types of end-users (graphical interface, Python interpreter, and C++ sources),

- industrial computing capabilities: to secure the challenging number of simulations required by uncertainty treatment.

As no software was fully answering the challenges mentioned above, EDF R&D, Airbus Group and Phimeca Engineering started a collaboration at the beginning of 2005, joined by EMACS in 2014, for the development of an open Source software platform dedicated to uncertainty propagation by probabilistic methods, named Open-TURNS for open source Treatment of Uncertainty, Risk 'N Statistics [10],[29]. Open-TURNS is actively supported by its core team of four industrial partners (IMACS joined the consortium in 2014) and its industrial and academic users community that meet through the web site `www.openturns.org` and annually during the OpenTURNS Users day. At EDF, OpenTURNS is the repository of all scientific developments on this subject, to ensure their dissemination within the several business units of the company. The software has also been distributed for several years via the integrating platform Salome [27].

Presentation of OpenTURNS

OpenTURNS is an open source software under the LGPL license, that presents itself as a C++ library and a Python TUI, and which works under Linux and Windows environment, with the following key features:

- open source initiative to secure the transparency of the approach, and its openness to ongoing Research and Development (R&D) and expert challenging,

- generic to the physical or industrial domains for treating of multi-physical problems;

- structured in a *practitioner-guidance* methodological approach,

- with advanced industrial computing capabilities, enabling the use of massive distribution and high performance computing, various engineering environments, large data models etc.,

- includes the largest variety of qualified algorithms in order to manage uncertainties in several situations,

- contains complete documentation (Reference Guide, Use Cases Guide, User manual, Examples Guide, and Developers' Guide).

All the methodological tools are described after this introduction in the different sections of this paper: uncertainty quantification, uncertainty propagation, sensitivity analysis and metamodeling. Before the conclusion, a section also explains the generic wrappers way to link OpenTURNS to any external code.

OpenTURNS can be downloaded from its dedicated website *www.openturns.org* which offers different pre-compiled packages specific to several Windows and Linux environments. It is also possible to download the source files from the *SourceForge* server (*www.sourceforge.net*) and to compile them within another environment: the OpenTURNS Developer's Guide provides advice to help compiling the source files.

At last, OpenTURNS has been integrated for more than 5 years in the major Linux distributions (for example debian, ubuntu, redhat and suze).

The uncertainty management methodology

The uncertainty management generic methodology [29] is schematized in Figure 1. It consists of the following steps:

- Step A: specify the random inputs $\boldsymbol{X}$, the deterministic inputs $\boldsymbol{d}$, the model G (analytical, complex computer code or experimental process), the variable of interest (model output) Y and the quantity of interest on the output (central dispersion, its distribution, probability to exceed a threshold, ...). The fundamental relation writes:

$$Y = G(\boldsymbol{X}, \boldsymbol{d}) = G(\boldsymbol{X}), \tag{1}$$

with $\boldsymbol{X} = (X_1, \ldots, X_d)$.

- Step B: quantify the sources of uncertainty. This step consists in modeling the joint probability density function (pdf) of the random input vector by direct methods (e.g. statistical fitting, expert judgment) [15].

- Step B': quantify the sources of uncertainty by indirect methods using some real observations of the model outputs [39]. The calibration process aims to estimate the values or the pdf of the inputs while the validation process aims to model the bias between the model and the real system.

- Step C: propagate uncertainties to estimate the quantity of interest. With respect to this quantity, the computational resources and the CPU time cost of a single model run, various methods will be applied: analytical formula, geometrical approximations, Monte Carlo sampling strategies, metamodel-based techniques, ... [21], [11].

- Step C': analyze the sensitivity of the quantity of interest to the inputs in order to rank uncertainty sources [36], [14].

For each of these steps, OpenTURNS offers a large number of different methods whose applicability depend on the specificity of the problem (dimension of inputs, model complexity, CPU time cost for a model run, quantity of interest, etc.).
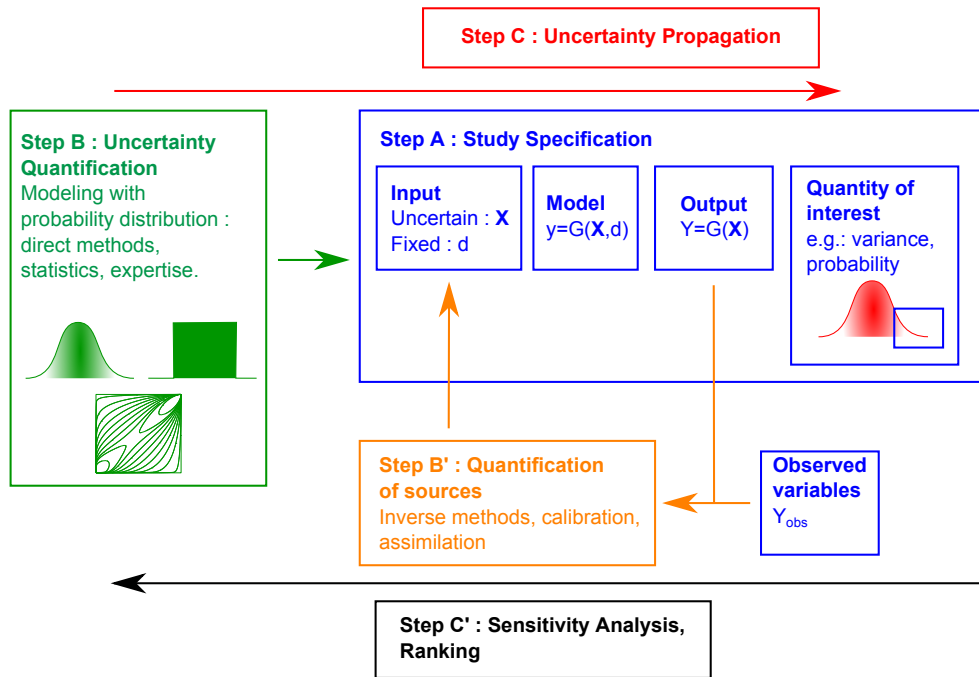

Fig. 1. The uncertainty management methodology.

Main originality of OpenTURNS

OpenTURNS is innovative in several aspects. Its input data model is based on the multivariate cumulative distribution function (CDF). This enables the usual sampling approach, as would be appropriate for statistical manipulation of large data sets, but also facilitates analytical approaches. Distributions are classified (continuous, discrete, elliptic, etc.) in order to take the best benefit of their properties in algorithms. If possible, the exact final cumulative density function is determined (thanks to charac-

teristic functions implemented for each distribution, the Poisson summation formula, the Cauchy integral formula, etc.).

OpenTURNS explicitly models the dependence with copulas, using the Sklar theorem. Furthermore, different sophisticated analytical treatments may be explored: aggregation of copulas, composition of functions from R^n into R^d, extraction of copula and marginals from any distribution.

OpenTURNS defines a domain specific oriented object language for probability modelling and uncertainty management. This way, the objects correspond to mathematical concepts and their inter-relations map the relations between these mathematical concepts. Each object proposes sophisticated treatments in a very simple interface.

OpenTURNS implements up-to-date and efficient sampling algorithms (Mersenne-Twister algorithm, Ziggurat method, the Sequential Rejection Method, etc.). Exact Kolmogorov statistics are evaluated with the Marsaglia Method and the Non Central Student and Non Central χ^2 distribution with the Benton & Krishnamoorthy method.

OpenTURNS is the repository of recent results of PhD research carried out at EDF R&D: for instance the sparse Polynomial Chaos Expansion method based on the LARS method [7], the Adaptive Directional Stratification method [25] which is an accelerated Monte Carlo sampling technique, and the maximum entropy order-statistics copulas [20].

The flooding model

Throughout this paper, the discussion is illustrated with a simple application model that simulates the height of a river and compares it to the height of a dyke that protects industrial facilities as illustrated in Figure 2. When the river height exceeds that of the dyke, flooding occurs. This academic model is used as a pedagogical example in [14]. The model is based on a crude simplification of the 1D hydro-dynamical equations

of SaintVenant under the assumptions of uniform and constant flowrate and large rectangular sections. It consists of an equation that involves the characteristics of the river stretch:

$$H = \left(\frac{Q}{BK_s\sqrt{\frac{Z_m-Z_v}{L}}}\right)^{0.6},\tag{2}$$

where the output variable H is the maximal annual height of the river, B is the river width and L is the length of the river stretch. The four random input variables Q, K_s, Z_v and Z_m are defined in Table 1 with their probability distribution. The randomness of these variables is due to their spatio-temporal variability, our ignorance of their true value or some inaccuracies of their estimation.
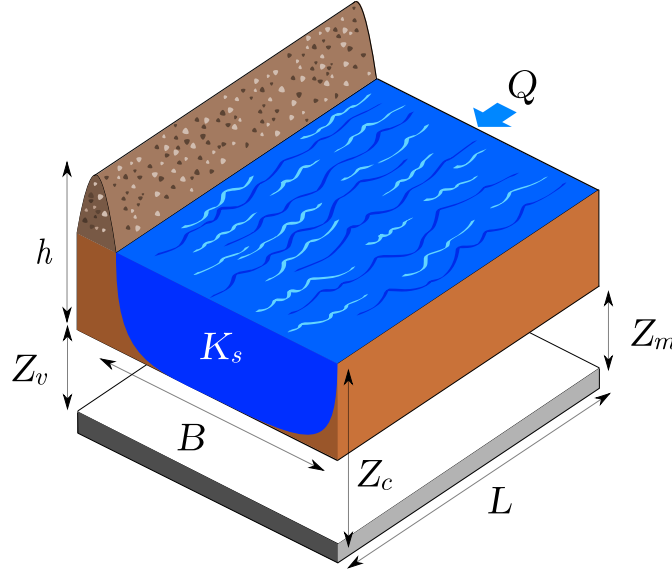

Fig. 2. The flood example: simplified model of a river.

Input	Description	Unit	Probability distribution
Q	Maximal annual flowrate	m³/s	Gumbel $\mathcal{G}(1.8e^{-3}, 1014)$
K_s	Strickler coefficient	-	Normal $\mathcal{N}(30, 7.5)$
Z_v	River downstream level	m	Triangular $\mathcal{T}(47.6, 50.5, 52.4)$
Z_m	River upstream level	m	Triangular $\mathcal{T}(52.5, 54.9, 57.7)$

Table 1. Input variables of the flood model and their probability distributions.

Uncertainty quantification

Modelling of a random vector

OpenTURNS implements more than 40 parametric distributions which are continuous (more than 30 families) and discrete (more than 10 families), with several sets of parameters for each one. Some are multivariate, such as the Student distribution or the Normal one.

Moreover, OpenTURNS enables the building of a wide variety of multivariate distributions thanks to the combination of the univariate margins and a dependence structure, the copula, according to the Sklar theorem: $F(x_1, \ldots, x_d) = C(F_1(x_1), \ldots, F_d(x_d))$ where F_i is the CDF of the margin X_i and $C : [0,1]^d \to [0,1]$ the copula.

OpenTURNS proposes more than 10 parametric families of copula: Clayton, Frank, Gumbel, Farlie-Morgenstein, etc. These copula can be aggregated to build the copula of a random vector whose components are dependent by blocks. Using the inverse relation of the Sklar theorem, OpenTURNS can extract the copula of any multivariate distribution, whatever the way it has been set up: for example, from a multivariate distribution estimated from a sample with the kernel smoothing technique.

All the distributions can be truncated in their lower and/or upper area. In addition to these models, OpenTURNS proposes other specific constructions. Among them, note the random vector which writes as a linear combination of a finite set of independent variables: $\boldsymbol{X} = a_0 + a_1\boldsymbol{X}_1 + \ldots a_N\boldsymbol{X}_N$ thanks to the python command, written for $N = 2$ with explicit notations:

```
>>>myX= RandomMixture([distX1,distX2], [a1, a2], a0)
```

In that case, the distribution of X is *exactly* determined, using the characteristic functions of the X_i distributions and the Poisson summation formula.

OpenTURNS also easily models the random vector whose probability density function (pdf) is a linear combination of a finite set of independent pdf: $f_{\boldsymbol{X}} = a_1 f_{\boldsymbol{X}_1} + \ldots a_N f_{\boldsymbol{X}_N}$ thanks to the python command, with the same notations as previously (the weights are automatically normalized):

```
>>>mypdfX= Mixture([distX1,distX2], [a1, a2])
```

Moreover, OpenTURNS implements a random vector that writes as the random sum of univariate independent and identically distributed variables, this randomness being distributed according to a Poisson distribution: $\boldsymbol{X} = \sum_{i=1}^{N} \boldsymbol{X}_i, \quad N \sim \mathcal{P}(\lambda)$, thanks to the python command:

```
>>>d= CompoundDistribution(lambda, distX)
```

where all the variables X_i are identically distributed according to $distX$. In that case, the distribution of X is *exactly* determined, using the characteristic functions of the X_i distributions and the Poisson summation formula.

In the univariate case, OpenTURNS exactly determines the pushforward distribution $\mathcal{D}$ of any distribution $\mathcal{D}_0$ through the function $f : \mathbb{R} \to \mathbb{R}$, thanks to the python command (with straight notations):

```
>>>d= CompositeDistribution(f,d0)
```

Finally, OpenTURNS enables the modeling of a random vector $(X_1, \ldots, X_d)$ which almost surely verifies the constraint $\boldsymbol{X} = X_1 \leq \cdots \leq X_d$, proposing a copula adapted to the ordering constraint [8]. OpenTURNS verifies the compatibility of the margins F_i with respect to the ordering constraint and then builds the associated distribution, thanks to the python command, written in dimension 2:

```
>>>d=MaximumEntropyOrderStatisticsDistribution([distX1, distX2])
```

Figure 3 illustrates the copula of such a distribution, built as the ordinal sum of some maximum entropy order statistics copulae.

The OpenTURNS python script to model the input random vector of the tutorial presented previously is as follows:

```
#Margin distributions:
>>>dist_Q = Gumbel(1.8e-3, 1014)
>>>dist_Q = TruncatedDistribution(dist_Q,0.0, TruncatedDistribution.LOWER)
>>>dist_K = Normal(30.0, 7.5)
>>>dist_K = TruncatedDistribution(dist_K,0., TruncatedDistribution.LOWER)
>>>dist_Zv = Triangular(47.6,50.5,52.4)
>>>dist_Zm = Triangular(52.5,54.9,57.7)
```
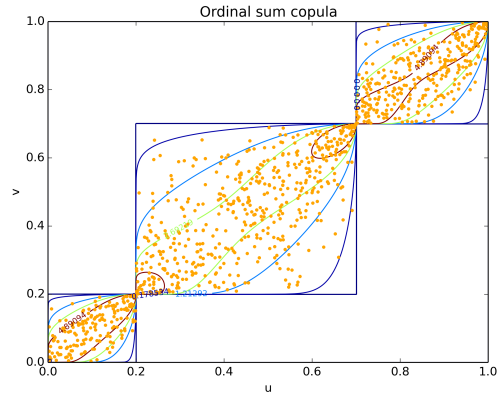
Fig. 3. An example of maximum entropy copula which almost surely satisfies the ordering constraint: $X_1 \leq X_2$.

```
# Copula in dimension 4 for (Q,K,Zv,Zm)
>>>R=CorrelationMatrix(2)
>>>R[0,1]=0.7
>>>copula = ComposedCopula([IndependentCopula(2),NormalCopula(R) ])
# Final distribution for (Q,K,Zv,Zm)
>>>distInput=ComposedDistribution([loi_Q, loi_K, loi_Zv, loi_Zm], copula)
# Final random vector (Q,K,Zv,Zm)
>>>inputVector=RandomVector(distInput)
```

Note that OpenTURNS can truncate any distribution to a lower, an upper bound or a given interval. Furthermore, a normal copula models the dependence between the variables Z_v and Z_m, with a correlation of 0.7. The variables (Q, K) are independent. Both blocks (Q, K) and (Z_v, Z_m) are independent.

Stochastic processes

OpenTURNS implements some multivariate random fields $\boldsymbol{X} : \Omega \times \mathcal{D} \to \mathbb{R}^d$ where $\mathcal{D} \in \mathbb{R}^s$ is discretized on a mesh. The User can easily build and simulate a random walk, a white noise as illustrated in Figures 4 and 5. The python commands write:

```
>>>myWN = WhiteNoise(myDist, myMesh)
>>>myRW = RandomWalk(myOrigin, myDist, myTimeGrid)
```
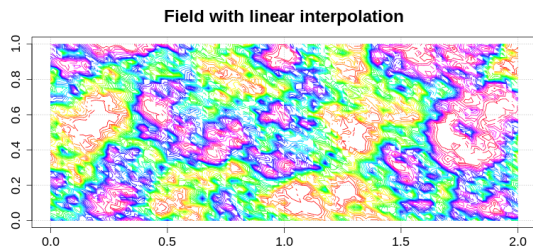
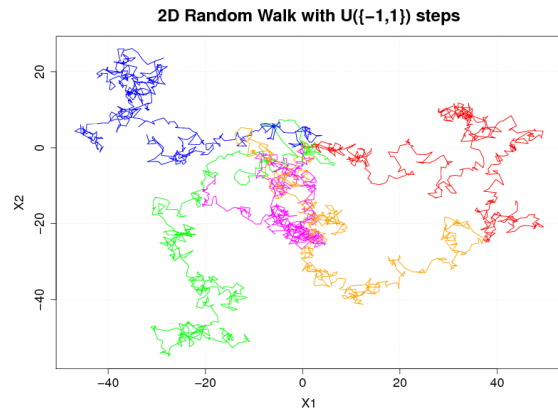**Fig. 4.** A Normal bivariate white noise.

Fig. 5. A Normal bivariate random walk.

Any field can be exported into the VTK format which allows it to be visualized using e.g.ParaView (www.paraview.org).

Multivariate ARMA stochastic processes $\boldsymbol{X} : \Omega \times [0, T] \to \mathbb{R}^d$ are implemented in OpenTURNS which enables some manipulations on times series such as the Box Cox transformation or the addition / removal of a trend. Note that the parameters of the Box Cox transformation can be estimated from given fields of the process.

OpenTURNS models normal processes, whose covariance function is a parametric model (e.g. the multivariate Exponential model) as well as defined by the User as illustrated in Figure 6. Stationary processes can be defined by its spectral density function (e.g. the Cauchy model).
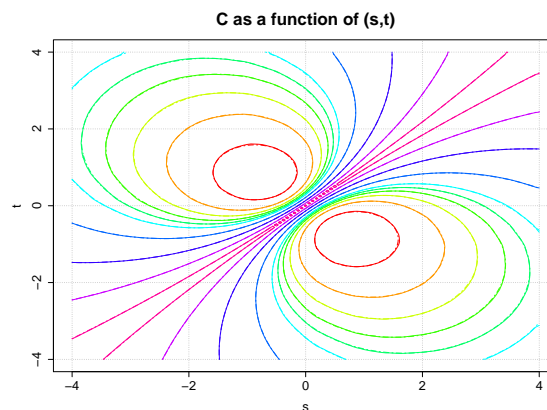

Fig. 6. A User Defined non stationary covariance function and its estimation from several given fields.

With explicit notations, the following python commands create a stationary Normal process defined by its covariance function, discretized on a mesh, with an additional trend:

```
>>>myNormalProcess=TemporalNormalProcess(myTrend, myCovarianceModel, myMesh)
```

Note that OpenTURNS enables the mapping of any stochastic processes $\boldsymbol{X}$ into a process $\boldsymbol{Y}$ through a function f: $\boldsymbol{Y} = f(\boldsymbol{X})$ where the function f can consist, for example, of adding or removing a trend, applying a Box Cox transformation in order to stabilize the variance of $\boldsymbol{X}$. The python command is, with explicit notations:

```
>>>myYprocess=CompositeProcess(f,myXprocess)
```

Finally, OpenTURNS implements multivariate processes defined as a linear combination of K deterministic functions $(\phi_i)_{i=1,\ldots,K} : \mathbb{R}^{d_1} \mapsto \mathbb{R}^{d_2}$:

$$X(\omega, \boldsymbol{x}) = \sum_{i=1}^{K} A_i(\omega)\phi_i(\boldsymbol{x})$$

where $(A_1, \ldots, A_K)$ is a random vector of dimension K. The python command writes:

```
>>>myX =FunctionalBasisProcess(myRandomCoeff, myBasis, myMesh)
```

Statistics estimation

OpenTURNS enables the User to estimate a model from data, in the univariate as well as in the multivariate framework, using the maximum likelihood principle or the moments based estimation.

Some tests, such as the Kolmogorov-Smirnov test, the Chi Square test and the Anderson Darling test (for normal distributions), are implemented and can help to select a model amongst others, from a sample of data. The python command to build a model and test it, writes:

```
>>>estimatedBeta = BetaFactory(sample)
>>>testResult = FittingTest.Kolmogorov(sample, estimatedBeta)
```

OpenTURNS also implements the kernel smoothing technique which is a non-parametric technique to fit a model to data: any distribution can be used as kernel. In the multivariate case, OpenTURNS uses the product kernel. It also implements

an optimized strategy to select the bandwidth, depending on the number of data in the sample, which is a mix between the Silverman rule and the plugin one. Note that OpenTURNS proposes a special treatment when the data are bounded, thanks to the mirroring technique. The python command to build the non-parametric model and to draw its pdf, is as simple as the following one:

```
>>>estimatedDist = KernelSmoothing().build(sample)
>>>pdfGraph = estimatedDist.drawPDF()
```

Figure 7 illustrates the resulting estimated distributions from a sample of size 500 issued from a Beta distribution: the Kernel Smoothing method takes into account the fact that data are bounded by 0 and 1. The histogram of the data is drawn to enable comparison.

Several visual tests are also implemented to help to select models: among them, the QQ-plot test and the Henry line test which writes (in the case of a Beta distributino for the QQ-plot test):

```
>>>graphQQplot = VisualTest.DrawQQplot(sample, Beta())
>>>graphHenryLine = VisualTest.DrawHenryLine(sample)
```

Figure 8 illustrates the QQ-plot test on a sample of size 500 issued from a Beta distribution: the adequation seems satisfying!

Stochastic processes also have estimation procedures from sample of fields or, if the ergodic hypothesis is verified, from just one field. Multivariate ARMA processes are estimated according to the BIC and AIC criteria and the Whittle estimator, which is based on the maximization of the likelihood function in the frequency domain. The python command to estimate an $ARMA(p, q)$ process of dimension d, based on a sample of time series, writes:

```
>>>estimatedARMA = ARMALikelihood(p,q,d).build(sampleTimeSeries)
```

Moreover, OpenTURNS can estimate the covariance function and the spectral density function of normal processes from given fields. For example, the python com-
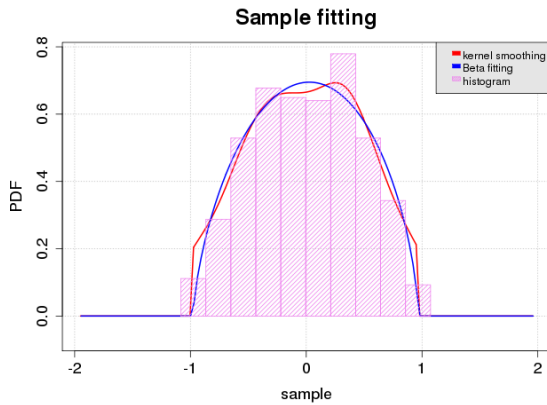
Fig. 7. Beta distribution estimation from a sample of size 500: parametric estimation versus kernel smoothing technique.
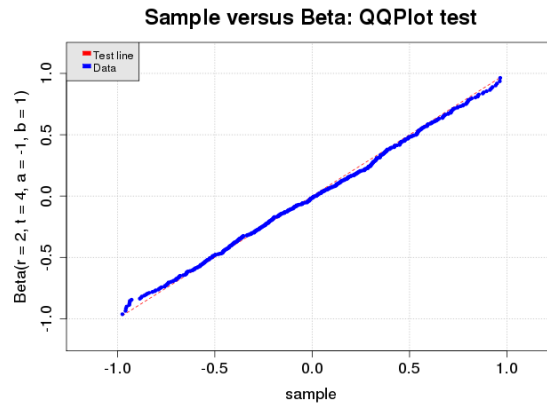

Fig. 8. QQ-plot test: theoretical model Beta versus the sample of size 500.

mand to estimate a stationary covariance model from a sample of realizations of the process:

>>>myCovFunc = $\mathrm{StationaryCovarianceModelFactory()\,.\,build(sampleProcess)}$

This estimation is illustrated in Figure 6.

Conditioned distributions

OpenTURNS enables the modeling of multivariate distributions by conditioning. Several types of conditioning are implemented.

At first, OpenTURNS enables the creation of a random vector $\boldsymbol{X}$ whose distribution $\mathcal{D}_{\boldsymbol{X}|\boldsymbol{\Theta}}$ whose parameters $\boldsymbol{\Theta}$ form a random vector distributed according to the distribution $\mathcal{D}_{\boldsymbol{\Theta}}$. The python command writes:

>>>myXrandVect = $\mathrm{ConditionalRandomVector(distXgivenTheta,\ distTheta)}$

Figure 9 illustrates a random variable X distributed according to a Normal distribution: $\mathcal{D}_{\boldsymbol{X}|\boldsymbol{\Theta}=(M,\Sigma)} = Normal(M, \Sigma)$, which parameters are defined by $M \sim Uniform([0,1])$ and $\Sigma \sim Exponential(\lambda = 4)$. The probability density function of X has been fitted with the kernel smoothing technique from $n = 10^6$ realizations of X with the normal kernel. It also draws, for comparison needs, the probability density function of X in the case where the parameters are fixed to their mean value.

Furthermore, when the random vector $\boldsymbol{\Theta}$ is defined as $\boldsymbol{\Theta} = g(\boldsymbol{Y})$ where the random vector follows a known distribution $\mathcal{D}_{\boldsymbol{Y}}$ and g is a given function, OpenTURNS creates the distribution of $\boldsymbol{X}$ with the python command:

```
>>>finalDist = ConditionalDistribution(distXGgivenTheta, distY, g)
```

Figure 10 illustrates the distribution of X that follows a $Uniform(A, B)$ distribution, with $(A, B) = g(Y)$, $g : \mathbb{R} \to \mathbb{R}^2$, $g(Y) = (Y, 1 + Y^2)$ and Y follows a $Uniform(-1, 1)$ distribution.
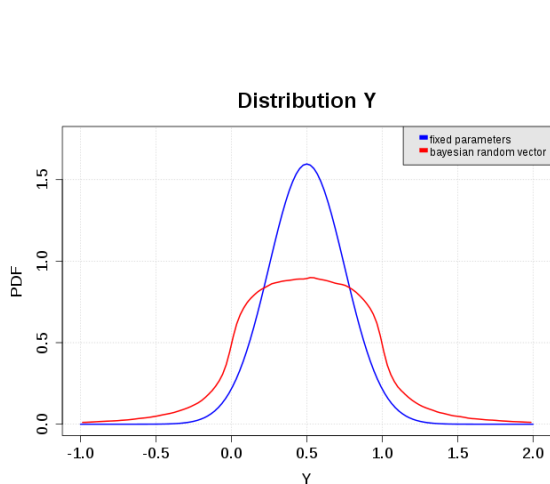

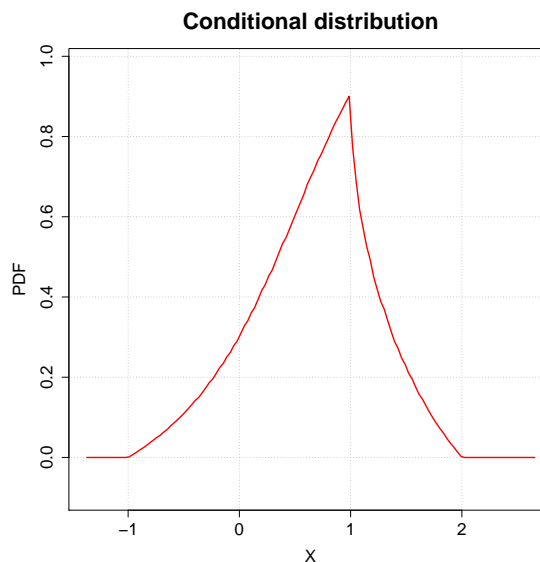**Fig. 9.** Normal distribution with random or fixed parameters.

Fig. 10. $Uniform(Y, 1 + Y^2)$, with $Y \sim Uniform(-1, 1)$.

Bayesian Calibration

Finally, OpenTURNS enables the calibration of a model (which can be a computer code) thanks to the Bayesian estimation, which is the evaluation of the model's parameters. More formally, let's consider a model G that writes: $\boldsymbol{y} = G(\boldsymbol{x}, \boldsymbol{\theta})$ where $\boldsymbol{x} \in \mathbb{R}^{d_1}$, $\boldsymbol{y} \in \mathbb{R}^{d_3}$ and $\boldsymbol{\theta} \in \mathbb{R}^{d_2}$ is the vector of unknown parameters to calibrate. The Bayesian calibration consists in estimating $\boldsymbol{\theta}$, based on a certain set of n inputs

$(\boldsymbol{x}^1, \ldots, \boldsymbol{x}^n)$ (an experimental design) and some associated observations $(\boldsymbol{z}^1, \ldots, \boldsymbol{z}^n)$ which are regarded as the realizations of some random vectors $(\boldsymbol{Z}^1, \ldots, \boldsymbol{Z}^n)$, such that, for all i, the distribution of $\boldsymbol{Z}^i$ depends on $\boldsymbol{y}^i = g(\boldsymbol{x}^i, \boldsymbol{\theta})$. Typically, $\boldsymbol{Z}^i = \boldsymbol{Y}^i + \boldsymbol{\varepsilon}^i$ where $\boldsymbol{\varepsilon}^i$ is a random measurement error. Once the User has defined the prior distribution of $\boldsymbol{\theta}$, OpenTURNS maximizes the likelihood of the observations and determines the posterior distribution of $\boldsymbol{\theta}$, given the observations, using the Metropolis-Hastings algorithm [5, 23].

Uncertainty propagation

Once the input multivariate distribution has been satisfactorily chosen, these uncertainties can be propagated through the G model to the output vector Y. Depending on the final goal of the study (min-max approach, central tendency, or reliability), several methods can be used to estimate the corresponding quantity of interest, tending to respect the best compromise between the accuracy of the estimator and the number of calls to the numerical, and potentially costly, model.

Min-Max approach

The aim here is to determine the extreme (minimum and maximum) values of the components of Y for the set of all possible values of $\boldsymbol{X}$. Several techniques enable it to be done :

- techniques based on design of experiments : the extreme values of Y are sought for only a finite set of combinations $(\mathbf{x}^1, \ldots, \mathbf{x}^n)$,

- techniques using optimization algorithms.

Techniques based on design of experiments

In this case, the min-max approach consists of three steps:

- choice of experiment design used to determine the combinations $(\mathbf{x}^1, \ldots, \mathbf{x}^n)$ of the input random variables,

- evaluation of $\mathbf{y}^i = G(\mathbf{x}^i)$ for $i = 1, \ldots, N$,

- evaluation of $\min_{1 \leq i \leq N} y_i^k$ and of $\max_{1 \leq i \leq N} y_i^k$, together with the combinations related to these extreme values: $\mathbf{x}_{k,\min} = \operatorname{argmin}_{1 \leq i \leq N} y_i^k$ and $\mathbf{x}_{k,\max} = \operatorname{argmax}_{1 \leq i \leq N} y_i^k$.

The type of design of experiments impacts the quality of the meta model and then on the evaluation of its extreme values. OpenTURNS gives access to two usual family of design of experiments for a min-max study :

- some stratified patterns (axial, composite, factorial or box patterns) Here are the two command lines that generate a sample from a 2-level factorial pattern.

```
>>>myCenteredReductedGrid = Factorial(2, levels)
>>>mySample = myCenteredReducedGrid.generate()
```

- some weighted patterns that include on the one hand, random patterns (Monte Carlo, LHS), and on the other hand, low discrepancy sequences (Sobol, Faure, Halton, Reverse Halton and Haselgrove, in dimension $n > 1$). The following lines illustrates the creation of a Faure sequence in diension 2 or a Monte Carlo design experiments form a bi-dimensional Normal(0,1) distribution.

```
# Sobol Sequence Sampling
>>>mySobolSample = FaureSequence(2).generate(1000)
# Monte Carlo Sampling
>>>myMCSample = MonteCarloExperiment(Normal(2), 100)
```

Figures 11 and 12 respectively illustrate a design of experiments issued from a Faure sequence or a Normal distribution in dimension 2.

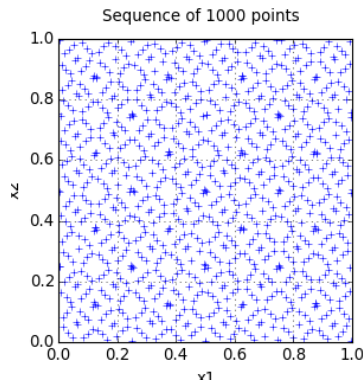**Techniques based on optimization algorithm**

Fig. 11. The first 1000 points according of a Faure sequence of dimension 2.
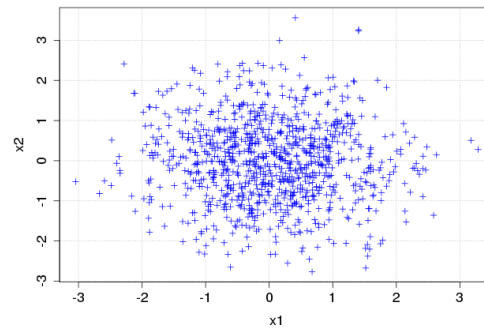

Fig. 12. Sample of 1000 points according of a Normal(0,1) distribution of dimension 2.

In this kind of approach, the min or max value of the output variable is sought thanks to an optimization algorithm. OpenTURNS offers several optimization algorithms for the several steps of the global methodology. Here the TNC (Truncated Newton Constrainted) is often used, which minimizes a function with variables subject to bounds, using gradient information. More details may be found in [26].

```
# For the research of the min value
>>>myAlgoTNC = TNC( TNCSpecificParameters() , limitStateFunction ,
                intervalOptim , startingPoint , TNC.MINIMIZATION)
# For the research of the max value
>>>myAlgoTNC = TNC( TNCSpecificParameters() , limitStateFunction ,
                intervalOptim , startingPoint , TNC.MAXIMIZATION)
# Run the research and extract the results
>>>myAlgoTNC.run()
>>>myAlgoTNCResult = BoundConstrainedAlgorithm(myAlgoTNC).getResult()
>>>optimalValue = myAlgoTNCResult.getOptimalValue()
```

Central tendency

A central tendency evaluation aims at evaluating a reference value for the variable of interest, here the water level H, and an indicator of the dispersion of the variable

around the reference. To address this problem, mean $\mu_Y = e(Y)$, and the standard deviation $\sigma_Y = \sqrt{\mathbb{V}(Y)}$ of Y are here evaluated using two different methods.

First, following the usual method within the Measurement Science community [12], $\mu_{\mathbf{Y}}$ and σ_Y have been computed under a Taylor first order approximation of the function $Y = G(\mathbf{X})$ (notice that the explicit dependence on the deterministic variable $\boldsymbol{d}$ is here omitted for simplifying notations):

$$\mu_Y \simeq G\left(\mathbb{E}(\boldsymbol{X})\right) \tag{3}$$

$$\sigma_Y \approx \sum_{i=1}^{d} \sum_{j=1}^{d} \left.\frac{\partial G}{\partial \boldsymbol{X}_i}\right|_{e(\boldsymbol{X})} \left.\frac{\partial G}{\partial \boldsymbol{X}_j}\right|_{e(\boldsymbol{X})} \rho_{ij}\sigma_i\sigma_j, \tag{4}$$

σ_i and σ_j being the standard deviation of the ith and jth component X_i and X_j of the vector $\boldsymbol{X}$ and ρ_{ij} their correlation coefficient. Thanks to the formulas above, the mean and the standard deviation of H are evaluated as 52.75m and 1.15m respectively.

```
>>>myQuadCum = QuadraticCumul(outputVariable)
# First order Mean
>>>meanFirstOrder =  myQuadCum.getMeanFirstOrder()[0]
# Second order Mean
>>>meanSecondOrder = myQuadCum.getMeanSecondOrder()[0]
# First order Variance
>>>varFirstOrder = myQuadCum.getCovariance()[0,0]
```

Then, the same quantities have been evaluated by a Monte Carlo evaluation : a set of 10000 samples of the vector $\boldsymbol{X}$ is generated and the function $G(\mathbf{X})$ is evaluated, thus giving a sample of H. The empirical mean and standard deviation of this sample are 52.75m and 1.42m respectively. Figure 13 shows the empirical histogram of the generated sample of H.

```
# Create a random sample of the output variable of interest of size 10000
>>>outputSample = outputVariable.getNumericalSample(10000)
# Get the empirical mean
>>>empiricalMean = outputSample.computeMean()
```
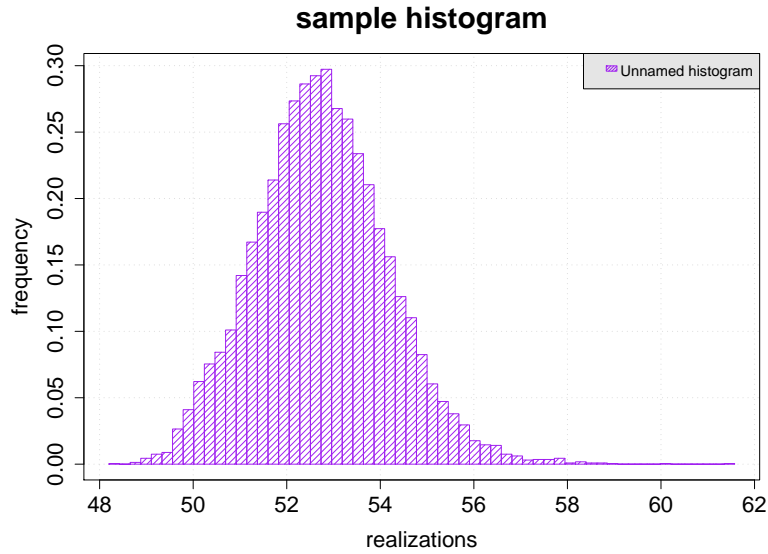
Fig. 13. Empirical histogram of 10000 samples of H.

```
# Get the empirical covariance matrix
>>>empiricalCovarianceMatrix = outputSample.computeCovariance()
```

Failure probability estimation

This section focuses on the estimation of the probability for the output Y to exceed a certain threshold s, noted P_f in the following. If s is the altitude of a flood protection dyke, then the above excess probability, P_f can be interpreted as the probability of an overflow of the dyke, i.e. a failure probability.

Note that an equivalent way of formulating this reliability problem would be to estimate the $(1 - p)$-th quantile of the output's distribution. This quantile can be interpreted as the flood height q_p which is attained with probability p each year. $T = 1/p$ is then seen to be a return period, i.e. a flood as high than $q_{1/T}$ occurs on average every T years.

Hence, the probability of overflowing a dyke with height s is less than p (where p, for instance, could be set according to safety regulations) if and only if $s \geq q_p$, i.e. if the dyke's altitude is higher than the flood with return period equal to $T = 1/p$.

FORM

A way to evaluate such failure probabilities is through the so-called First Order Reliability Method (FORM) [9]. This approach allows, by using an equiprobabilistic transformation and an approximation of the limit-state function, the evaluation with a much reduced number of model evaluations, of some low probability as required in the reliability field. Note that OpenTURNS implements the Nataf transformation where the input vector X has a normal copula, the generalized Nataf transformation when X has an elliptical copula, and the Rosenblatt transformation for any other cases [16, 19, 17, 18].

The probability that the yearly maximal water height H exceeds s=58m is evaluated using FORM. The Hasofer-Lind Reliability index was found to be equal to: $\beta_{HL} = 3.04$, yielding a final estimate of:

$$\hat{P}_{f,FORM} = 1.19 \times 10^{-3}.$$

The method gives also some importance factors that measure the weight of each input variable in the probability of exceedance, as shown on Figure 14
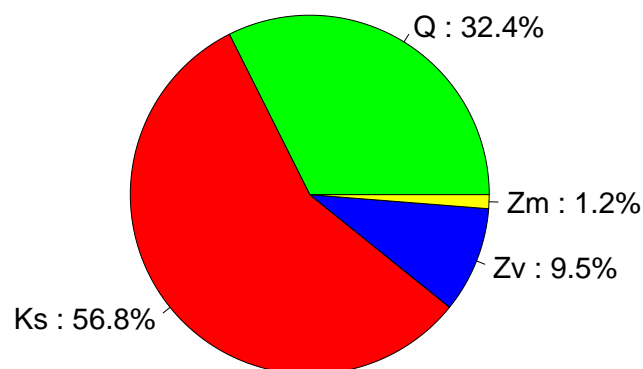

Fig. 14. FORM Importance Factors.

```
>>>myFORM = FORM( Cobyla ( ) , myEvent , meanInputVector )
```

```
>>>myFORM.run()
>>>FormResult = myFORM.getResult()
>>>pFORM = FormResult.getEventProbability()
>>>HasoferIndex = FormResult.getHasoferReliabilityIndex()
# Importance factors
>>>importanceFactorsGraph = FormResult.drawImportanceFactors()
```

Monte Carlo

Whereas the FORM approximation relies on strong assumptions, the Monte Carlo method is always valid, independently from the regularity of the model. It is nevertheless much more computationally intensive, covering all the input domain to evaluate the probability of exceeding a threshold. It consists in sampling many input values $(\boldsymbol{X^{(i)}})_{1 \leq i \leq N}$ from the input vector joint distribution, then computing the corresponding output values $Y^{(i)} = g(\boldsymbol{X^{(i)}})$. The excess probability P_f is then estimated by the proportion of sampled values $Y^{(i)}$ that exceed t :

$$\hat{P}_{f,MC} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{1}_{\{Y^{(i)}>s\}}. \tag{5}$$

The sample average of the estimation error $\hat{P}_{f,MC} - P_f$ decreases as $1/\sqrt{N}$, and can be precisely quantified by a confidence interval derived from the central limit theorem. In the present case the results are:

$$\hat{P}_{f,MC} = 1.50 \times 10^{-3},$$

with the following 95% confidence interval:

$$I_{P_f,MC} = \left[1.20 \times 10^{-3}, 1.79 \times 10^{-3} \right].$$

These results are coherent with those of the FORM approximation, confirming that the assumptions underlying the latter are correct. Figure 15 shows the convergence of the estimate depending on the size of the sample, obtained with OpenTURNS .
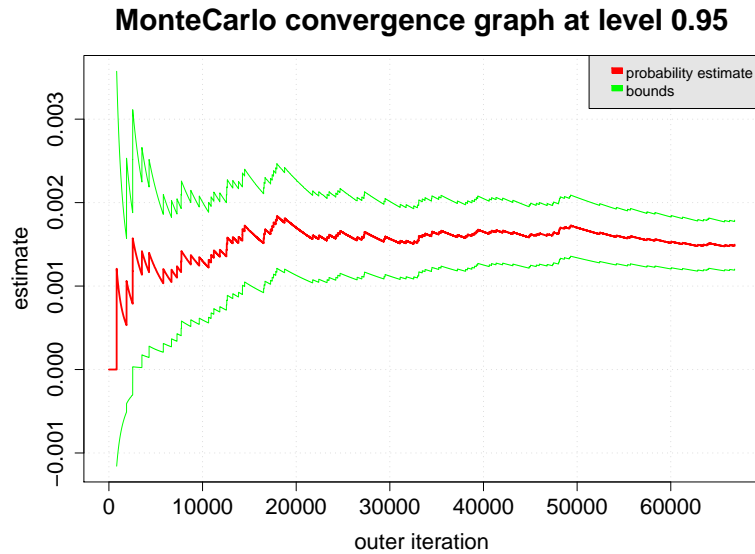
MonteCarlo convergence graph at level 0.95

Fig. 15. Monte Carlo Convergence graph.

```
>>>myEvent = Event(outputVariable, Greater(), threshold)
>>>myMonteCarlo = MonteCarlo(myEvent)
# Specify the maximum number of simulations
>>>numberMaxSimulation = 100000
>>>myMonteCarlo.setMaximumOuterSampling(numberMaxSimulation)
# Perform the algorithm
>>>myMonteCarlo.run()
# Get the convergence graph
>>>convergenceGraph = myMonteCarlo.drawProbabilityConvergence()
>>>convergenceGraph.draw("MonteCarloCovergenceGraph")
```

Importance Sampling

An even more precise estimate can be obtained through importance sampling [31], using the Gaussian distribution with identity covariance matrix and mean equal to the design point u^* as the proposal distribution. Many values $(U^{(i)})_{1 \leq i \leq N}$ are sampled from this proposal. Because $\phi_n(u - u^*)$ is the proposal density from which the $U^{(i)}$ have been sampled, the failure probability can be estimated without bias by:

$$\hat{P}_{f,IS} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{1}_{\{G\circ T^{-1}U^{(i)}>s\}}\frac{\phi_n(U^{(i)})}{\phi_n(U^{(i)}-u^*)} \tag{6}$$

The rationale of this approach is that by sampling in the vicinity of the failure domain boundary, a larger proportion of values fall within the failure domain than by sampling around the origin, leading to a better evaluation of the failure probability, and a reduction in the estimation variance. Using this approach, the results are :

$$\hat{P}_{f,IS} = 1.40 \times 10^{-3}$$

As in the simple Monte-Carlo approach, a 95%-level confidence interval can be derived from the output of the Importance Sampling algorithm. In the present case, this is equal to:

$$I_{P_f,IS} = \left[1.26\times 10^{-3}, 1.53\times 10^{-3}\right],$$

and indeed provides tighter confidence bounds for P_f.

```
# Specify the starting point from FORM algorithm
>>>standardPoint = FormResult.getStandardSpaceDesignPoint()
# Define the importance distribution
>>>sigma = [1.0, 1.0, 1.0, 1.0]
>>>importanceDistrib = Normal(standardPoint,sigma,CorrelationMatrix(4))
# Define the IS algorithm : event, distribution, criteria of convergence
>>>myAlgoImportanceSampling = ImportanceSampling (myStandardEvent,importanceDistrib)
>>>myAlgoImportanceSampling.setMaximumOuterSampling(maximumOuterSampling_IS)
>>>myAlgoImportanceSampling.setMaximumCoefficientOfVariation(0.05)
```

Directional Sampling

The directional simulation method is an accelerated sampling method, that involves as a first step a preliminary iso-probabilistic transformation as in FORM method. The basic idea is to explore the space by sampling in several directions in the standard space. The final estimate of the probability P_f after N simulations is the following:

$$\widehat{P}_{f,DS} = \frac{1}{N} \sum_{i=1}^{N} q_i$$

where q_i is the probability obtained in each explored direction. A central limit theorem allows to access to some confidence interval on this estimate. More details on this specific method can be found in [32].

In practice in OpenTURNS , the Directional Sampling simulation requires the choice of several parameters in the methodology : a sampling strategy to choose the explored directions, a "root strategy" corresponding to the way to seek the limit state function (i.e. a sign change) along the explored direction and a non-linear solver to estimate the root. A default setting of these parameters allows the user to test the method in one command line :

>>>myAlgo = DirectionalSampling(myEvent)

Subset Sampling

The subset sampling is a method for estimating rare event probability, based on the idea of replacing rare failure event by a sequence of more frequent events F_i.

$$F_1 \supset F_2 \supset \cdots \supset F_m = F$$

The original probability is obtained conditionaly to the more frequent events :

$$P_f = P(F_m) = P(\bigcap_{i=1}^{m} F_i) = P(F_1) \prod_{i=2}^{m} P(F_i|F_{i-1})$$

In practice, the subset simulation shows a substantial improvement $(N_T \sim \log P_f)$ compared to crude Monte Carlo $(N_T \sim \frac{1}{P_f})$ sampling when estimating rare events. More details on this specific method can be found in [2].

OpenTURNS provides this method through a dedicated module. Here also, some parameters of the methods have to be chosen by the user : a few command lines allows the algorithm to be set up before its launch.

>>>mySSAlgo=SubsetSampling(myEvent)

```
# Change  the  target  conditional  probability  of  each  subset  domain
>>>mySSAlgo.setTargetProbability(0.9)
# Set  the  width  of  the  MCMC  random  walk  uniform  distribution
>>>mySSAlgo.setProposalRange(1.8)
# This  allows  to  control  the  number  of  samples  per  step
>>>mySSAlgo.setMaximumOuterSampling(10000)
# Run  the  algorithm
>>>mySSAlgo.run()
```

Sensitivity analysis

The sensitivity analysis aims to investigate how a given computational model answers to variations in its inputs. Such knowledge is useful for determining the degree of resemblance of a model and a real system, distinguishing the factors that mostly influence the output variability and those that are insignificant, revealing interactions among input parameters and correlations among output variables, etc. A detailed description of sensitivity analysis methods can be found in [36] and in the *Sensitivity analysis* chapter of the Springer Handbook. In the global sensitivity analysis strategy, the emphasis is put on apportioning the output uncertainty to the uncertainty in the input factors, given by their uncertainty ranges and probability distributions.

Graphical tools

In sensitivity analysis, graphical techniques have to be used first. With all the scatterplots between each input variable and the model output, one can immediately detect some trends in their functional relation. The following instructions allow scatterplots of Figure 16 to be obtained from a Monte Carlo sample of size $N = 1000$ of the flooding model.

```
>>> inputSample = inputRandomVector.getNumericalSample(1000)
```

```
>>> inputSample.setDescription(['Q', 'K', 'Zv', 'Zm'])
>>> outputSample = finalModelCrue(inputSample)
>>> outputSample.setDescription(['H'])
# Here, stack both samples in one
>>> inputSample.stack(outputSample)
>>>myPairs = Pairs(inputSample)
>>>myGraph = Graph()
>>>myGraph.add(myPairs)
```

In the right column of Figure 16,it is clear that the strong and rather linear effects of Q and Z_v on the output variable H. In the plot of third line and fourth column, it is also clear that the dependence between Z_v and Z_m, which comes from the large correlation coefficient introduced in the probabilistic model.
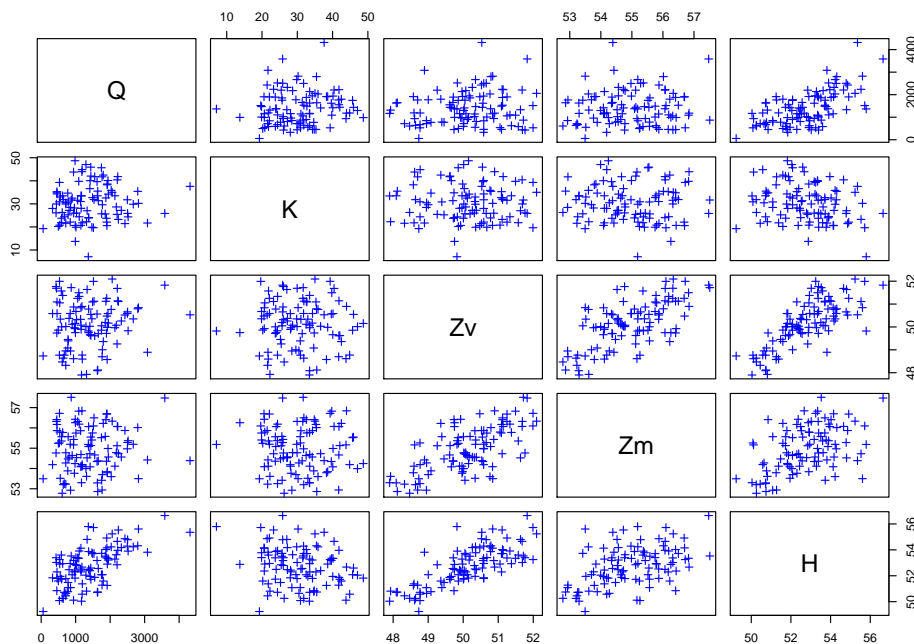

Fig. 16. Scatterplots between the inputs and the output of the flooding model: each combination (input i, input j) and (input i, output) is drawn, which enables to exhibit some correlation patterns.

However scatterplots do not capture some interaction effects between the inputs. Cobweb plots are then used to visualize the simulations as a set of trajectories. The

following instructions allow the cobweb plots of Figure 17 to be obtained where the simulations leading to the largest values of the model output H have been colored in red.

```
>>>inputSample = inputRandomVector.getNumericalSample(1000)
>>>outputSample = finalModelCrue(inputSample)
# Graph 1 : value based scale to describe the Y range
>>>minValue = outputSample.computeQuantilePerComponent(0.05)[0]
>>>maxValue = outputSample.computeQuantilePerComponent(0.95)[0]
>>>myCobweb = VisualTest.DrawCobWeb(inputSample, outputSample,
                    minValue, maxValue, 'red', False)
```

The cobweb plot allows us to immediately understand that these simulations correspond to large values of the flowrate Q and small values of the Strickler coefficient K_s.
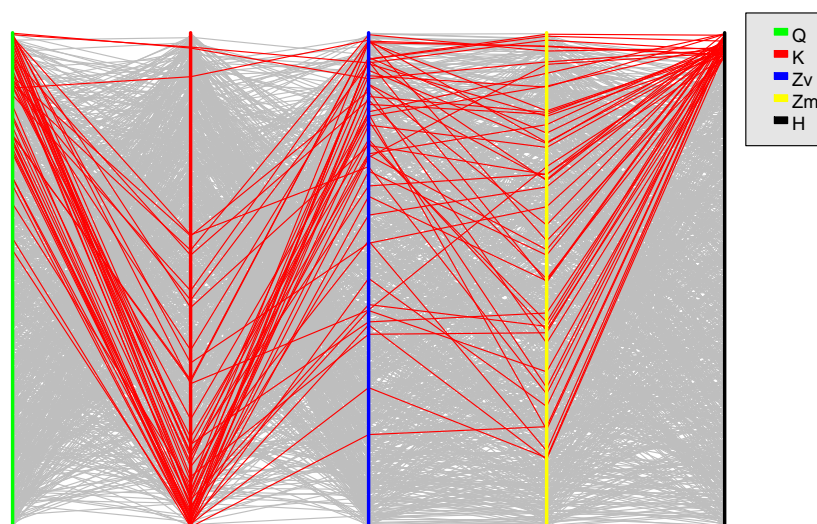

Fig. 17. Cobweb plot for the flooding model: each simulation is drawn. The input marginal values are linked to the output value (last column). All the simulations that led to a high quantile of the output are drawn in red: the cobweb plot enables to detect all the combinations of the inputs they come from.

Sampling-based methods

In order to obtain quantitative sensitivity indices rather than qualitative information, one may use some sampling-based methods which often suppose that the input variables are independent. The section illustrates some of these methods on the flooding model with independence between its input variables.

If the behavior of the output Y compared to the input vector $\boldsymbol{X}$ is overall linear, it is possible to obtain quantitative measurements of the inputs influences from the regression coefficients α_i of the linear regression connecting Y to the $X = (X_1, \ldots, X_p)$. The Standard Regression Coefficient (SRC), defined by

$$\mathrm{SRC}_i = \alpha_i \frac{\sigma_i}{\sigma_Y} \text{ (for } i = 1 \ldots p), \tag{7}$$

with σ_i (resp. σ_Y) the standard deviation of X_i (resp. Y), measures the variation of the response for a given variation of the parameter X_i. In practice, the coefficient R^2 (the variance percentage of the output variable Y explained by the regression model) also helps to check the linearity: if R^2 is close to one, the relation connecting Y to all the parameters X_i is almost linear and the SRC sensitivity indices make sense.

The following instructions allow the results of Table 2 to be obtained from a Monte Carlo sample of size $N = 1000$.

```
>>>inputSample = inputRandomVector.getNumericalSample(1000)
>>>outputSample = finalModelCrue(inputSample)
>>>SRCCoefficient = CorrelationAnalysis.SRC(inputSample, outputSample)
>>>linRegModel=LinearModelFactory().build(inputSample,outputSample,0.90)
>>>Rsquared = LinearModelTest.LinearModelRSquared(inputSample,
                                    outputSample, linRegModel,0.90)
```

The SRC values confirm our first conclusions drawn from the scatterplots visual analysis. As $R^2 = 0.97$ is very close to one, the model is quasi-linear. The SRC coefficients are sufficient to perform a global sensitivity analysis.

Table 2. Regression coefficients and SRC of the flood model inputs ($\alpha_0 = -0.1675$ and $R^2 = 0.97$).

	Q	K_s	Z_v	Z_m
α_i	3.2640	0.0012	-0.0556	1.1720
SRC_i	0.3462	0.0851	0.6814	0.0149

Several other estimation methods are available in OpenTURNS for a sensitivity analysis purpose:

- derivatives and Pearson correlation coefficients (linearity hypothesis between output and inputs),

- Spearman correlation coefficients and Standard Rank Regression Coefficients (monotonicity hypothesis between output and inputs),

- reliability importance factors with the FORM/SORM importance measures presented previously (section),

- variance-based sensitivity indices (no hypothesis on the model). These last indices, often known as Sobol' indices and defined by

$$S_i = \frac{\mathrm{Var}[\mathbb{E}(Y|X_i)]}{\mathrm{Var}(Y)} \text{ (first order index) and } S_{T_i} = \sum_{i=1}^{p} S_i + \sum_{i<j} S_{ij} + \ldots \text{ (total index)},$$

(8)

are estimated in OpenTURNS with the classic pick-freeze method based on two independent Monte Carlo samples [34]. In OpenTURNS, other ways to compute the Sobol' indices are the Extended FAST method [35] and the coefficients of the polynomial chaos expansion [38].

Metamodels

When each model evaluation is time consuming, it is usual to build a surrogate model which is a good approximation of the initial model and which can be evaluated at negligible cost. OpenTURNS proposes some usual polynomial approximations: the lin-

ear or quadratic Taylor approximations of the model at a particular point, or a linear approximation based on the least squares method. Two recent techniques implemented in OpenTURNS are detailed here: the polynomial chaos expansion and the kriging approximation.

Polynomial chaos expansion

The polynomial chaos expansion enables the approximation of the output random variable of interest $\boldsymbol{Y} = G(\boldsymbol{X})$ with $g : \mathbb{R}^d \to \mathbb{R}^p$ by the surrogate model:

$$\tilde{\boldsymbol{Y}} = \sum_{k \in K} \boldsymbol{\alpha}_k \Psi_k \circ T(\boldsymbol{X})$$

where $\boldsymbol{\alpha}_k \in \mathbb{R}^p$, T is an isoprobabilistic transformation (e.g. the Rosenblatt transformation) which maps the multivariate distribution of $\boldsymbol{X}$ into the multivariate distribution $\mu = \prod_{i=1}^d \mu_i$, and $(\Psi_k)_{k \in \mathbb{N}}$ a multivariate polynomial basis of $\mathcal{L}^2_\mu(\mathbb{R}^d, \mathbb{R}^p)$ which is orthonormal according to the distribution μ. K is a finite subset of $\mathbb{N}$. $\boldsymbol{Y}$ is supposed to be of finite second moment.

OpenTURNS proposes the building of the multivariate orthonornal basis $(\Psi_k(\boldsymbol{x}))_{k \in \mathbb{N}}$ as the cartesian product of orthonormal univariate polynomial family $(\Psi^i_l(z_i))_{l \in \mathbb{N}}$:

$$\Psi_k(\boldsymbol{z}) = \Psi^1_{k_1}(z_1) * \Psi^2_{k_2}(z_2) * \cdots * \Psi^d_{k_d}(z_d)$$

The possible univariate polynomial families associated to continuous measures are :

- Hermite, which is orthonormal with respect to the $Normal(0,1)$ distribution,

- Jacobi(α, β, *param*), which is orthonormal with respect to the $Beta(\beta + 1, \alpha + \beta + 2, -1, 1)$ distribution if $param = 0$ (default value) or to the $Beta(\alpha, \beta, -1, 1)$ distribution if $param = 1$,

- Laguerre(k), which is orthonormal with respect to the $Gamma(k + 1, 1, 0)$ distribution,

- Legendre, which is orthonormal with respect to the $Uniform(-1,1)$ distribution.

OpenTURNS proposes three strategies to truncate the multivariate orthonormal basis to the finite set K : these strategies select different terms from the multivariate basis, based on a convergence criterion of the surrogate model and the cleaning of the less significant coefficients.

The coefficients of the polynomial decomposition writes:

$$\boldsymbol{\alpha} = argmin_{\boldsymbol{\alpha} \in \mathbb{R}^K} E_\mu \left[\left(g \circ T^{-1}(\boldsymbol{Z}) - \sum_{k \in K} \alpha_k \Psi_k(\boldsymbol{Z}) \right)^2 \right] \tag{9}$$

as well as:

$$\boldsymbol{\alpha} = \left(E_\mu \left[g \circ T^{-1}(\boldsymbol{Z}) \Psi_k(\boldsymbol{Z}) \right] \right)_k \tag{10}$$

where $\boldsymbol{Z} = T(\boldsymbol{X})$ is distributed according to μ.

It corresponds to two points of view implemented by OpenTURNS : the relation (9) means that the coefficients $(\alpha_k)_{k \in K}$ minimize the mean quadratic error between the model and the polynomial approximation; the relation (10) means that α_k is the scalar product of the model with the $k-th$ element of the orthonormal basis $(\Psi_k)_{k \in K}$. In both cases, the expectation E_μ is approximated by a linear quadrature formula that writes, in the general case:

$$E_\mu \left[f(\boldsymbol{Z}) \right] \simeq \sum_{i \in I} \omega_i f(\Xi_i) \tag{11}$$

where f is a function $L_1(\mu)$. The set I, the points $(\Xi_i)_{i \in I}$ and the weights $(\omega_i)_{i \in I}$ are evaluated from weighted designs of experiments which can be random (Monte Carlo experiments, and Importance sampling experiments) or deterministic (low discrepancy experiments, User given experiments, and Gauss product experiments).

At last, OpenTURNS gives access to:

- the composed model $h : \boldsymbol{Z} \mapsto \boldsymbol{Y} = G \circ T^{-1}(\boldsymbol{Z})$, which is the model of the reduced variables $\boldsymbol{Z}$. Then $h = \sum_{k \in \mathbb{N}} \boldsymbol{\alpha}_k \Psi_k$,

- the coefficients of the polynomial approximation : $(\boldsymbol{\alpha}_k)_{k \in K}$,

- the composed meta model: $\hat{h}$, which is the model of the reduced variables reduced to the truncated multivariate basis $(\Psi_k)_{k \in K}$. Then $\hat{h} = \sum_{k \in K} \boldsymbol{\alpha}_k \Psi_k$,

- the meta model: $\hat{g} : \boldsymbol{X} \mapsto Y = \hat{h} \circ T(\boldsymbol{X})$ which is the polynomial chaos approximation as a NumericalMathFunction. Then $\hat{g} = \sum_{k \in K} \boldsymbol{\alpha}_k \Psi_k \circ T$.

When the model is very expensive to evaluate, it is necessary to optimize the number of coefficients of the polynomials chaos expansion to be calculated. Some specific strategies have been proposed by [6] for enumerating the infinite polynomial chaos series: OpenTURNS implements the hyperbolic enumeration strategy which is inspired by the so-called sparsity-of-effects principle. This strategy states that most models are principally governed by main effects and low-order interactions. This enumeration strategy selects the multi-indices related to main effects.

The following lines illustrates the case where the model $\mathcal{G} : \boldsymbol{x} \mapsto x \sin x$ and where the input random vector follows a Uniform distribution on $[-1, 1]$

```
# Define the model
>>> model = NumericalMathFunction(['x'], ['x*sin(y)'])
# Create the input distribution
>>> distribution = Uniform()
# Construction of the  orthonormal basis
>>> polyColl = [0.]
>>> polyColl[0] = StandardDistributionPolynomialFactory(distribution)
>>> enumerateFunction = LinearEnumerateFunction(1)
>>> productBasis = OrthogonalProductPolynomialFactory(polyColl, enumerateFunction)
# Truncature strategy of the multivariate orthonormal basis
# Choose all the polynomials of degree <= 4
>>> degree = 4
>>> indexMax = enumerateFunction.getStrataCumulatedCardinal(degree)
# Keep all the polynomials of degree <= 4
```

```
# which corresponds to the 5 first ones
>>> adaptiveStrategy = FixedStrategy(productBasis, indexMax)
# Evaluation strategy of the approximation coefficients
>>> samplingSize = 50
>>> experiment = MonteCarloExperiment(samplingSize)
>>> projectionStrategy = LeastSquaresStrategy(experiment)
# Creation of the Functional Chaos Algorithm
>>> algo = FunctionalChaosAlgorithm(model, distribution, adaptiveStrategy,
...                                          projectionStrategy)
>>> algo.run()
# Get the result
>>> functionalChaosResult = algo.getResult()
>>> metamodel = functionalChaosResult.getMetaModel()
```
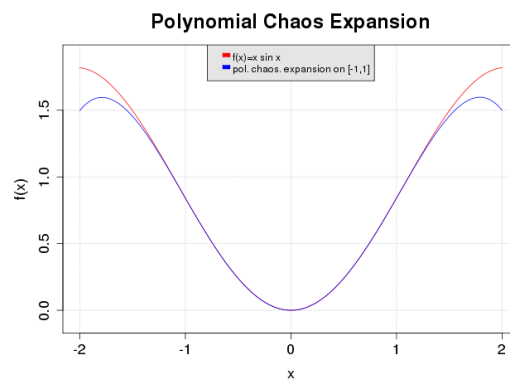
Figure 18 illustrates the result.

Fig. 18. An example ofa polynomial chaos expansion: the blue line is the reference function $\mathcal{G} : \boldsymbol{x} \mapsto x \sin x$ and the red one its approximation only valid on $[-1, 1]$.

The Kriging approximation

Kriging (also known as Gaussian process regression) [33, 37, 30, 24] is a Bayesian technique that aims at approximating functions (most often in order to surrogate them because they are expensive to evaluate). In the following it is assumed the aim is to

surrogate a scalar-valued model $G : \boldsymbol{x} \mapsto y$. Note the OpenTURNS implementation of Kriging can deal with vector-valued functions ($G : \boldsymbol{x} \mapsto \boldsymbol{y}$), with simple loops over each output. It is also assumed the model was run over a design of experiments in order to produce a set of observations gathered in the following dataset: $((\boldsymbol{x}^i, y^i), i = 1, \ldots, n)$. Ultimately Kriging aims at producing a predictor (also known as a response surface or metamodel) denoted as $\tilde{G}$.

It is assumed that the model G is a realization of the normal process $Y : \Omega \times \mathbb{R}^d \to \mathbb{R}$ defined by:

$$Y(\omega, \boldsymbol{x}) = m(\boldsymbol{x}) + Z(\omega, \boldsymbol{x}) \tag{12}$$

where $m(\boldsymbol{x})$ is the trend and $Z(\boldsymbol{x})$ is a zero-mean Gaussian process with a covariance function $c_{\boldsymbol{\theta}} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ which depends on the vector of parameters $\boldsymbol{\theta} \in \mathbb{R}^{n_\theta}$:

$$\mathbb{E}[Z(\boldsymbol{x}), Z(\boldsymbol{y})] = c_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{y}) \tag{13}$$

The trend is generally taken equal to the generalized linear model:

$$m(\boldsymbol{x}) = (\boldsymbol{f}(\boldsymbol{x}))^t \boldsymbol{\beta} \tag{14}$$

where $(\boldsymbol{f}(\boldsymbol{x}))^t = (f_1, \ldots, f_p)$ and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)$. Then, the Kriging method approximates the model f by the mean of the Y given that:

$$Y(\omega, \boldsymbol{x}^{(i)}) = y^{(i)} \quad \forall i = 1, \ldots, n \tag{15}$$

The Kriging meta model $\tilde{G}$ of G writes:

$$\tilde{G}(\boldsymbol{x}) = \mathbb{E}[Y(\omega, \boldsymbol{x}) | Y(\omega, \boldsymbol{x}^{(i)}) = y^{(i)}, \forall i = 1, \ldots, n] \tag{16}$$

The meta model is then defined by:

$$\tilde{G}(\boldsymbol{x}) = (\boldsymbol{f}(\boldsymbol{x}))^t \tilde{\boldsymbol{\beta}} + \left(\boldsymbol{c}_{\boldsymbol{\theta}}(\boldsymbol{x})\right)^t C_{\boldsymbol{\theta}}^{-1} (\boldsymbol{y} - F\tilde{\boldsymbol{\beta}}) \tag{17}$$

where $\tilde{\boldsymbol{\beta}}$ is the least squares estimator for $\boldsymbol{\beta}$ defined by:

$$\tilde{\boldsymbol{\beta}} = \left(F^t C_{\boldsymbol{\theta}}^{-1} F\right)^{-1} F^t C_{\boldsymbol{\theta}}^{-1} \boldsymbol{y} \qquad (18)$$

and $C_{\boldsymbol{\theta}} = [c_{\boldsymbol{\theta}}(x_i, x_j)]_{i,j=1...n}$, $F = [f(x_i)^t]_{i=1...n}$ and $\boldsymbol{c}_{\boldsymbol{\theta}}^t(\boldsymbol{x}) = [c_{\boldsymbol{\theta}}(x, x_i)]_{i=1...n}$. The line command writes:

```
>>> algo = KrigingAlgorithm(inputSample, outputSample, basis, covarianceModel)
>>> algo.run()
>>> result = algo.getResult()
>>> metamodel = result.getMetaModel()
>>> graph = metamodel.draw()
```

Figure 19 approximates the previously defined model $\mathcal{G} : \boldsymbol{x} \mapsto x \sin x$ with a realization of a Gaussian process based on 6 observations.
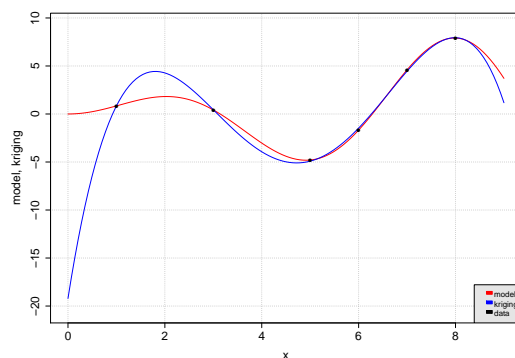

Fig. 19. An example of kriging approximation based on 6 observations: the blue line is the reference function $\mathcal{G} : \boldsymbol{x} \mapsto x \sin x$ and the red one its approximation by a realization of a Gaussian process.

Using an external code

The external simulator

Fast evaluations of G

On the practical side, the OpenTURNS software provides features which make the connection to the simulator G easy, and make its evaluation generally fast. Within the OpenTURNS framework, the method to connect to G is called "wrapping".

In the simplest situations, the function G is analytical and the formulas can be provided to OpenTURNS with a character string. Here, the Muparser C++ library [4] is used to evaluate the value of the mathematical function. In this case, the evaluation of G by OpenTURNS is quite fast.

In the following Python script, consider the function $G : \mathbb{R}^3 \rightarrow \mathbb{R}^2$, where $G_1(\mathbf{x}) = x_1 + x_2 + x_3$ and $G_2(\mathbf{x}) = x_1 - x_2 x_3$, for any real numbers x_1, x_2 and x_3. The input argument of the `NumericalMathFunction` class is a Python `tuple`, where the first item describes the three inputs variables, the second item describes the two output variables and the last item describes the two functions G_1 and G_2.

```
>>>G = NumericalMathFunction(
    ("x0","x1","x2"),
    ("y0","y1"),
    ("x0+x1+x2","x0-x1*x2"))
```

Once created, the function `G` can be used as a regular Python function, or can be passed as an input argument of other OpenTURNS classes.

In most cases, the function G is provided as a Python function, which can be connected to OpenTURNS with the `PythonFunction` class. This task is easy (for those who are familiar with this language), and allows the scientific packages already available in Python to be combined. For example, if the computational code uses XML files on input or output, it is easy to make use of the XML features of Python (e.g. the `minidom` package). Moreover, if the function evaluation can be

vectorized (e.g. with the `numpy` package), then the `func_sample` option of the `PythonFunction` class can improve the performance a lot.

The following Python script creates the function G associated with the flooding model. The `flood` function is first defined with the `def` Python statement. This function takes the variable `X` as input argument, which is an array with four components, `Q`, `K_s`, `Z_v` and `Z_m`, which corresponds to the input random variables in the model. The body of the `flood` function is a regular Python script, so that all Python functions can be used at this point (e.g. the `numpy` or `scipy` functions). The last statement of the function returns the overflow `S`. Then the `PythonFunction` class is used in order to convert this Python function into an object that OpenTURNS can use. This class takes as input arguments the number of input variables (in this case, 4), the number of outputs (in this case, 1) and the function and returns the object `G`.

```
>>>from openturns import PythonFunction
>>>def flood (X) :
    L = 5.0 e3 ;       B = 300.0
    Q, K_s, Z_v, Z_m = X
    alpha = (Z_m − Z_v)/L
    H = (Q/(K_s∗B∗sqrt(alpha)))∗∗(0.6)
    return H
>>>G = PythonFunction(4, 1, flood)
```

If, as many of the computational codes commonly used, the data exchange is based on text files, OpenTURNS provides a component (`coupling_tools`) which is able to read and write structured text files based, for example, on line indices and perhaps containing tables (using line and column indices). Moreover, OpenTURNS provides a component which can evaluate such a Python function using the multi-thread capabilities that most computers have.

Finally, when the computational code G is provided as a C or Fortran library, OpenTURNS provides a generic component to exchange data by memory, which is much faster than with files. In this case, the evaluation of G is automatically multi-thread. This component can be configured by Python, based on a XML file. If this method is not flexible enough, then the connection can be done with the C++ library.

The previous techniques are documented in the OpenTURNS Developer's Guide [1].

Figure 20 compares the performance of three methods to connect to the function G : the `PythonFunction` class, the `PythonFunction` class with the `func_sample` option and the analytical function. This test was performed with a basic MS Windows laptop computer. Obviously, the fastest method is the analytical function, which can provide as many as 0.2 million samples per second, a performance which is four times the performance of the `PythonFunction` class.
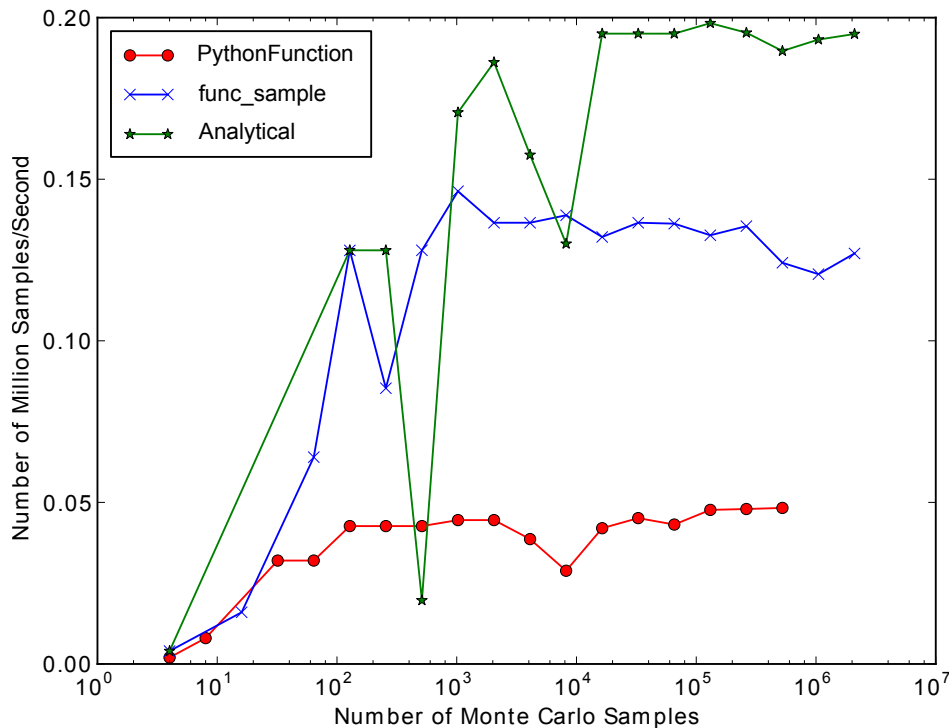

Fig. 20. Performance of various connection methods in OpenTURNS

Evaluation of the derivatives

When the algorithm involves an optimization step (e.g. in the FORM-SORM method) or a local approximation of G (e.g. in the Taylor development used to approximate the expectation and variance), the derivatives of G are required.

When the computer code can compute the gradient and Hessian matrix of G, this information can be used by OpenTURNS . This happens sometimes, for example when the computer code has been differentiated with automatic differentiation methods, such as forward or adjoint techniques.

In the case where the function is analytical and is provided as a character string, OpenTURNS is able to compute the exact derivatives of G. In order to do this, the software uses the Ev3 C++ library [22] to perform the symbolic computation of the derivatives and MuParser [4] to evaluate it.

In most common situations, however, the code does not compute its derivatives. In this case, OpenTURNS provides a method to compute the derivatives based on finite difference formulas. By default a centered finite difference formula for the gradient and a centered formula for the Hessian matrix are used.

High performance computing

For most common engineering practices, OpenTURNS can evaluate G with the multi-thread capabilities of most laptop and scientific workstations. However, when the evaluation of G is more CPU consuming or when the number of evaluations required is larger, these features are not sufficient by themselves and it is necessary to use a high performance computer such as the Zumbrota, Athos or Ivanhoe supercomputers available at EDF R&D which have from 16 000 to 65 000 cores [40].

In this case, two solutions are commonly used. The first one is to use a feature which can execute a Python function on remote processors, connected on the network with `ssh`. Here, the data flow is based on files, located in automatically generated directories, which prevents the loss of intermediate data. This feature (the `DistributedPythonFunction`) allows each remote processor to use its multi-thread capabilities, providing two different levels of parallel computing.

The second solution is to use the OpenTURNS component integrated in the Salome platform. This component, along with a graphical user interface, called "Eficas", makes use of a software, called "YACS", which can call a Python script. The YACS module allows calculation schemes in Salome to be built, edited and executed. It provides both a graphical user interface to chain the computations by linking the inputs and outputs of computer codes, and then to execute these computations on remote machines.

Several studies have been conducted at EDF based on the OpenTURNS component of Salome. For example, an uncertainty propagation study (the thermal evaluation of the storage of high-level nuclear waste) was making use of a computer code where one single run required approximately 10 minutes on the 8 cores of a workstation (with shared memory). Within Salome, the OpenTURNS simulation involving 6000 unitary evaluations of the function G required 8000 CPU hours on 32 nodes [3].

Conclusions

This educational example has shown a number of questions and problems that can be addressed by UQ methods: uncertainty quantification, central tendency evaluation, excess probability assessment and sensitivity analysis, that can require the use of a metamodel.

Different numerical methods have been used for solving these three classes of problems, leading substantially to the same (or very similar) results. In the industrial practice of UQ, the main issue (which actually motivates the choice of one mathematical method instead of another) is the computational budget, which is actually given by the number of allowed runs of the deterministic model G. When the computer code implementing G is computationally expensive, one needs specifically designed mathematical and software tools.

OpenTURNS is specially intended to meet these issues : (i) it includes a set of efficient mathematical methods for UQ and (ii) it can be easily connected to any external black box model G. Thanks to these two main features, OpenTURNS is a software that can address many different physics problems, and thus help to solve industrial problems. From this perspective, the partnership around OpenTURNS focuses efforts on the integration of the most efficient and innovative methods required by the industrial applications that takes into account both the need of genericity and of ease to communicate. The main projects for 2015 concern the improvement of the kriging implementation to integrate some very smart methods of optimization. Around this theme some other classical optimization methods will also be generalized or newly implemented.

A growing need for model exploration and analysis of uncertainty problem in industrial applications is to better visualise the information provided by such a volume of data. In this area, specific visualization software, such as Paraview, can provide very efficient and interactive features. Taking the advantage of the integration of OpenTURNS in the Salome platform, EDF is working on a better link between the Paraview module in Salome (called ParaVIS) and the uncertainty analysis with OpenTURNS : in 2012, functional boxplot ([13]) has been implemented. Some recent work around in-situ visualization for uncertainty analysis should also be developed and implemented and so benefit very computationaly expensive model physics that generate an extremely high volume of data.

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