"Benchmark" of integrated solutions for uncertainty quantification

Quantifying uncertainty makes it easier

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Problématique

The strategy for encouraging the use of uncertainty quantification at the DAM is based on three pillars:

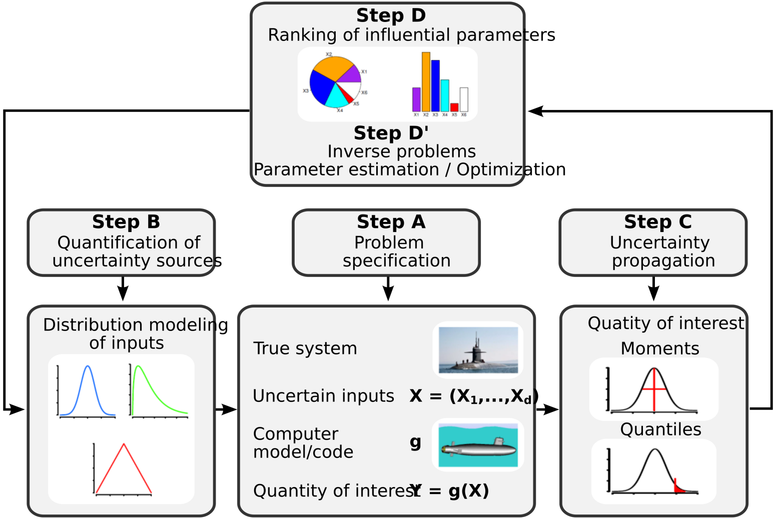
1. Training in these methods $\rightarrow$ internal DAM training.
2. Identifying "experts" $\rightarrow$ the role of my laboratory.
3. Highlight of asoftware for "simple" problems $\rightarrow$ Choise of Persalys in 2021.

Question :

What software tools can be made available to DAM units for simple uncertainty quantification studies?

- This presentation takes the choice made in 2021 as a starting point and questions this choice on the basis of 3 new examples.

Uncertainty quantification method



The user

Needs

- Design of multiphysics systems.
- Interface with complex computer codes.

Knowledge of the use

- The basics of statistics.
- The basics of the ABCD method.
- A very advanced understanding of the problem to be solved.

Outline

Problem

Softwares

Performances

Outline

Problem

Softwares

Performances

Finding the best software for uncertainty quantification

An uncertainty quantification aproach

Inputs / Outputs

- Inputs : 2 test cases.
  - a drone flying
  - Hydrogen's equation of state
- Outputs
  - Global sensity analysis
  - Surrogate models (not just linear regression)
  - Optimisation (option for multi-objective optimization)

Conditions to be evaluated

- Available on Linux and Windows, with documentation.
- Free and able to run the computation on the user's computer (to protect the user's data).
- (CEA condition) Installation should be possible offline (in less than 2 hours).

How the softwares are evaluated

Criteria or multi-objective

- User Interface
- Methods available
- Software's ergonomy

Important things we have assessed without drawing any conclusions

- Sensitivity indices computation
- Surrogate models computation
- Optimization performances

Outline

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Candidats

Name	Main Developpers	HCI	Based on	Reference
Lagun	Safran IFPEN, FR	Point and click		https://gitlab.com/drti/lagun
UQpy	SURG (M. Shields), US			uppyproject.readthedoc.io/en/latest/
UQLab	ETH Zurich, CH			www.uqlab.com/
PyApprox	Sandia NL, US			sandialabs.github.io/pyapprox/index.html
Cossan	Univ. of Liverpool, UK	Point and click		www.cossan.co.uk/software/open-cossan-e
OpenTURNS	Airbus EDF IMACS ONERA Phymeca, FR			openturns.github.io/www/index.html
Persalys	EDF Phymeca FR	Point and click		persalys.fr/
UQTk	Sandia NL, US			www.sandia.gov/uqtoolkit/
URANIE	CEA, FR			sourceforge.net/projets/uranie/
SmartUQ	SmartUQ, US	Point and click		www.smartuq.com
DAKOTA	Sandia NL, US	Point and		dakota.sandia.gov/

Softwares

Small presentation of the 3 softwares

The evaluated softwares

Dakota	Persalys	Lagun
Sandia National Lab 1997	Phymeca, EDF $\sim$ 2019	Safran, IFPEN 2019

Persalys

Parameters

- V 14.1 (Not the most recent, but the most recent at the time of the study)

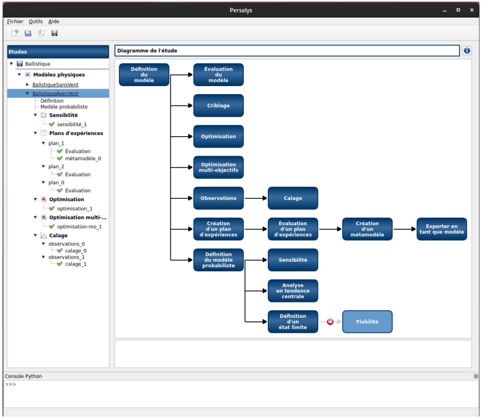
Features

- Design of Experiment
- Surrogate model
- Global sensitivity analysis
- Optimization (simple and multi-objective)
- Calibration

Problem

- Relatively slow for the RHEL installation that I use on a daily basis (no impact on my laptop opensource red hat).

Persalys



Let see

LAGUN

Parameters

- V 1.0.0

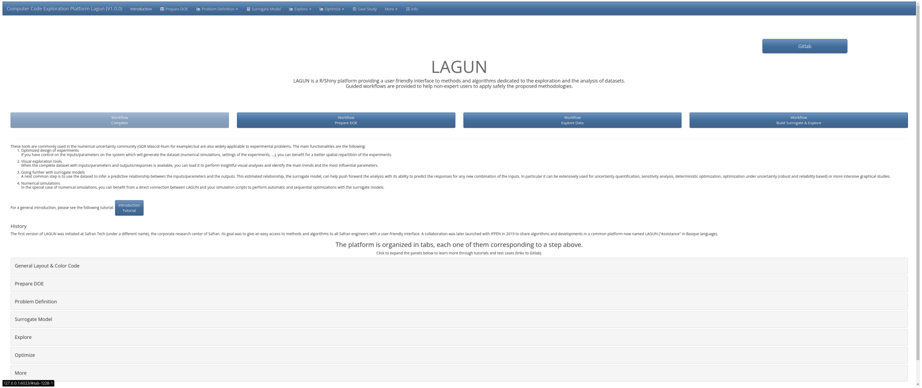
Features

- Design of Experiment
- Surrogate model
- Global sensitivity analysis
- Optimization (simple and multi-objective)

Problem

- I was not able to use the simulator mode

LAGUN

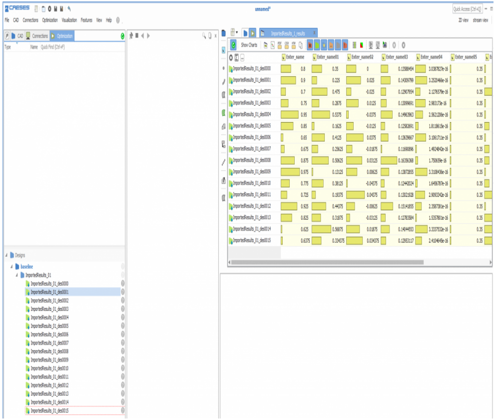


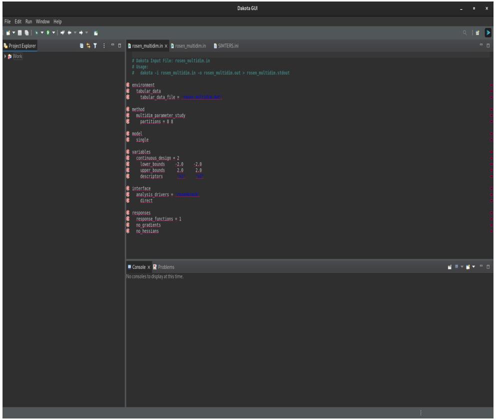
Let see

Why I will not use DAKOTA

Explore and predict with confidence.

- Too hard to install
- Graph are very poor
- Old school for french engineers





Test Cases

How we plan to use the softwares

1D drone ballistic trajectory

Newton's laws for drone ballistic

- Drone without engine with drag and leaft
- Simple very fast simulator

Random wind

Target

1D drone ballistic trajectory

Technical details of the problem

- 4 inputs of the code + 3 parameters + 1 random variable
- Code in Python and R
- Maximum 80 code's calls

Goals

- Global sensitivity analysis
- Calibration of the code
- Optimization of the parameters for maximum distance

Equation of State Hydrogen

Compute the quantum two-body problem

- Equation between ρ, T and Z, P, E, F of hydrogen.
- Very large dataset (90000 points)

Goals

- Global sensitivity analysis and data analysis
- Surrogate model

Reason of this example

- Test the limits of softwares
- Tested software on a well-known example

This example did not work for more than 1000 points

Equation of State Hydrogen

Compute the quantum two-body problem

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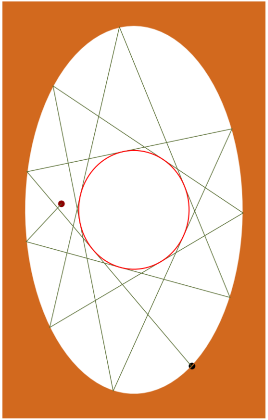
Elliptical billiard table

Technical details of the problem

- 4 inputs of the code + 2 parameters
- Code in
- Maximum 1000 code's calls

Goals

- Global sensitivity analysis
- Calibration of the code
- Optimization 2 inputs for surface optimisation



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Surrogate models- Linear regression

R^2 for the same training set

	Persalys	Lagun
Drone Y_1	0.80	0.76
Drone Y_2	0.93	0.92
Billard Y_0	2.210^{-16}	??
Billard Y_2	0.34	??

Persalys : Linear Model, order 1 without interactions

Lagun : Lasso Model

- The best linear model, order 2 with interactions, gives much better results (ex drone Y_1 : 0.95 and Y_2 : 0.99)

Surrogate models- Kriging

Q^2 for the same training set

	Persalys	Lagun
Drone Y_1	0.94	0.96
Drone Y_2	0.99	0.99
Billard Y_0	-0.00037	??
Billard Y_2	0.92	??

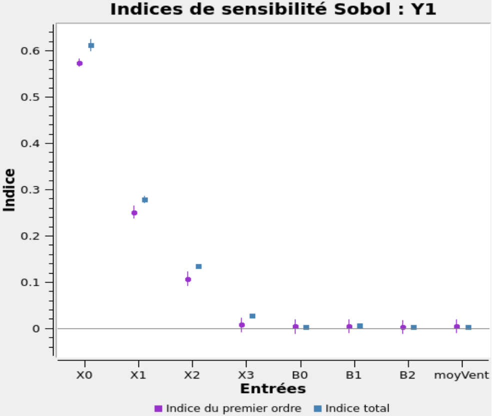
Persalys : Krigin Model with constant trend Matèrn $\frac{5}{2}$ kernel
Lagun : Kriging Model with constant trend (kernel seems to be an optimization between 4 options)

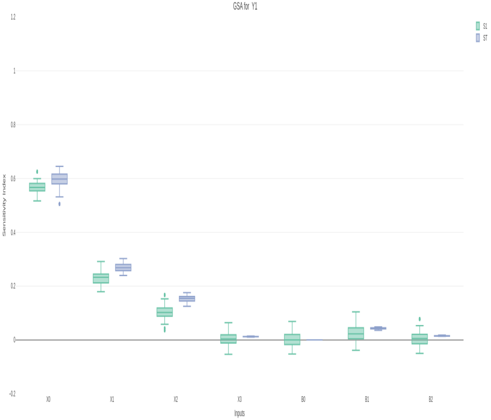
- For Persalys I have test all possible model and takes the one that gives the best performances in Q^2.

Global sensitivity analysis

The GSA for both softwares solutions are based on Sobol indices on surrogates.

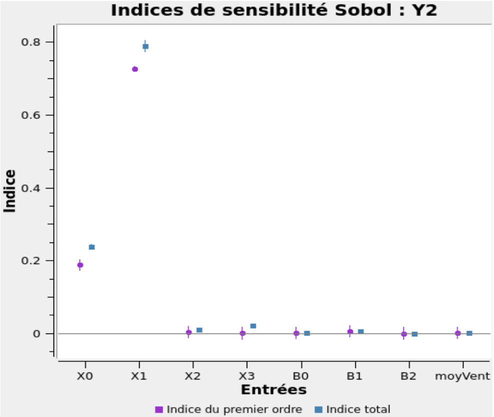
Differences will therefore appear in the results due to the metamodel. In this study we did not attempt to evaluate the computation of the indices.

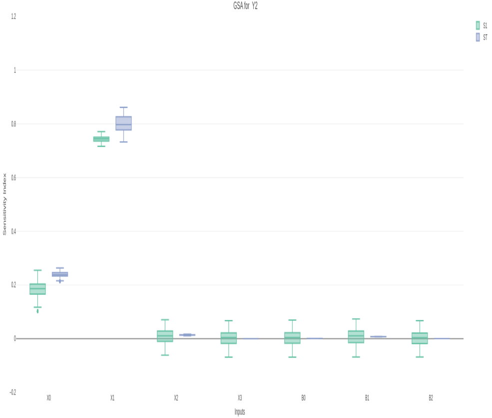




Global sensitivity analysis

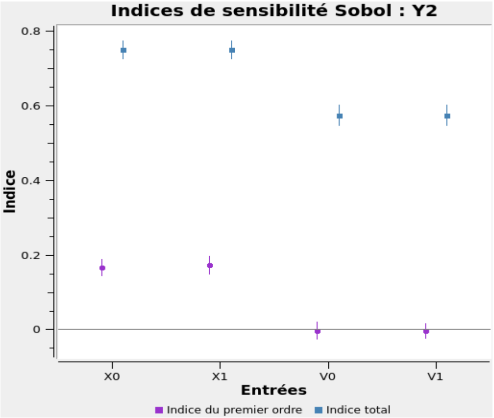
Drone

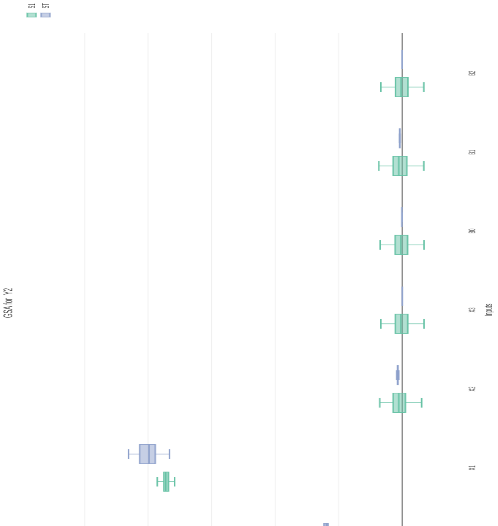




Global sensitivity analysis

Billard

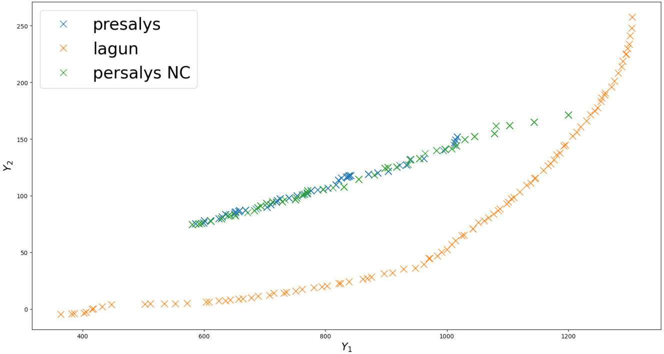




Optimization

The problem

- Maximize Y_1, Minimize Y_2
- Constraints : $Y_2 > 60$ and $Y_2 < 152.4$ (This constraint is not available on Lagun)



Calibration

Drone

- Easy to set experimental data
- 4 differents choices for calibration algorithm : linear and non-linear least squares and linear and non-linear Gaussian (3D-Var).
- Results :

Entrée	Valeur	Intervalle de confiance à 95%
B0	0.112615	[0.103109, 0.122121]
B1	0.0390973	[0.0279607, 0.0502339]
B2	9.79157	[9.77498, 9.80815]

β_0	β_1	β_2
0.095	0.03	9.8050

Calibration

Billard

- Easy to set experimental data
- 4 differents choices for calibration algorithm : linear and non-linear least squares and linear and non-linear Gaussian (3D-Var).
- Results :

Entrée	Valeur	Intervalle de confiance à 95%
A0	2.97425	[2.97363, 2.97478]
A1	2.0008	[2.00077, 2.00083]

A_1	A_2
3	2

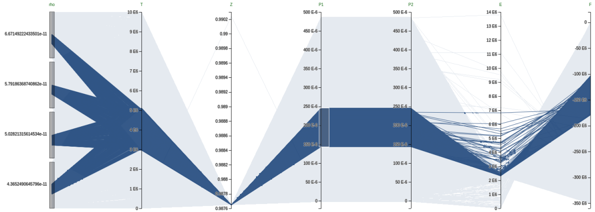
The little details that makes all the differences

LAGUN

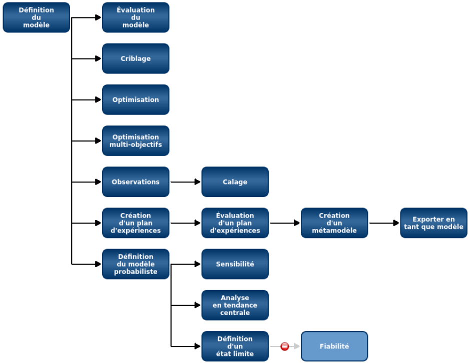
- Surrogate model combination

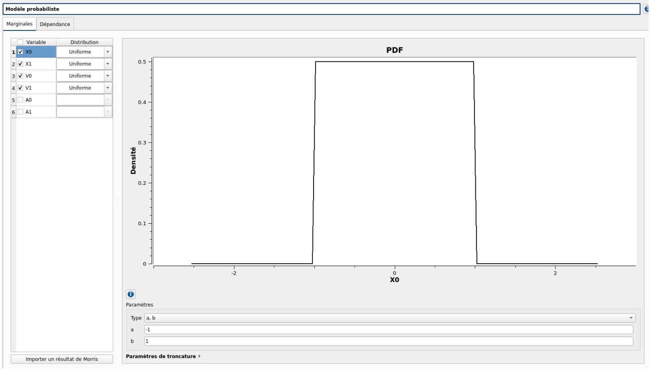
Type	Var	Trend	Z	P1	P2	E	F
BestQ2			**0.7789**	**0.986**	**0.986**	**1**	**1**
Lasso			0.1263	0.986	0.986	1	1
Acosso1			0.3731	0.9828	0.9828		
Acosso2	All						
Acosso2	Acosso1						
Kriging	All	Constant	0.7789	0.9796	0.9798	1	1

- Parallel plot



The little details that makes all the differences





Conclusion

Powerful tools for speed and efficiency

- Complete all the steps in the ABCD method faster than we can in R/python
- Very, Very fast compared to simulations for most of the industrial cases.
- Advanced methods that are easy to use

There are still a few points that raise questions

- Tools vulnerable to defects in the basic software bricks. For example, a package required by Lagun is archived in CRAN because it no longer works on the new version of R?
- Some parts (Kriging Lagun and GSA all) are still black boxes for me, although I wanted to find out what was going on.

My use

- I use them to save time in my engineering studies.
- I give them to physicists and engineers to facilitate their UQ.

Thank you for your attention