OpenTURNS and its graphical interface

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Contents

OpenTURNS: www.openturns.org

OpenTURNS

An Open source initiative for the Treatment of Uncertainties, Risks'N Statistics

- Multivariate probabilistic modeling including dependence
- Numerical tools dedicated to the treatment of uncertainties
- Generic coupling to any type of physical model
- Open source, LGPL licensed, C++/Python library

OpenTURNS: `www.openturns.org`

- Linux, Windows
- First release : 2007
- 5 full time developers
- Users $\approx$ 1000, mainly in France (208 000 Total Conda downloads)
- Project size (2018) : 720 classes, more than 6000 services

OpenTURNS: content

Data analysis

Visual analysis: QQ-Plot, Cobweb
Fitting tests: Kolmogorov, Chi2
Multivariate distribution: kernel smoothing (KDE), maximum likelihood
Process: covariance models, Welch and Whittle estimators
Bayesian calibration: Metropolis-Hastings, conditional distribution

Probabilistic modeling

Dependence modelling: elliptical, archimedian copulas.
Univariate distribution: Normal, Weibull
Multivariate distribution: Student, Dirichlet, Multinomial, User-defined
Process: Gaussian, ARMA, Random walk.
Covariance models: Matern, Exponential, User-defined

Meta modeling

Functional basis methods: orthogonal basis (polynomials, Fourier, Haar, Soize Ghanem)
Gaussian process regression: General linear model (GLM), Kriging
Spectral methods: functional chaos (PCE), Karhunen-Loeve, low-rank tensors

Reliability, sensitivity

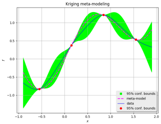
Sampling methods: Monte Carlo, LHS, low discrepancy sequences
Variance reduction methods: importance sampling, subset sampling
Approximation methods: FORM, SORM
Indices: Spearman, Sobol, ANCOVA
Importance factors: perturbation method, FORM, Monte Carlo

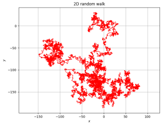
Functional modeling

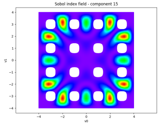
Numerical functions: symbolic, Python-defined, user-defined
Function operators: addition, product, composition, gradients
Function transformation: linear combination, aggregation, parametrization
Polynomials: orthogonal polynomial, algebra

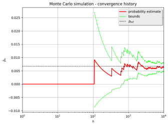
Numerical methods

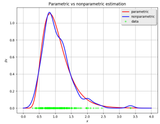
Integration: Gauss-Kronrod
Optimization: NLopt, Cobyla, TNC
Root finding: Brent, Bisection
Linear algebra: Matrix, HMat
Interpolation: piecewise linear, piecewise Hermite
Least squares: SVD, QR, Cholesky









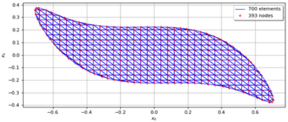


OpenTURNS: documentation

LevelSetMesher

(Source code, png, hires.png, pdf)

Mesh of a level set



class **LevelSetMesher**(**args*)

Creation of mesh of box type.

Available constructor:

LevelSetMesher(*discretization*)

Parameters: **discretization** : sequence of int, of dimension ≤ 3.

Discretization of the levelset bounding box.

solver : `OptimizationAlgorithm`

Optimization solver used to project the vertices onto the level set. It must be able to solve nearest point problems. Default is `AbdoRackwitz`.

Notes

The meshing algorithm is based on the `IntervalMesher` class. First, the bounding box of the level set (provided by the user or automatically computed) is meshed. Then, all the simplices with all vertices outside of the level set are rejected, while the simplices with all vertices inside of the level set are kept. The remaining simplices are adapted the following way :

- The mean point of the vertices inside of the level set is computed
- Each vertex outside of the level set is projected onto the levelset using a linear interpolation
- If the *project* flag is *True*, then the projection is refined using an optimization solver.

Examples

Create a mesh:

```
>>> import openturns as ot
>>> mesher = ot.LevelSetMesher([5, 10])
>>> level = 1.0
>>> function = ot.SymbolicFunction(['x0', 'x1'], ['x0^2+x1^2'])
>>> levelSet = ot.LevelSet(function, level)
>>> mesh = mesher.build(levelSet)
```

Methods

`build`(*args)	Build the mesh of levelset type.
`getClassName`()	Accessor to the object's name.
`getDiscretization`()	Accessor to the discretization.

- Content: programming interface, examples, theory.
- The doc is generated: *all* classes and methods are documented, partly automatically.
- Examples are automatically tested at *each* update of the code and outputs are checked.

OpenTURNS: estimate the mean sequentially

Two sequential algorithms based on asymptotic statistics: the mean and Sobol' sensitivity indices.

Part 1 : Estimate the mean with an sequential algorithm.

- The "classical" way of estimating the mean : set the sample size n, then use the sample mean $\bar{\mu} = (1/n)\sum_{j=1}^{n} y^{(j)}$ and estimate the accuracy (e.g. C.V.).
- Goal: use the smallest possible sample which achieves a given accuracy. Increase the sample size until a stopping criteria is met.
- The sample mean is asymptotically gaussian:

$$\bar{\mu} \xrightarrow{D} \mathcal{N}\left(E(Y), \frac{V(Y)}{n}\right).$$

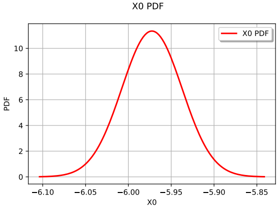
- The absolute accuracy of the estimate $\bar{\mu}$ can be evaluated based on the sample standard deviation of the estimator $\hat{s}/\sqrt{n}$
- To get good performances on distributed supercomputers and multi-core workstations, the size of the sample increases by block.

OpenTURNS: estimate the mean sequentially

```
[... Define the Y RandomVector ...]
algo = ot.ExpectationSimulationAlgorithm(Y)
algo.setMaximumOuterSampling(1000)
algo.setBlockSize(10) # Sample size is 0, 10, 20, 30, 40, ...
algo.setMaximumCoefficientOfVariation(0.001)
algo.run()
result = algo.getResult()
expectation = result.getExpectationEstimate()
print("Mean = %f " % expectation[0])
meanDistr = result.getExpectationDistribution()
View(meanDistr.drawPDF())
```

Output:

Mean $= -5.972516$



Asymptotic distribution of the sample mean.

OpenTURNS: estimate Sobol' indices sequentially

Part 2 : Estimate Sobol' sensitivity indices with an incremental algorithm based on asymptotic statistics, extending the work of (Janon et al., 2014).

- Assume that the Sobol' estimator is:

$$\bar{S} = \Psi\left(\overline{U}\right)$$

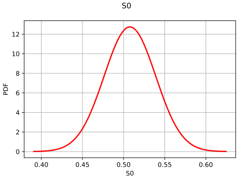
  where Ψ is a multivariate function, U is a multivariate sample and $\overline{U}$ is its sample mean.
- Each Sobol' estimator (e.g. Saltelli, Jansen, etc...) can be associated with a specific choice of function Ψ and vector U.
- Therefore, the multivariate delta method implies:

$$\sqrt{n}\left(\overline{U} - \mu\right) \xrightarrow{D} \mathcal{N}\left(0, \nabla\psi(\mu)^T \Gamma \nabla\psi(\mu)\right)$$

  where μ is the expected value of the Sobol' indice, $\nabla\psi(\mu)$ is the gradient of the function Ψ and Γ is the covariance matrix of $\overline{U}$.
- An implementation of the exact gradient $\nabla\psi(\mu)$ was derived for all estimators in OpenTURNS (Dumas, 2018).

OpenTURNS: estimate Sobol' indices sequentially

```
[... Define the X Distribution, define the g Function...]
estimator = ot.SaltelliSensitivityAlgorithm()
estimator.setUseAsymptoticDistribution(True)
algo = ot.SobolSimulationAlgorithm(X, g, estimator)
algo.setMaximumOuterSampling(100) # number of iterations
algo.setBlockSize(50)  # size of experiment at each iteration
algo.setIndexQuantileLevel(0.1) # the confidence interval level
algo.setIndexQuantileEpsilon(0.2) # length of confidence interval
algo.run()
```



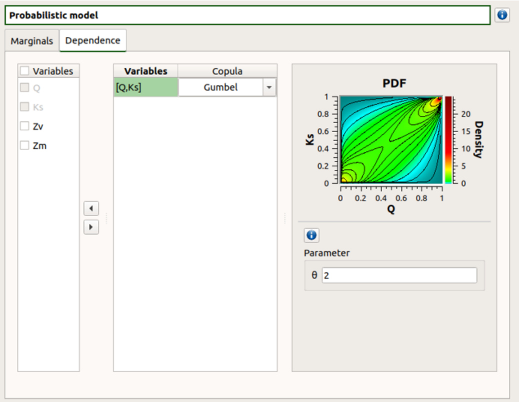
Asymptotic distribution of the first order Sobol' indices for the first variable.

PERSALYS, the graphical user interface of OpenTURNS

- Main goal : provide a graphical interface of OpenTURNS in the SALOME integration platform
- Features
  - Uncertainty quantification : definition of the probabilistic model (including dependence), distribution fitting (including copulas), central tendency, sensitivity analysis, probability estimate, meta-modeling (polynomial chaos, kriging), screening with Morris, optimization, design of experiments
  - Generic (not dedicated to a specific application)
  - GUI language : English, French
- Partners : EDF, Phiméca
- Licence : LGPL
- Schedule :
  - Since summer 2016, one EDF release per year
  - On the internet (free) : SALOME_EDF since 2018 on `https://www.salome-platform.org`

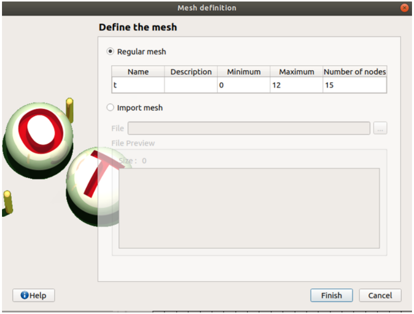
PERSALYS: define the dependence

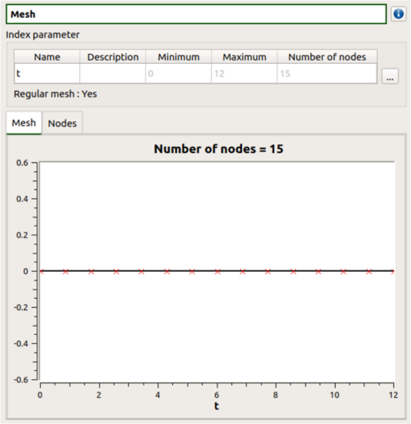
- Dependence is defined using copulas
- Define arbitrary groups of dependent variables
- Available copulas (same as in OT): gaussian, Ali-Mikhail-Haq, Clayton, Farlie-Gumbel-Morgenstern, Frank, Gumbel
- Dependence inference from a sample : Bayesian Information Criteria (BIC) or Kendall plot



PERSALYS: 1D fields

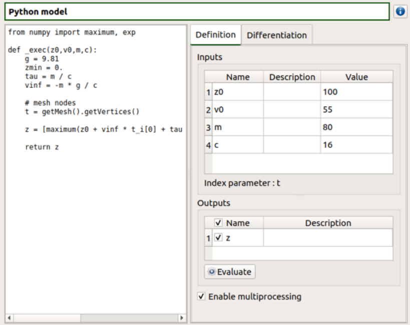
- Mesh definition and visualization
- Import from text or csv file

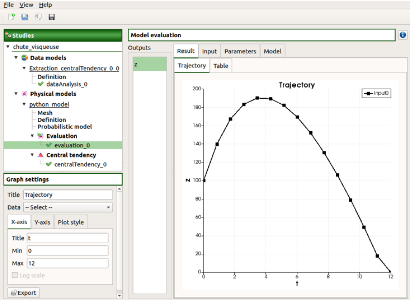




PERSALYS: 1D fields

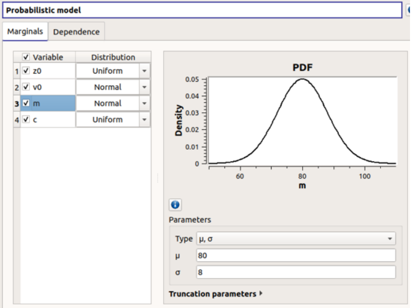
- Functional model definition and probabilistic model
- Python or symbolic

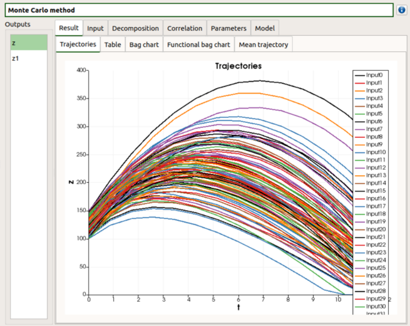




PERSALYS: 1D fields

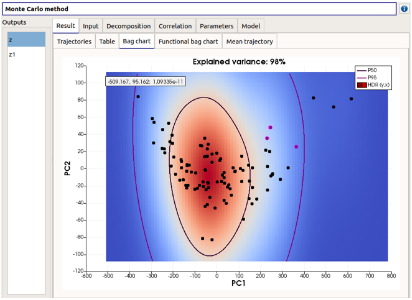
- Probabilistic model
- Uncertainty propagation with simple Monte-Carlo sampling

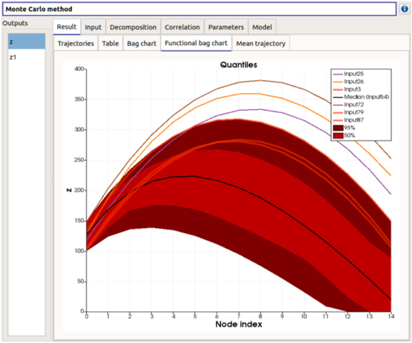




PERSALYS: 1D fields

- BagChart and Functional Bagchart (from Paraview) based on High Density Regions (Hyndman, 1996).
- To do this, Paraview uses a principal component analysis decomposition.
- Linked and interactive selections in the views.

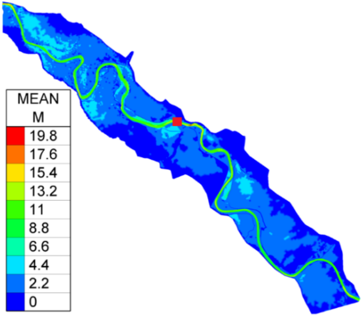




What's next ?

PERSALYS Roadmap :

- Calibration
- 2D Fields, 3D Fields
- In-Situ fields based on the MELISSA library (with INRIA): when we cannot store the whole sample in memory or on the hard drive, update the statistics (e.g. the mean, Sobol' indices) sequentially, with distributed computing.



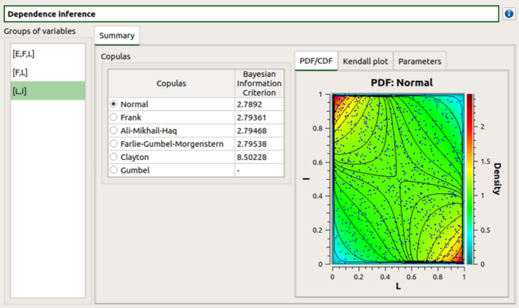
The end

Thanks !

Questions ?

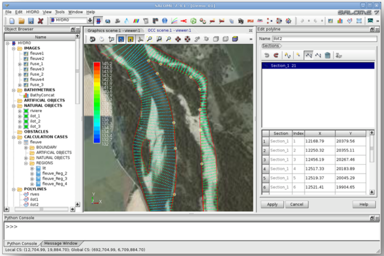
PERSALYS: estimate the parameters of the copulas

- Inference of the dependence of the multivariate sample
- Guided choice according to the BIC and Kendall plot



SALOME

- Integration platform for pre and post processing, and 2D/3D numerical simulation
- Features : geometry, mesh, distributed computing
- Visualization, data assimilation, uncertainty treatment
- Partners : EDF, CEA, Open Cascade
- Licence : LGPL
- Linux, Windows
- `www.salome-platform.org`



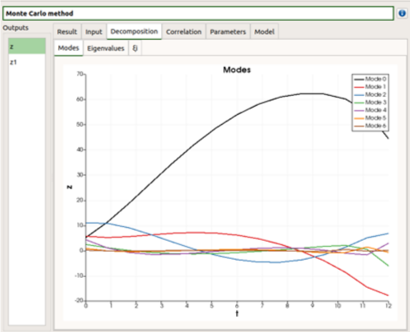
OpenTURNS: estimate Sobol' indices sequentially

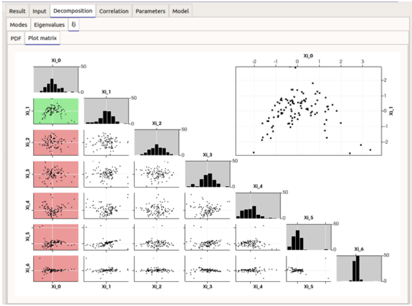
Part 2 : Estimate Sobol' sensitivity indices with an incremental algorithm.

- Let us denote by Φ_k^F (resp. Φ_k^T) the cumulated distribution function of the gaussian distribution of the first (resp. total) order sensitivity indice of the k-th input variable.
- We set $\alpha \in [0, 1]$ a quantile level and $\epsilon \in (0, 1]$ a quantile precision.
- The algorithms stops when, on all components, first and total order indices haved been estimated with enough precision.
  The precision is said to be sufficient if
  $$\Phi_k^F(1-\alpha) - \Phi_k^F(\alpha) \leq \epsilon$$
  and
  $$\Phi_k^T(1-\alpha) - \Phi_k^T(\alpha) \leq \epsilon$$
  for $k = 1, ..., n_X$.

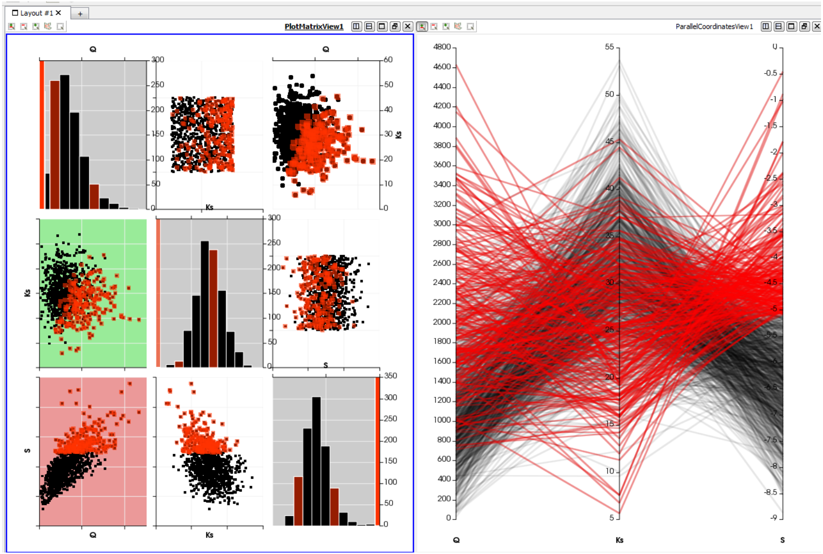
PERSALYS: 1D fields

- Karhunen Loeve decomposition
- Show modes, eigenvalues and projection coefficients

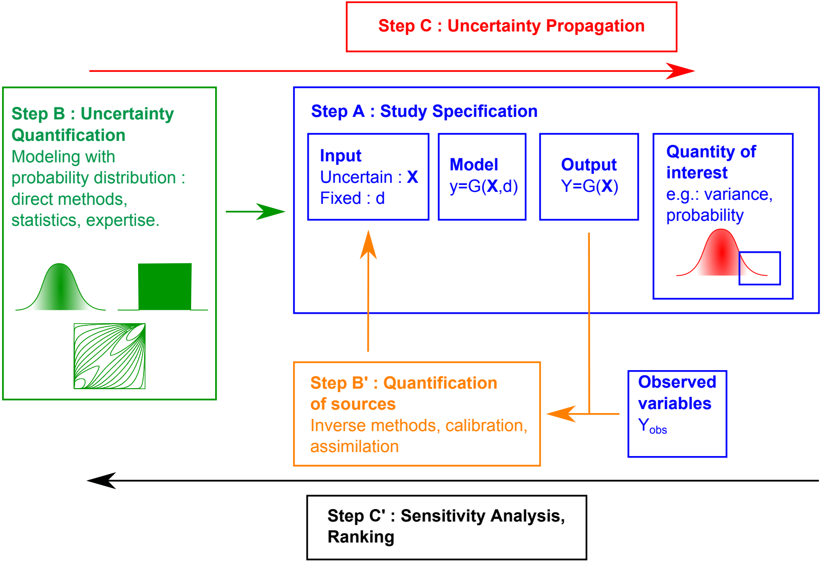




Interactive uncertainty visualization with Paraview



Methodology



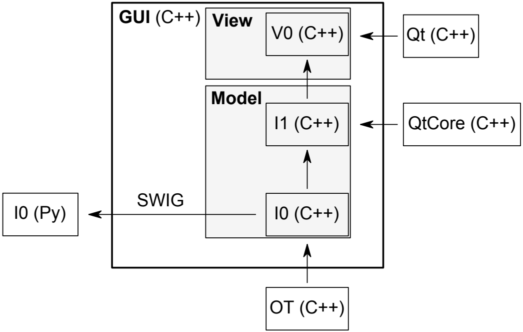
Software architecture

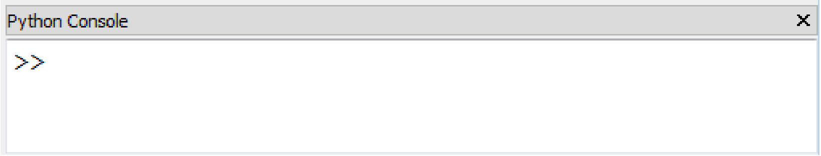
Two entry points:

- interactive,
- Python.

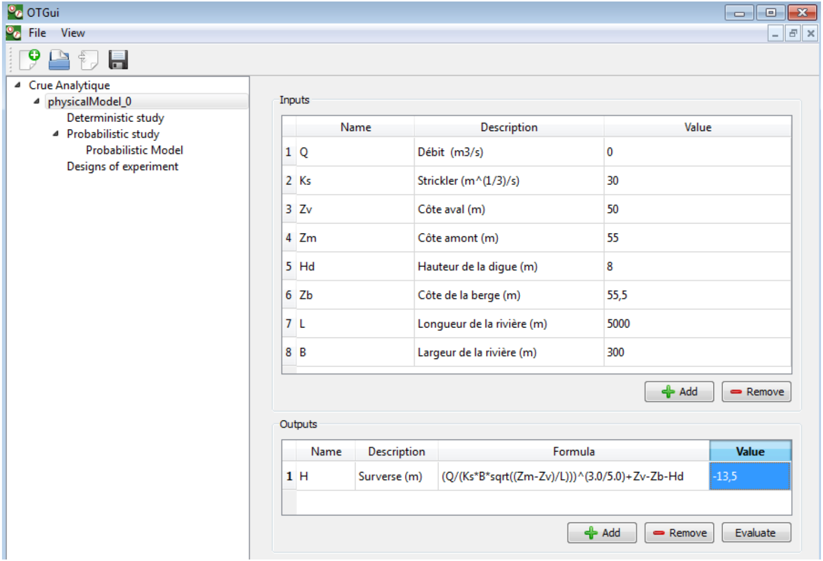
Advantages of the Python programming of the GUI:

- unit tests,
- going beyond the GUI

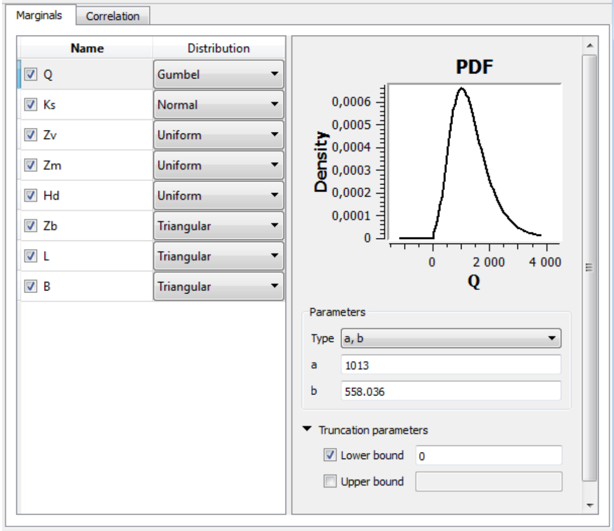




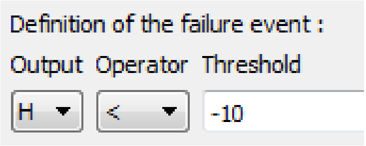
Symbolic physical model



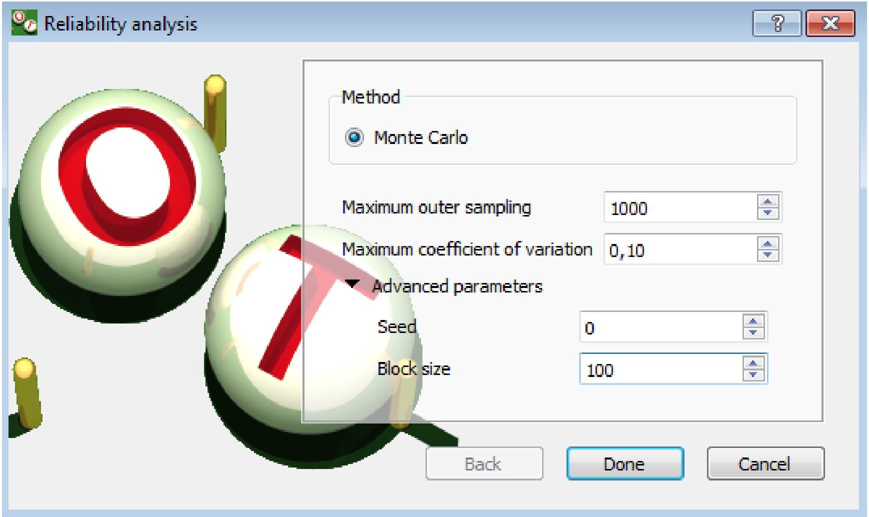
Probabilistic model



Limit state study : definition of the threshold



Limit state study : algorithm parameters



Limit state study : summary

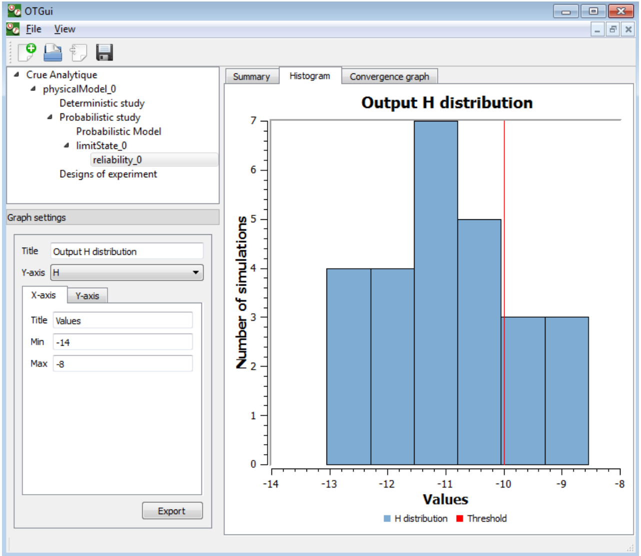
Summary | Histogram | Convergence graph

Output H

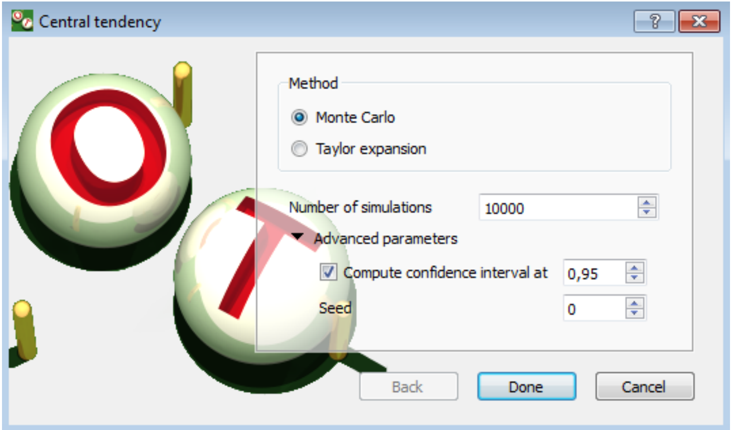
Number of simulations: 26

Estimate	Value	Confidence interval at 95%	
		Lower bound	Upper bound
Failure probability	0.807692	0.656203	0.959182
Coefficient of variation	0.0956949		

Limit state study : histogram



Central tendency : algorithm parameters



Central tendency : summary results

Moments estimate

Estimate	Value	Confidence interval at 95%	
		Lower bound	Upper bound
Mean	-11.0178	-11.0417	-10.9938
Standard deviation	1.22309	1.20637	1.24028
Skewness	0.20005		
Kurtosis	3.01907		
First quartile	-11.8721		
Third quartile	-10.2129		

Probability 0,50 **Quantile** -11,04288948

Central tendency : summary results

Result table | Summary | PDF/CDF | Box plots | Sca

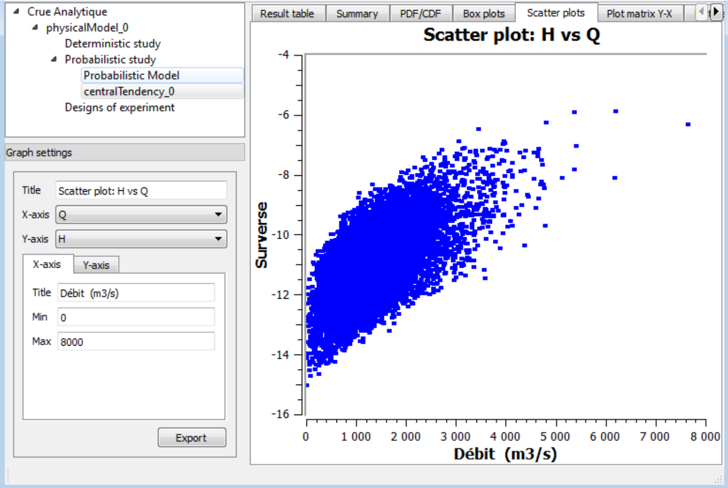
Output H

Number of simulations: 10000

Minimum and Maximum

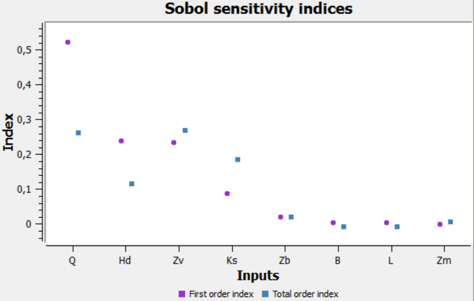
	Variable	Minimum	Maximum
Output	H	-15.0155	-5.88758
Inputs at extremum	Q	7.97827	6187.43
	Ks	27.132	25.5926
	Zv	49.1681	50.9071
	Zm	54.5469	55.3994
	Hd	8.76082	8.49391
	Zb	55.5436	55.4935
	L	4999.26	4997.37
	B	303.187	300.871

Central tendency : scatter plots



Sensitivity analysis : Sobol' indices

Result



Input	First order index	Total order index
Zv	0.2366	0.2707
Q	0.5246	⚠ 0.2646
Ks	0.08843	0.1881
Hd	0.2411	⚠ 0.1179
Zb	0.02115	0.02203
Zm	0.0002773	0.008043

Interactions -2.784 ⚠

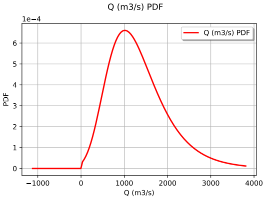
OpenTURNS: estimate the mean

See the Jupyter Notebook.

```python
from openturns.viewer import View
import openturns as ot
from math import sqrt

ot.RandomGenerator.SetSeed(0)

# 1. The function G
def functionCrue(X) :
    Q, Ks, Zv, Zm = X
    alpha = (Zm - Zv)/5.0e3
    H = (Q/(Ks*300.0*sqrt(alpha)))**(3.0/5.0)
    S = [H + Zv - (55.5 + 3.0)]
    return S

# Creation of the problem function
g = ot.PythonFunction(4, 1, functionCrue)
g = ot.MemoizeFunction(g)
```

OpenTURNS: estimate the mean

```
# 2. Random vector definition
myParamQ = ot.GumbelAB(1013., 558.)
Q = ot.ParametrizedDistribution(myParamQ)
otLOW = ot.TruncatedDistribution.LOWER
Q = ot.TruncatedDistribution(Q, 0, otLOW)
Ks = ot.Normal(30.0, 7.5)
Ks = ot.TruncatedDistribution(Ks, 0, otLOW)
Zv = ot.Uniform(49.0, 51.0)
Zm = ot.Uniform(54.0, 56.0)

# 3. View the PDF
Q.setDescription(["Q (m3/s)"])
View(Q.drawPDF()).show()
```



OpenTURNS: estimate the mean

```
# 4. Create the joint distribution function,
#    the output and the event.
X = ot.ComposedDistribution([Q, Ks, Zv, Zm])
Y = ot.RandomVector(g, ot.RandomVector(X))

# 5. Estimate expectation with simple Monte-Carlo
sampleSize = 10000
sampleX = X.getSample(sampleSize)
sampleY = g(sampleX)
sampleMean = sampleY.computeMean()
print("Mean=%f" % (sampleMean[0]))
```

Output:

```
Mean by MC =-5.937845
```

GUI : the demo

Demo time.

GUI : outline

- From scratch : 3 inputs, 2 outputs, sum, central dispersion study with default parameters
- Open axialStressedBeam-python.xml : central dispersion with sample size 1000, Threshold P(G<0) with CV=0.05
- Import crue-4vars-analytique.py : S.A. with sample size 1000, sort by size

UQ, the easy way

Main goal : make UQ easy to use

- classical user-friendly algorithms with a state-of-the-art implementation,
- default parameters of the algorithms whenever possible,
- an easy access to the HPC resources,
- an automated connection to the computer code.

Produce standard results :

- numerical results e.g. tables,
- classical graphics.

Overview (1/2)

Inputs from the user :

- Physical model : symbolic, Python code or SALOME component
- Probabilistic model : joint probability distribution function of the input.

Then :

- Central dispersion: estimates the central dispersion of the output Y (e.g. mean).
- Threshold probability: estimates the probability that the output exceeds a given threshold S.
- Sensitivity analysis: estimates the importance of the inputs to the variability of the output.

Overview (2/2)

Probabilistic modeling :

- Distribution fitting from a sample
- Dependence modeling (Gaussian copula)

Meta-modeling :

- Polynomial chaos (full or sparse)
- Kriging