Overview of OpenTURNS and its graphical user interface Persalys

J. Muré [1] M. Baudin [1] J. Pelamatti [1]
J. Schueller [2] A. Marion [2]

[1]EDF R&D. 6, quai Watier, 78401, Chatou Cedex - France, joseph.mure@edf.fr

[2]Phimeca Engineering. 18/20 boulevard de Reuilly, 75012 Paris - France, schueller@phimeca.com

May 22nd 2024, BEPU 2024, Lucca, Italy

Contents

OpenTURNS: www.openturns.org

OpenTURNS

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

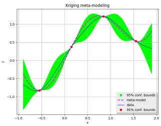
- Multivariate probabilistic modeling including dependence
- Numerical tools dedicated to the treatment of uncertainties
- Generic coupling to any type of physical model
- Open source, LGPL licensed, C++/Python library

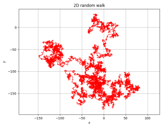
OpenTURNS: www.openturns.org

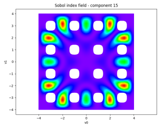
- Linux, Windows, macOS
- First release : 2007
- 5 full time developers
- Users $\approx$ 1000, mainly in France (1 078 000 Total Conda downloads)
- Project size : 800 classes, more than 6000 services

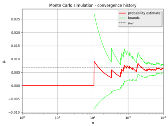
OpenTURNS: content

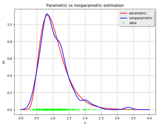
- Data analysis
  - Distribution fitting
  - Statistical tests
  - Estimate dependency and copulas
  - Estimate stochastic processes
- Probabilistic modeling
  - Dependence modeling
  - Univariate distributions
  - Multivariate distrbutions
  - Copulas
  - Processes
  - Covariance kernels
- Surrogate models
  - Linear regression
  - Polynomial chaos expansion
  - Gaussian process regression
  - Spectral methods
  - Low rank tensors
  - Fields metamodel
- Reliability, sensitivity
  - Sampling methods
  - Approximation methods
  - Sensitivity analysis
  - Design of experiments
- Calibration
  - Least squares calibration
  - Gaussian calibration
  - Bayesian calibration
- Numerical methods
  - Optimization
  - Integration
  - Least squares
  - Meshing
  - Coupling with external codes







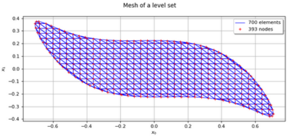




OpenTURNS: documentation

LevelSetMesher

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



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.

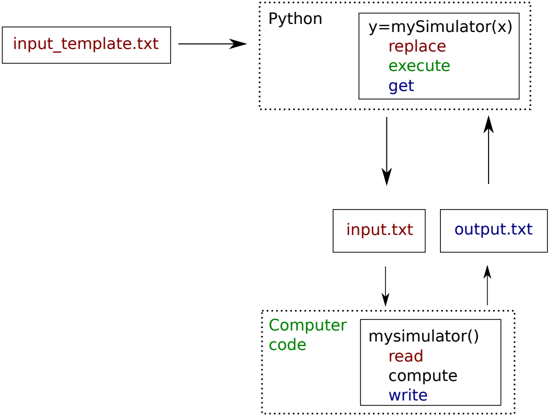
- <u>Content</u>:
  - Programming interface (API)
  - Examples
  - Theory
- *All* classes and methods are documented, partly automatically.
- Examples are automatically tested at *each* update of the code and outputs are checked.

OpenTURNS: practical use

- C++ and Python interface
- Parallel computations with shared memory (TBB)
- Optimized linear algebra with LAPACK and BLAS
- Possibility to interface with a computation cluster
- Focused towards handling numerical data
- Installation through conda, pip, packages for various Linux distros and source code
-
```python
import numpy as np
import openturns as ot
from openturns.viewer import View
ot.ResourceMap.SetAsString("Contour-DefaultColorMap", "viridis")
ot.ResourceMap.SetAsBool("Contour-DefaultIsFilled", True)
ot.ResourceMap.SetAsUnsignedInteger("Contour-DefaultLevelsNumber", 15)
```

Coupling OpenTURNS with computer codes

OpenTURNS provides a text file exchange based interface in order to perform analyses on complex computer codes

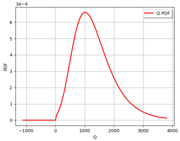


- Replaces the need for input/output text parsers
- Wraps a simulation code under the form of a standard python function
- Allows to interface OpenTURNS with a cluster
- otwrapy: interfacing tool to allow easy parallelization

Probabilistic modeling

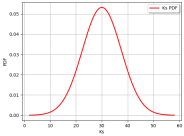
Random variables distributions:

Q: Gumbel(scale=558, mode=1013)>0



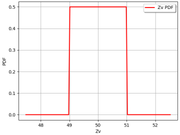

```
d = ot.Gumbel(558.0, 1013.0)
tr = ot.TruncatedDistribution.LOWER
Q = ot.TruncatedDistribution(d, 0.0, tr)
```

Ks: Normal(mean=30, std=7.5)>0

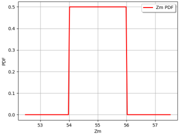



```
d = ot.Normal(30.,7.5)
tr = ot.TruncatedDistribution.LOWER
Ks = ot.TruncatedDistribution(d, 0.0, tr)
```

Zv: Uniform(min=49, max=51)



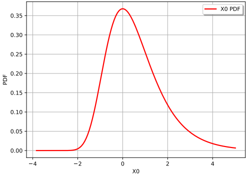
Zm: Uniform(min=54, max=56)

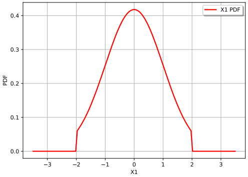


Probabilistic modeling

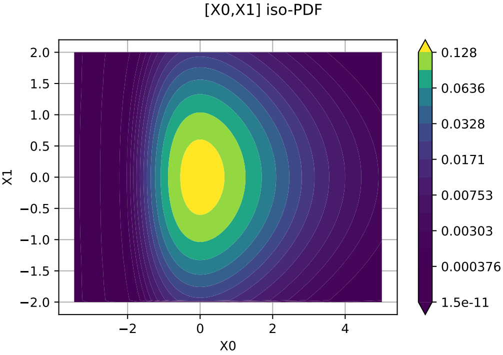
- We consider a 2-dimensional distribution with the following marginals:
  - Gumbel(min = -1, max = 1)
  - Truncated normal (mean = 0, std = 1, min = -2, max = 2)

Marginals

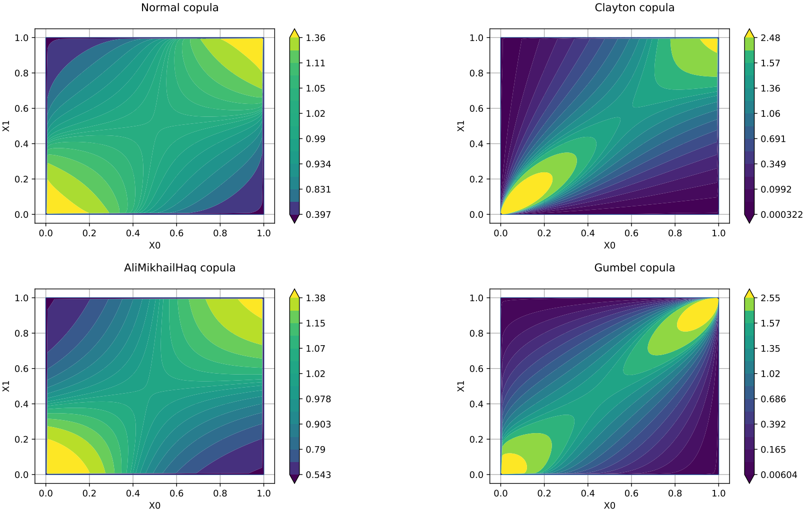




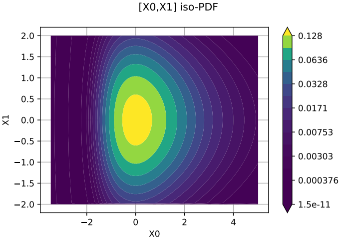
Joint distributions

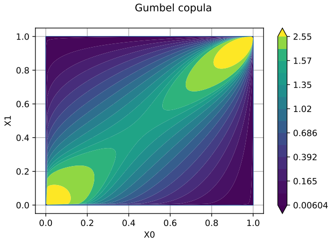


Beyond independent marginals: Copulas

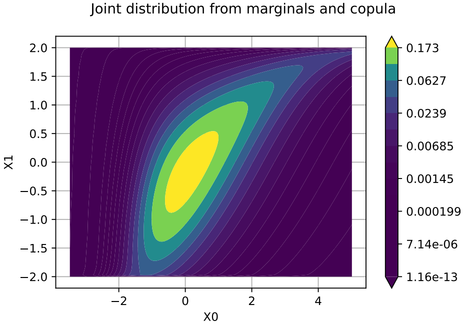


Composing marginal distributions and copulas



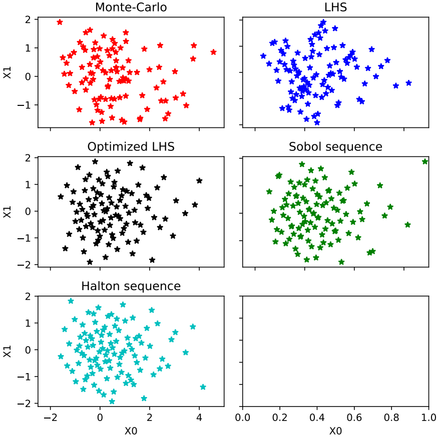


We obtain:




```
marg1 = ot.Gumbel(1.0, 0.0)
marg2 = ot.TruncatedNormal(0.0, 1.0, -2.0, 2.0)
copula = ot.GumbelCopula()
joint = ot.JointDistribution([marg1, marg2],
     copula)
graph = joint.drawPDF()
title = "Joint distribution "
title += "from marginals and copula"
graph.setTitle(title)
```

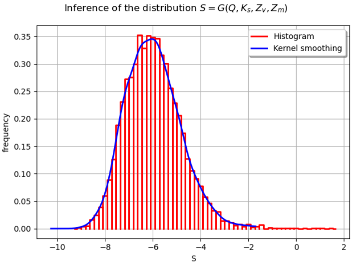
Design of experiments




```
dim = 2
X=[ot.Gumbel(),ot.TruncatedNormal(0,1,-2,2)]
dist = ot.JointDistribution(X)
bounds = dist.getRange()
sampleSize = 100

sample1 = dist.getSample(sampleSize)

experiment = ot.LHSExperiment(dist,
  sampleSize, False, False)
sample2 = experiment.generate()

lhs = ot.LHSExperiment(dist, sampleSize)
lhs.setAlwaysShuffle(True) # randomized
space_filling = ot.SpaceFillingC2()
temperatureProfile = ot.GeometricProfile
      (10.0, 0.95, 1000)
algo = ot.SimulatedAnnealingLHS(lhs,
 space_filling, temperatureProfile)
sample3 = algo.generate()

sequence = ot.SobolSequence(dim) # or Halton
experiment = ot.LowDiscrepancyExperiment(
  sequence, dist, sampleSize, False)
sample4 = experiment.generate()
```

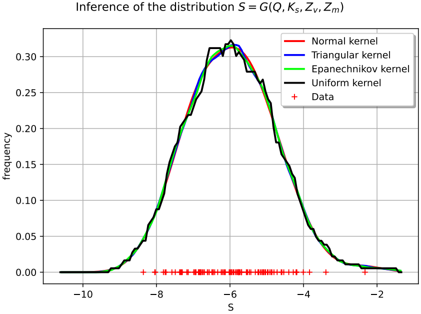
Monte-Carlo sampling

- The input distribution and relative output value are evaluated 10000 times
- The output distribution can be infered as a parametric function or through histogram or kernel smoothing methods




```
Distribution = ot.JointDistribution([Q,Ks,Zv,Zm])

#Python model
def floodFunction(X):
    Q, Ks, Zv, Zm = X
    alpha = (Zm - Zv)/5.0e3
    H = (Q/(300.0*Ks*np.sqrt(alpha)))**0.6
    S = [H + Zv - 58.5]
    return S

fun = ot.PythonFunction(4,1,floodFunction)

#We define the output as a random vector
inputVector = ot.RandomVector(Distribution)
outputVector = ot.CompositeRandomVector(fun,
     inputVector)

#We sample and infere the output distribution
size = 10000
sampleY = outputVector.getSample(size)
hist = ot.HistogramFactory().build(sampleY)
graph = hist.drawPDF()
loiKS = ot.KernelSmoothing().build(sampleY)
graph2 = loiKS.drawPDF()
```

Distribution and dependence inference



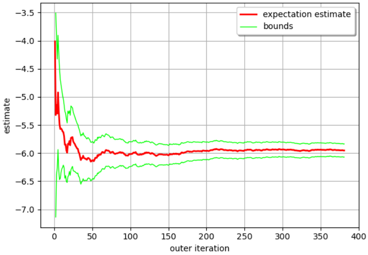

```
size = 100
sampleY = outputVector.getSample(
     size)
graph = ot.KernelSmoothing(ot.
     Normal()).build(sampleY).
     drawPDF()
loiKS = ot.KernelSmoothing(ot.
     Triangular()).build(sampleY)
graph2 = loiKS.drawPDF()
graph.add(graph2)
loiKS = ot.KernelSmoothing(ot.
     Epanechnikov()).build(sampleY)
graph2 = loiKS.drawPDF()
graph.add(graph2)
loiKS = ot.KernelSmoothing(ot.
     Uniform()).build(sampleY)
graph2 = loiKS.drawPDF()
```

- Parametric ($1d - Nd$) distribution inference
- Non-parametric ($1d - Nd$) distribution inference
- Parametric copula inference
- Non-parametric copula inference (Bernstein copula)
- Resampling w.r.t. inferred distributions

Iterative Monte-Carlo: Central tendency anaysis

- The expected value and associated standard deviation are computed iteratively
- Different stopping criteria can be used
- Batch computation can be used

Expectation convergence graph at level 0.95



$$\widehat{m_y} = \frac{1}{N}\sum_{1}^{N} G(\mathbf{X}_i)$$

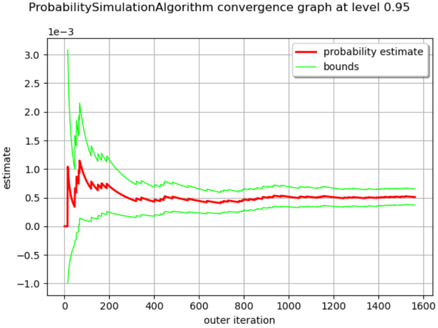
$$\widehat{\sigma_y} = \sqrt{\frac{1}{N}\sum_{1}^{N}(G(\mathbf{X}_i) - \hat{m}_y)^2}$$

$$\widehat{\sigma_{m_y}} = \widehat{\sigma_y}/\sqrt{N}$$

```
algo = ot.ExpectationSimulationAlgorithm(
     outputVector)
algo.setMaximumOuterSampling(100000)
algo.setBlockSize(1)
algo.setCoefficientOfVariationCriterionType("MAX")
algo.setMaximumCoefficientOfVariation(0.01)
algo.run()
graph = algo.drawExpectationConvergence()
```

Iterative Monte-Carlo: Reliability analysis

- We now consider the probability of flooding: $(P(S > 0.))$
- Same as before, but the function $\mathbb{I}_{G(\mathbf{X}_i)>0}$ is considered



$$
\begin{aligned}
\widehat{p_y} &= \frac{1}{N}\sum_{1}^{N} \mathbb{I}_{G(\mathbf{X}_i)>0} \\
\widehat{\sigma} &= \sqrt{\frac{1}{N}\sum_{1}^{N} (\mathbb{I}_{G(\mathbf{X}_i)>0} - \hat{p}_y)^2} \\
\widehat{\sigma_{p_y}} &= \widehat{\sigma}/\sqrt{N}
\end{aligned}
$$

```
eventF = ot.ThresholdEvent(outputVector, ot.
     GreaterOrEqual(), 0.0)
exp = ot.MonteCarloExperiment()
algo = ot.ProbabilitySimulationAlgorithm(
     eventF, exp)
algo.setMaximumOuterSampling(100000)
algo.setMaximumCoefficientOfVariation(0.01)
algo.setBlockSize(10)
algo.run()
```

FORM/SORM reliability analysis

- We estimate the probability of flooding through FORM/SORM procedures
- MC estimation requires $\simeq$ 1500 function evaluations
- FORM and SORM only use $\simeq$ 150
- Estimated probability:
  - MC: 5.09999999999998 1e-4
  - FORM: 5.340929030055227 1e-4
  - SORM: 6.793780433482759 1e-4

```
#FORM
OptAlgo = ot.Cobyla()
startingPoint = Distribution.getMean()
algoFORM = ot.FORM(OptAlgo, eventF,
startingPoint)
algoFORM.run()

#SORM
OptAlgo = ot.Cobyla()
startingPoint = Distribution.getMean()
algoSORM = ot.SORM(OptAlgo, eventF,
startingPoint)
algoSORM.run()
```

Different types and parameterizations of finite difference gradient computation are available

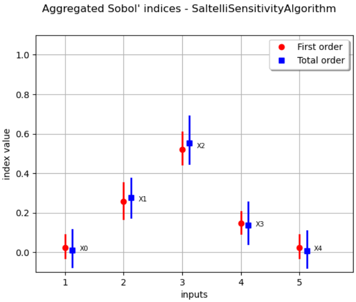
Also:

- Directional sampling
- Importance sampling (FORM-IS, NAIS, Adaptive IS-Cross-entropy)
- Subset sampling

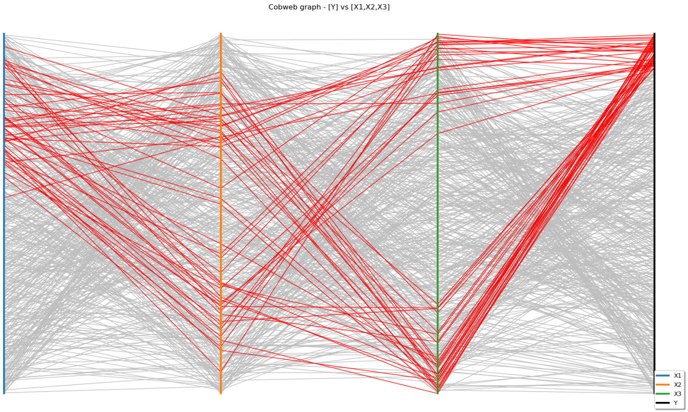
Sensitivity analysis

Various sensitivity analysis methods are available

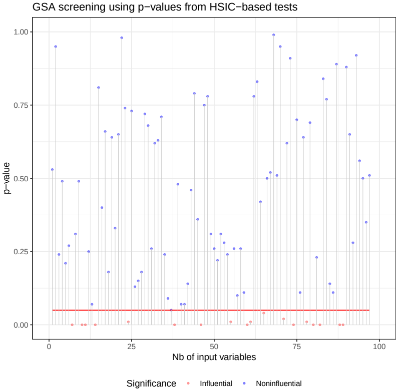
- Graphical analysis
  - Pair plots
  - Parallel coordinates plots
  - Cross-cuts
- Quantitative indices
  - SRC, SRRC, PRC, PRCC
  - Sobol' indices (multiple estimators)
  - FAST indices
  - ANCOVA indices
  - HSIC indices
  - Shapley Indices (available as a module)



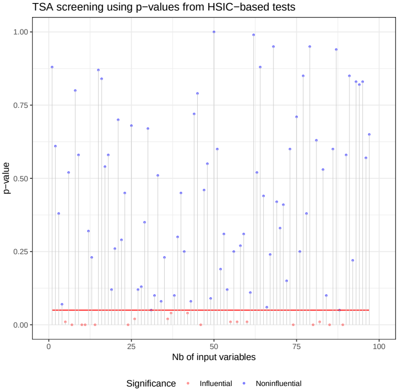
Sensitivity analysis: Parallel coordinates plot



Sensitivity analysis: HSIC indices and associated p-values



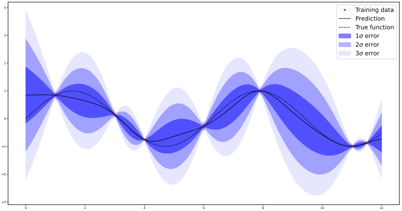
GSA-oriented screening.



TSA-oriented screening.

Surrogate modeling: Gaussian process regression

- Different surrogate modeling methods are available
  - Kriging
  - Polynomial chaos expansion
  - Linear regression & step-wise basis selection
  - Low rank tensors
  - automatic validation tools



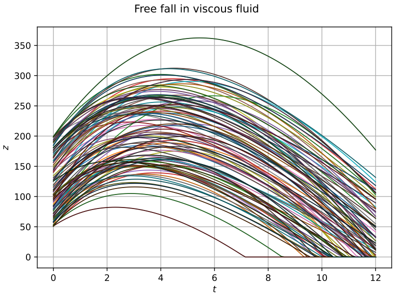
- Gaussian process regression
  - Different types of covariance functions and function basis can be used
  - User-defined options are also available
  - MLE optimization can be parameterized
  - Large number of optimization algorithms available

```
inputSample = Distribution.getSample(100)
outputSample = fun(inputSample)

dimension = 4
basis = ot.ConstantBasisFactory(dimension).
     build()
covarianceModel = ot.SquaredExponential()

algo = ot.KrigingAlgorithm(inputSample,
     outputSample, covarianceModel, basis)

algo.run()
result = algo.getResult()
KrigingMM = result.getMetaModel()
```

Optimization

- OpenTURNS provides an interface with several optimization libraries
  - Bonmin
  - NLopt
  - dlib
  - pagmo
- Ad-hoc implementation of the COBYLA algorithm
- Constrained and unconstrained optimization
- Gradient-based and derivative-free optimizaiton
- Bounded and unbounded optimization
- Single and multi-objective optimization
- Multi-start wrapper

Field function modeling

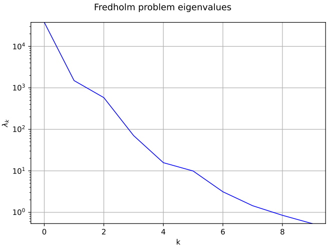



```python
def free_fall(X):
    g  = 9.81
    z0,v0,m,c = X
    tau=m/c
    vinf=-m*g/c
    t = np.array(mesh.getVertices().asPoint())
    z=z0+vinf*t+tau*(v0-vinf)*(1-np.exp(-t/tau))
    z=np.maximum(z,0.0)
    return ot.Field(mesh, z.reshape(-1, 1))

tmin=0.
tmax=12.
gridsize=100
mesh = ot.IntervalMesher([gridsize-1]).build(
ot.Interval(tmin, tmax))

alti = ot.PythonPointToFieldFunction(4, mesh,  1,
      free_fall)

distZ0 = ot.Uniform(50.0, 200.0)
distV0 = ot.Normal(55.0, 10.0)
distM = ot.Normal(80.0, 8.0)
distC = ot.Uniform(0.0, 30.0)
distX = ot.JointDistribution([distZ0, distV0,
 distM, distC])

size = 100
inputSample = distX.getSample(size)
outputField = alti(inputSample)
```

Dimension reduction: Karhunen-Loeve decomposition

- We wish to reduce the dimension of the problem from a infinite dimensional output to a finite dimensional one
- We can perform a Karhunen-Loeve decomposition with a finite truncature
- This requires to solve a Fredholm's problem in order to identify the eigenfunctions and associated eigenvalues of the considered process

$$Y(\omega, \underline{t}) = \sum_{k=1}^{\infty} \sqrt{\lambda_k} \xi_k(\omega) \underline{\varphi}_k(\underline{t}) \rightarrow \tilde{Y}(\omega, \underline{t}) = \sum_{k=1}^{p} \sqrt{\lambda_k} \xi_k(\omega) \underline{\varphi}_k(\underline{t})$$

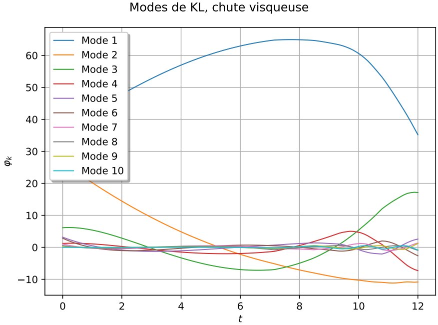



```
meanField = outputField.computeMean()
meanFunction = ot.P1LagrangeEvaluation(
 meanField)
trend = ot.TrendTransform(meanFunction, mesh
     )
invTrend = trend.getInverse()
outputFieldCentered = invTrend(outputField)

truncThreshold = 1.0e-5
algo = ot.KarhunenLoeveSVDAlgorithm(
 outputFieldCentered, truncThreshold)
algo.run()
KLResult = algo.getResult()

eigenValues = KLResult.getEigenvalues()
```

Dimension reduction: Karhunen-Loeve decomposition

$$\tilde{Y}(\omega, \underline{t}) = \sum_{k=1}^{p} \sqrt{\lambda_k}\xi_k(\omega)\underline{\varphi}_k(\underline{t})$$

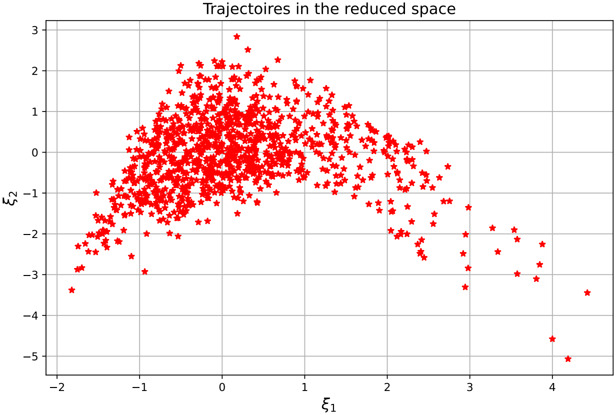
Main modes:




```
scaledModes =
 KLResult.getScaledModesAsProcessSample()
graph = scaledModes.drawMarginal(0)
graph.setTitle('Modes de KL, chute visqueuse
     ')
graph.setXTitle(r'$t$')
graph.setYTitle(r'$\varphi_k$')
leg = ot.Description([ 'Mode '+str(i +1) for
  i in range(eigenValues.getDimension()) ])
graph.setLegends(leg)
graph.setLegendPosition('topleft')
view=View(graph)
```

Dimension reduction: Karhunen-Loeve decomposition

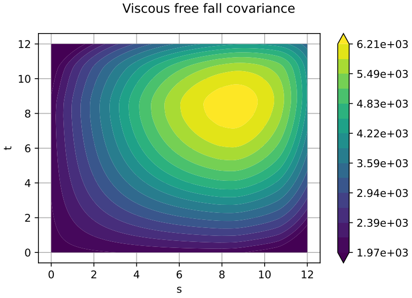
We only consider the first 2 terms of the decomposition:

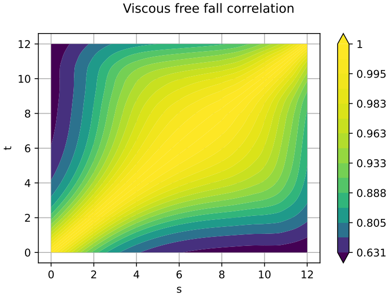



```
projectionFunction = ot.KarhunenLoeveProjection(KLResult)
sampleKsi = projectionFunction(outputFieldCentered)
sampleKsi = sampleKsi[:,:2]
```

Field function analysis

We center the trajectories with respect to the mean field:






```
cov = KLResult.getCovarianceModel()

# As a covariance function
isStationary = False
asCorrelation = False
graph = cov.draw(0, 0, tmin, tmax, 128, isStationary, asCorrelation)

# As a correlation function
asCorrelation = True
graph = cov.draw(0, 0, tmin, tmax, 128, isStationary, asCorrelation)
```

Contents

Project overview

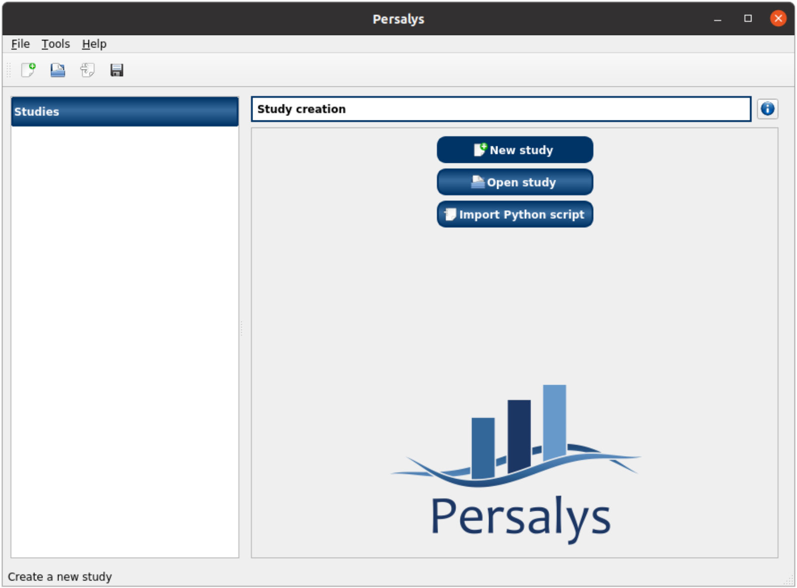
- Partnership between EDF and Phimeca since 2015
  - Developed in C++ using Qt
  - Aiming at maximizing the use of OpenTURNS - through a dedicated GUI - for engineers/researchers without a strong coding experience
  - As easy to use as possible while providing the user with help and guidelines
  - Benefit from the advanced visualization capability of Paraview

- Features:
  - Uncertainty quantification:
  - Probabilistic model definition
  - Distribution fitting
  - Probability estimate
  - Metamodeling
  - Screening
  - Optimization
  - Design of experiments
  - As generic as possible
  - Allows for a wide variety of models
  - Can be coupled to external code
  - GUI language in both English and French
- LGPL license
- Two releases per year, follows OpenTURNS development
- Available for free on demand at `https://persalys.fr`

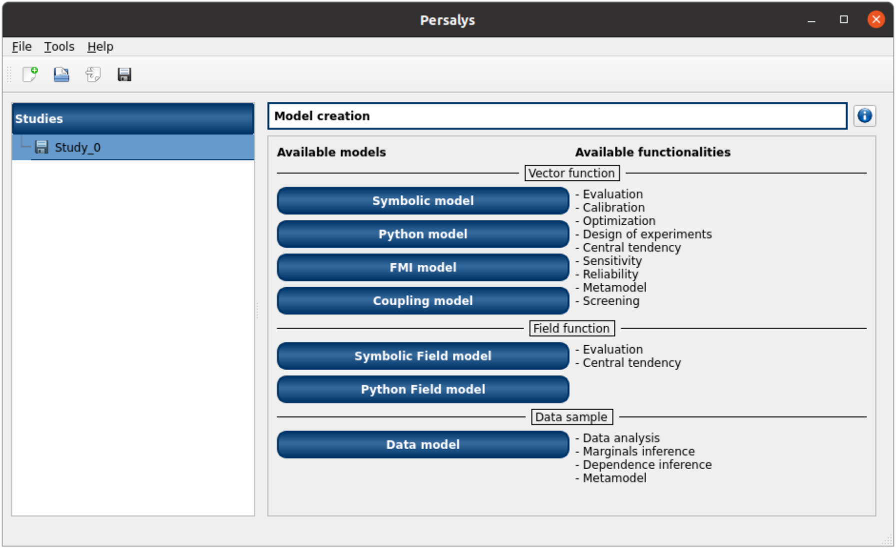
Persalys installation

- Github: sources
- You can request executables at `https://persalys.fr/obtenir.php?la=en`
- Depending on your OS
  - Linux → .AppImage (600 Mo)
  - Windows → .exe will create a shortcut on your Desktop (program is 1.45 Go)
- Also distributed by Debian-based GNU/Linux distributions (e.g. Debian, Ubuntu...)

Open Persalys and click on “New study”



Create a study



Definition/Evaluation

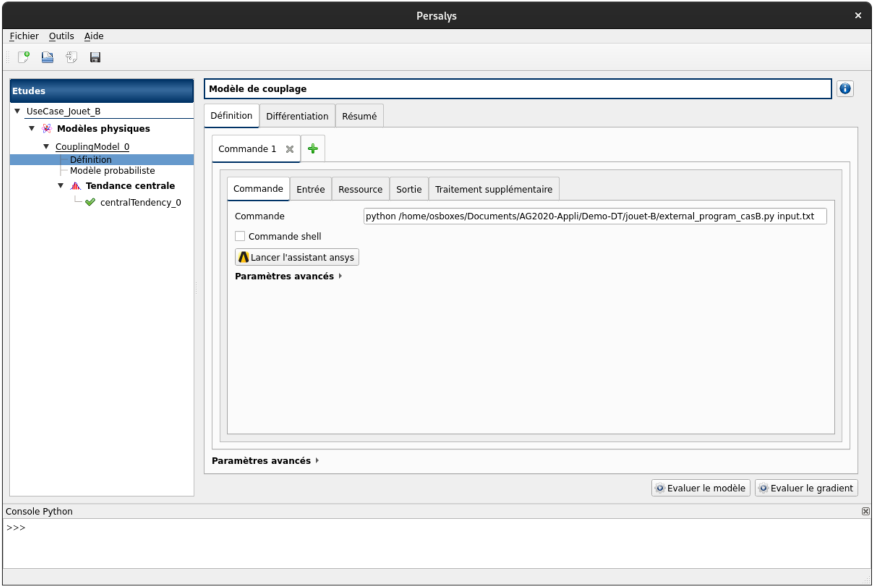
Models are viewed as a “black box” with inputs, outputs and a transfer function (TF). Persalys supports two model categories:

- vector to vector ($X_i \to Y_i$, emphasized here)
- vector to 1D field ($X_i \to Y_i(t)$)

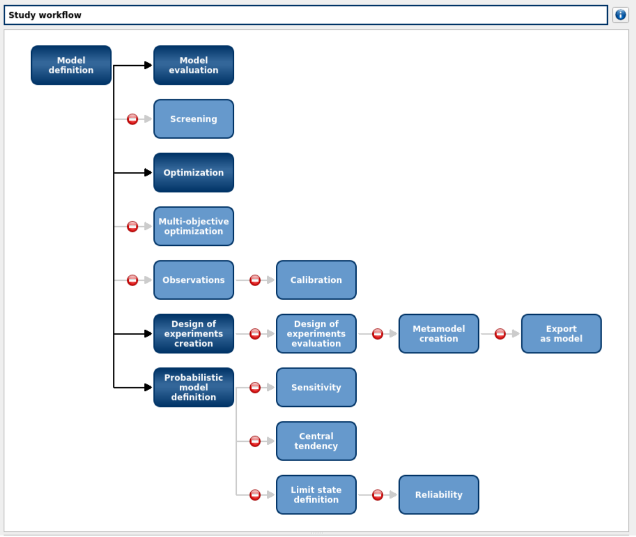
Vector to vector models can be of the following type:

- Symbolic, TF is a mathematical formula
- Python, TF is a Python function
- FMI, TF is provided by an FMU model
- Coupling, TF is an executable command which reads/writes input/output files

Coupling model definition



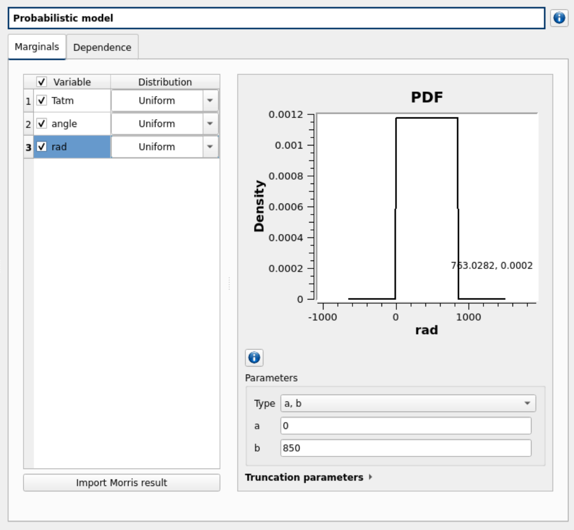
Study workflow



Blocks become available as study content grows and prerequisites are fulfilled.

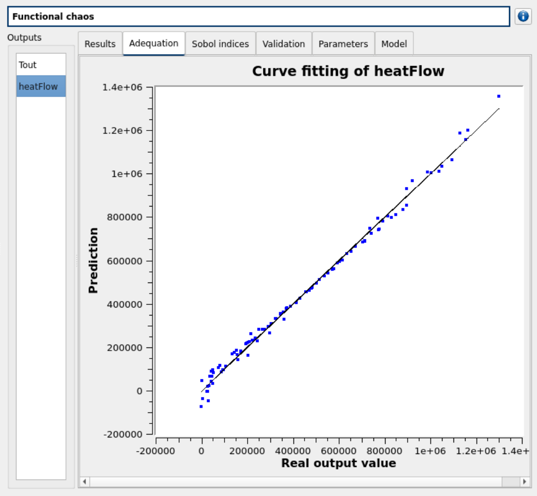
Probabilistic models

Each input variable can be associated to a distribution.
Dependencies between variables are specified as copulas.



Metamodel (surrogate model) creation

Using an evaluated design of experiments, the user can build a surrogate model (linear regression, functional chaos or Gaussian process regression). Validation tests are run to check the approximation being made.



OpenTURNS resources

- Website and documentation: `www.openturns.org`
- GitHub: `https://github.com/openturns/openturns`
- Forum: `https://openturns.discourse.group`

Persalys resources

- Website and documentation: `https://persalys.fr/?la=en`
- Forum: `https://persalys.discourse.group`