

DE LA RECHERCHE À L'INDUSTRIE



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General overview of the Uranie platform

Uncertainty PRACE formation session



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In a nutshell

ROOT
Uranie

Focusing on Uranie

Schematic workflow examples
The modular organisation

Tools for interoperability

Dealing with external pieces of code
Communication with other platforms

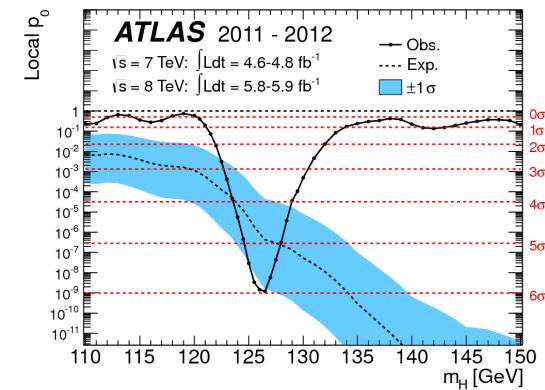
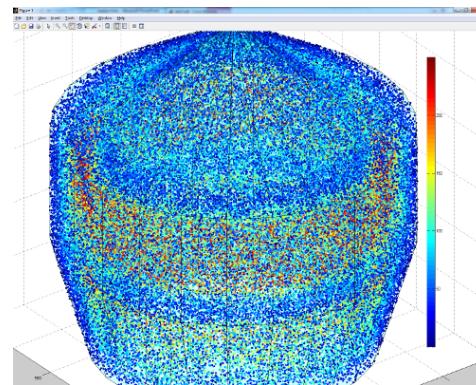
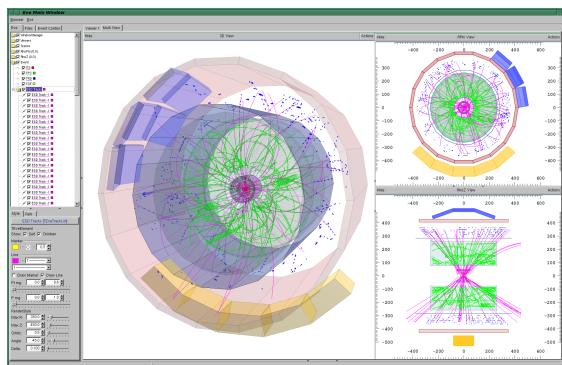
Module description

The ROOT platform



Developed at CERN to help analyse the huge amount of data delivered by the successive particle accelerators

- Written in C++ (3/4 releases a year)
- Multi platform (Unix/Windows/Mac OSX)
- Started and maintained over more than 20 years
- It brings:
 - a **C++ on-the-flight compiler**, but also **Python** and **Ruby** interface
 - a hierarchical object-oriented database (machine independent and highly compressed)
 - advanced visualisation tool (graphics are very important in HEP)
 - statistical analysis tools (*RooStats*, *RooFit*...)
 - and many more (3D object modelling, distributed computing interface...)
- **LGPL**



Many sources for documentation

Online

- Reference guide: <https://root.cern.ch/root/html/ClassIndex.html>
 - Details all the methods (inherited or not) of a given class
- User-guide: <https://root.cern.ch/root/html/guides/users-guide/ROOTUsersGuideA4.pdf>
 - Description of what can be done from installation to high level usage. Nicely illustrated !
- How-to: <https://root.cern.ch/howtos>
 - Example to answer most answered questions
- A dedicated forum: <https://root-forum.cern.ch/>
 - Very reactive forum, to help people with the many different usage one can do with ROOT.

On your machine, once installed

- User guide and manual: They are provided in markdown, ready to be compiled
 - \$ROOTSYS/documentation/users-guide and \$ROOTSYS/documentation/primer
- Tutorials: plenty of examples to be run
 - \$ROOTSYS/tutorials
- Macros: place to store your own macros that you might call from anywhere
 - \$ROOTSYS/macros

This is a structure that we acknowledge and try to follow as well

The Uranie platform

Developed at CEA/DEN to help partners handling sensitivity, meta-modelling and optimisation problems.

- Written in C++ (~2 releases a year), based on ROOT
- Multi platform (developed on Unix and tested on Windows)
- It brings simple data access:
 - Flat [ASCII](#) file, [XML](#), [JSON](#) ...
 - [TTree](#) (internal ROOT format)
 - [SQL](#) database access
- Provides advanced visualisation tools (on top of ROOT's one)
- Allows some analysis to be run in parallel through various mechanism
 - simple [fork](#) processing
 - shared-memory distribution ([pthread](#))
 - split-memory distribution ([mpirun](#))
 - through graphical card ([GPU](#))
- Main purpose is tools for:
 - construction of design-of-experiment
 - uncertainty propagation
 - surrogate models generation
 - sensitivity analysis
 - optimisation problem
 - reliability analysis
- [LGPL](#)



General organisation: version 4.3.0

Unit Testing Report

General description:

- ROOT version: 6.18.04
- 11 modules / 246 classes
~ 134 000 lines of code
- Compilation using CMAKE

	DataServer	Launcher	Relauncher	Sampler	Sensitivity	Optimizer	reOptimizer	Modeler	UncertModeler	reliability	XMLProblem
Status	PASSED										
Duration											
Num. test	328	112	39	176	115	139	46	429	53	2	13
Total Failures	0	0	0	0	0	0	0	0	0	0	0
Num. Errors	0	0	0	0	0	0	0	0	0	0	0
Num. Failures	0	0	0	0	0	0	0	0	0	0	0
Start	2018-01-09 20:15:10	2018-01-09 20:16:38	2018-01-09 20:31:36	2018-01-09 20:32:26	2018-01-09 20:33:03	2018-01-09 20:59:22	2018-01-09 21:11:42	2018-01-09 21:38:09	2018-01-09 22:09:47	2018-01-09 22:09:51	2018-01-09 22:09:51
End	2018-01-09 20:16:38	2018-01-09 20:31:35	2018-01-09 20:32:26	2018-01-09 20:33:03	2018-01-09 20:59:19	2018-01-09 21:11:40	2018-01-09 21:38:07	2018-01-09 22:09:45	2018-01-09 22:09:50	2018-01-09 22:09:51	2018-01-09 22:12:45

Regularly tested:

- 7 Linux platforms and Windows 10 every night
- ~ 1500 unitary tests with CPPUNIT
- ~ 83% coverage with GCOV (without logs)
- Memory leak check with VALGRIND

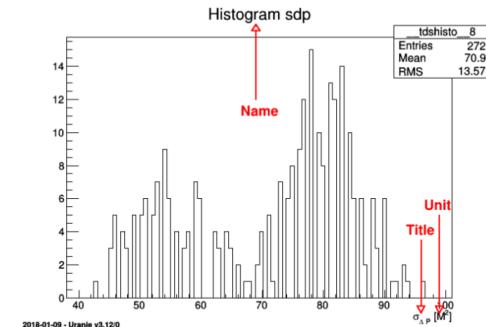
- Name + title: constructor defined from the name and the title of the variable

```
Attribute *psdp = new TAttribute("sdp", "#sigma_{#Delta P}");
psdp->setUnity("M^2");
```

A pointer `psdp` to a variable "`sdp`" is available with title being `#sigma_{#Delta P}`. The command `setUnity()` precises the unit. In this case, by default, the field `key` is identical to the field `name`. We will use the ability given by ROOT to write LaTeX expressions in graphics to improve graphics rendering without weighing down the manipulation of variables: as a matter of fact, we can plot the histogram of the variable `sdp` by:

```
tdsGeyser->addAttribute("newx2","x2","#sigma_{#Delta P}","M^2");
tdsGeyser->draw("newx2");
```

The result of this piece of code is shown in Figure II.3



Documentation: 3 different levels

2 using DocBook, generating both PDF and HTML formats.

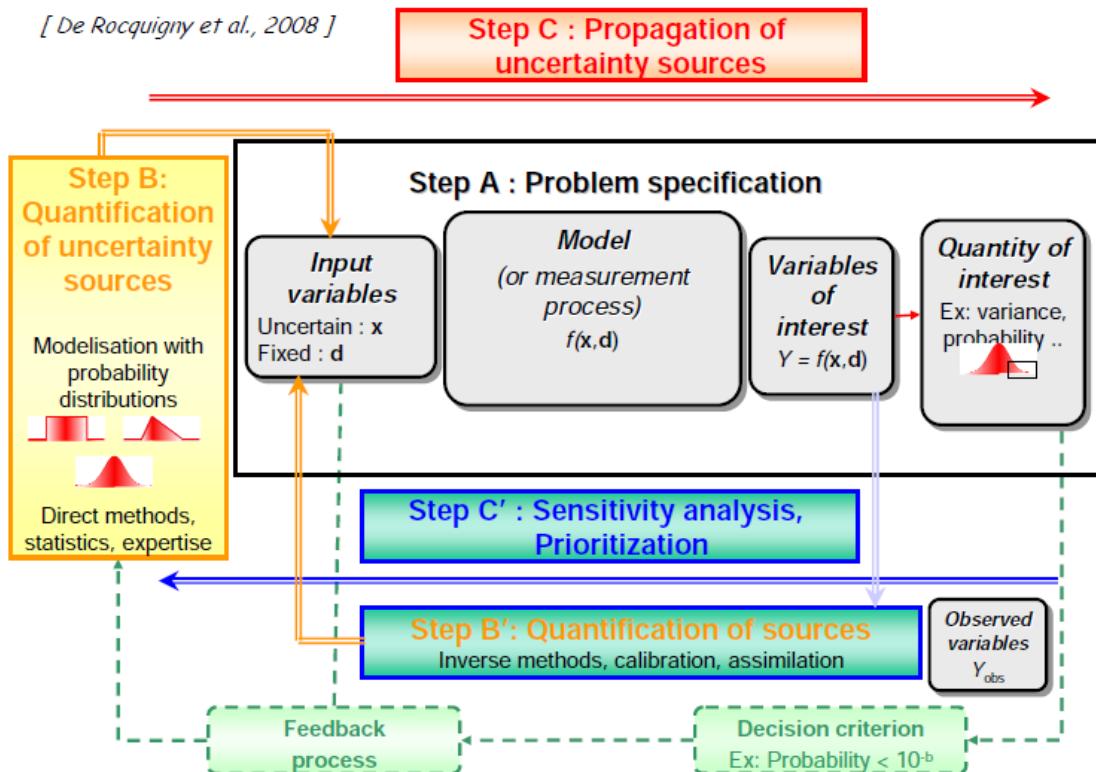
- Methodological reference (~ 75 pages)
- User manual: ~ 930 pages
 - ~ 280 pages: describing methods and their options.
 - ~ 320 pages: C++ macros (~ 125 examples)
 - ~ 320 pages: Python macros (~ 125 examples)

Developer's guide using DOXYGEN (HTML only)

- describing methods from comments in the code

Workflow: breakdown into steps

[De Rocquigny et al., 2008]



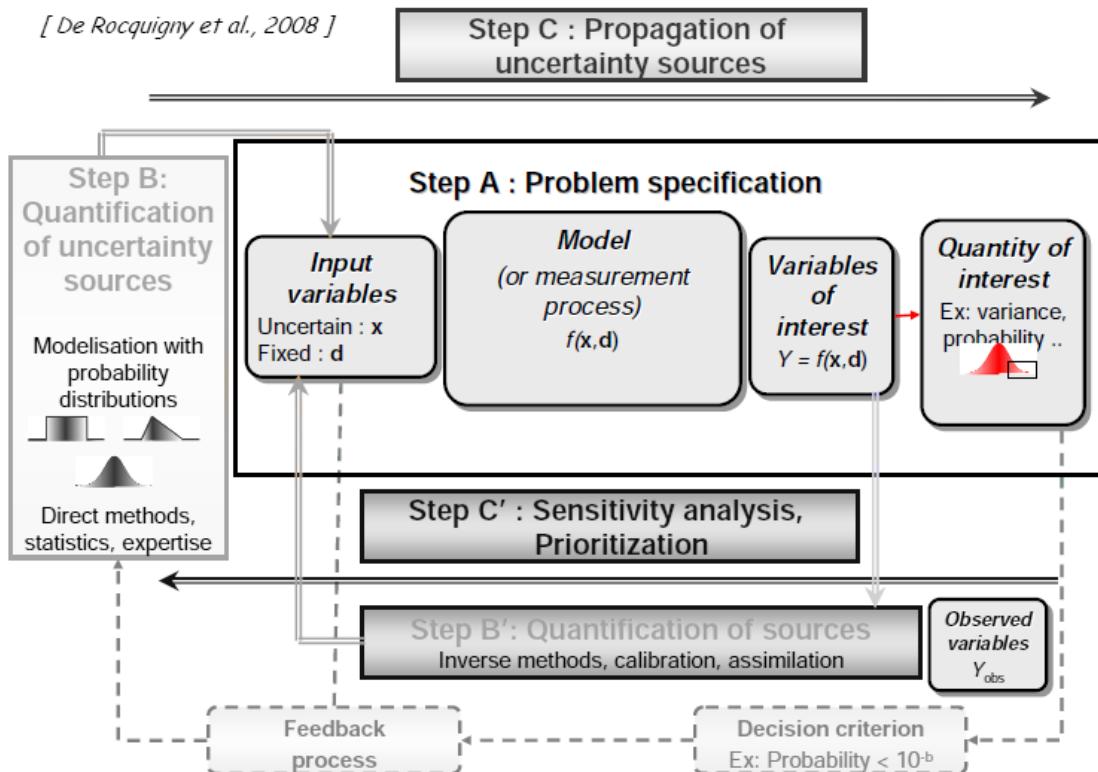
Main steps:

- A: problem definition
 - Uncertain input variables
 - Variable/quantity of interest
 - Model construction
- B: uncertainty quantification
 - Choice of pdfs
 - Choice of correlations
- B': quantification of sources
 - Inverse methods using data to constrain input values and uncertainties
- C: uncertainty propagation
 - Evolution of output variability w.r.t input uncertainty
- C': sensitivity analysis
 - Uncertainty source sorting

These steps are usually model dependent, it might be useful to iterate to help converging to proper conclusions

Workflow: breakdown into steps

[De Rocquigny et al., 2008]



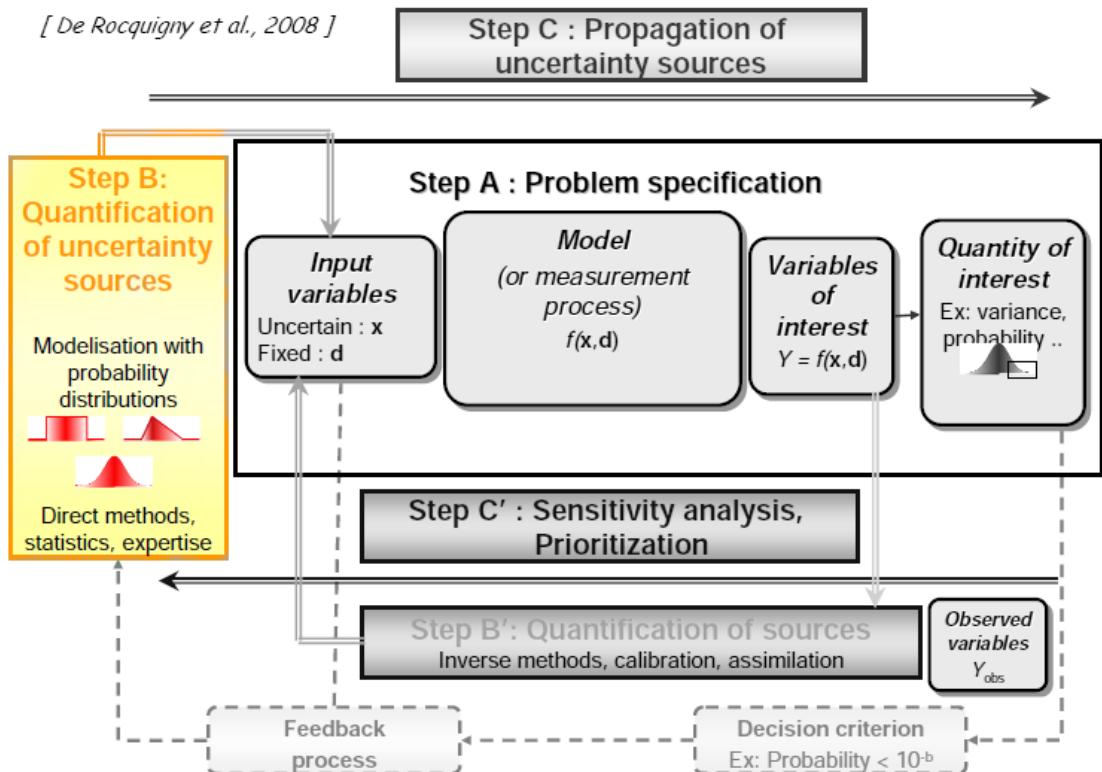
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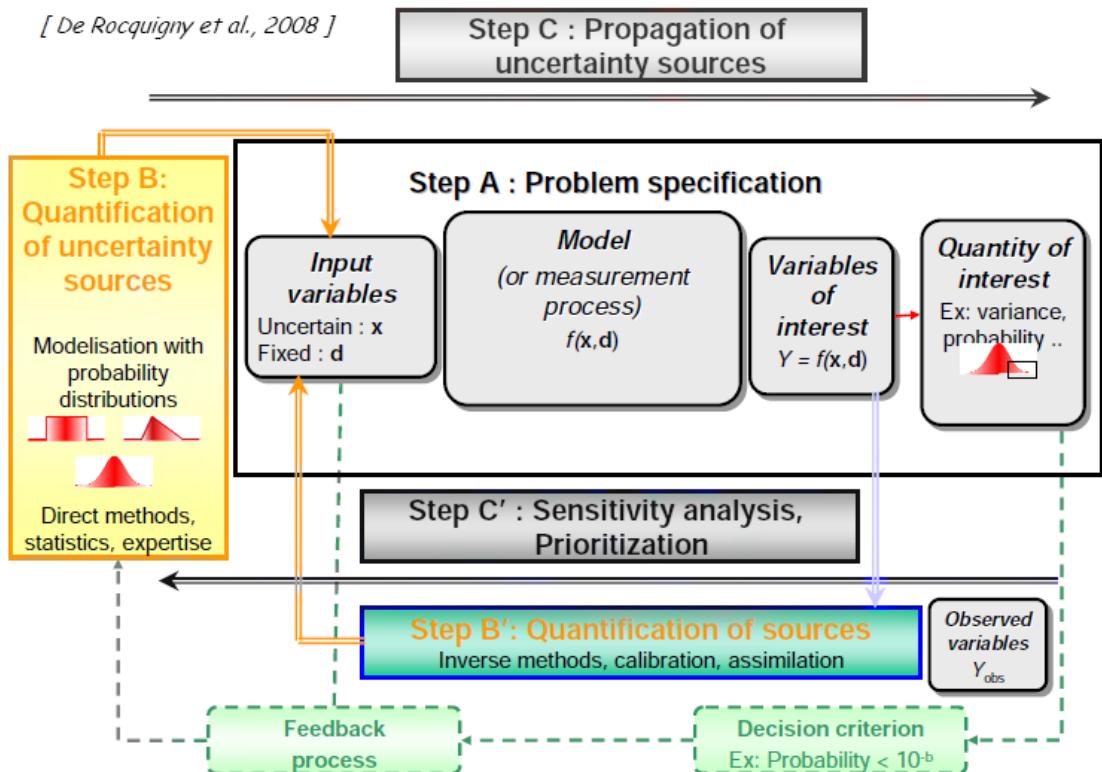
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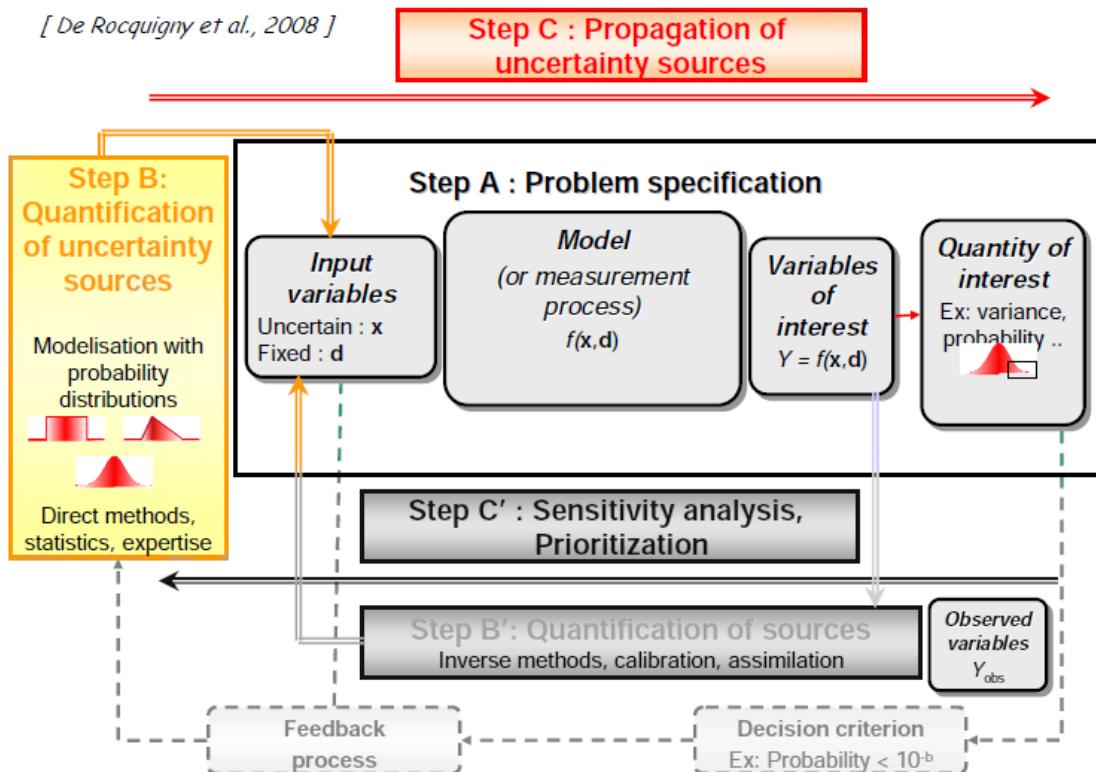
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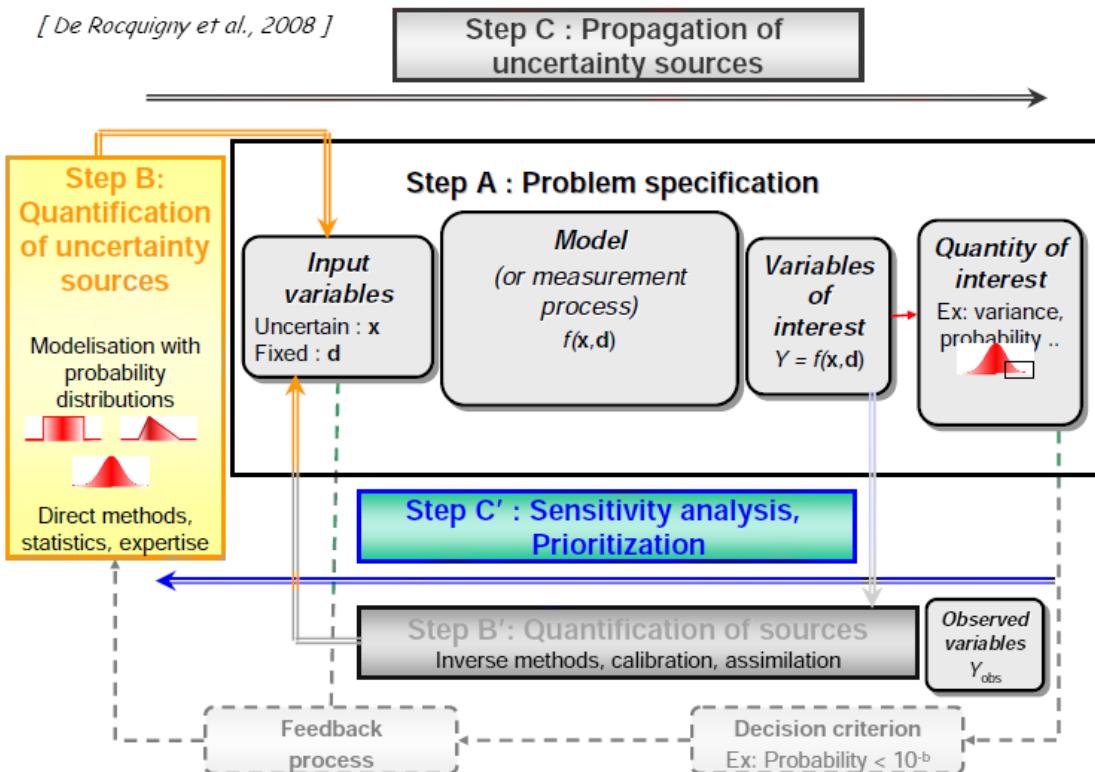
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The module point of view

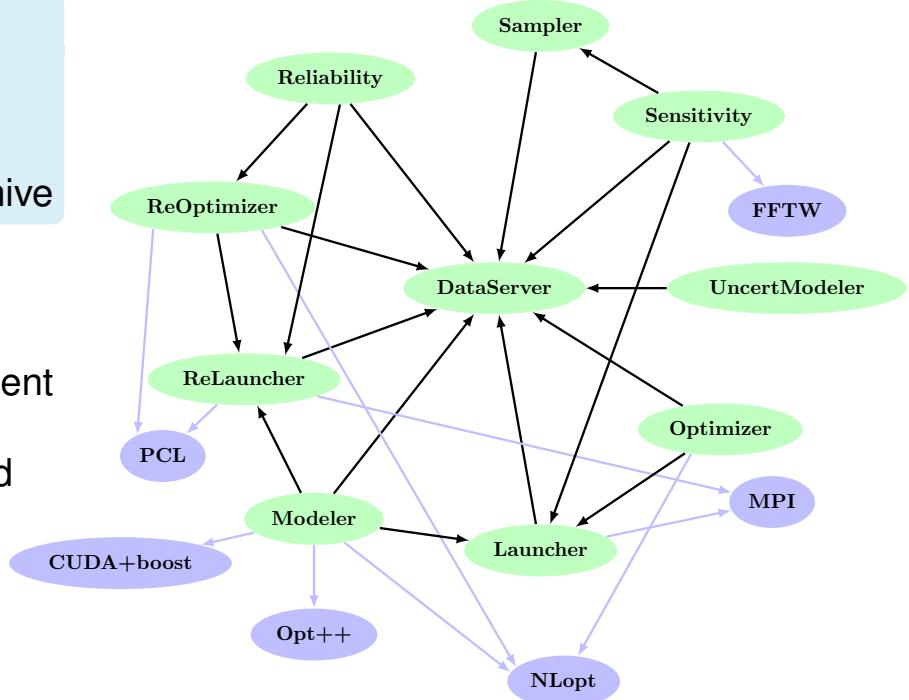
█ Uranie's module █ Uranie's dependence

Few dependencies:

- █ Compulsory: ROOT, CPPUNIT, CMAKE
 - █ Optional: PCL, NLOPT, OPT++, MPI, FFTW, CUDA
- (*) a patched version of OPT++ is brought along in the archive

Organised in modules:

- █ Some are more technical ones:
 - DataServer: data handling and first statistical treatment
 - (Re)Launcher: interfaces to code/function handling.
Can deal with code, PYTHON-function, C++-interpreted and compiled functions
- █ Many are dedicated ones:
 - Sampler: creation of design-of-experiments
 - Modeler: surrogate-model generation
 - (Re)Optimizer: mono/multi criteria optimisation
 - Sensitivity: ranking inputs w.r.t impact on the output



The next following slides will discuss the content of the main dedicated modules

Tools for interoperability



Submitting code computations

Launching functions:

- Analytic C++ functions: myFunction (double *x, double *y)
 - inputs/outputs are double-precision.
- Analytic PYTHON functions and compiled C++ functions
 - inputs/outputs are double-precision, strings or varying-size vectors of double.

Launching external codes (considering them as black boxes):

- inputs/outputs are double-precision, strings or varying-size vectors of double.

Non-intrusive approach: communication is done through input/output file with many possible formats

- line format: every input/output has its own line
- column format: every input/output has its own column
- XML format:
- key=value: every input/output has its own key and corresponding value is separated by “=”
- flag format: input file is modified to put specific flags in the text (“@rw@” in next slide)
- Can specify boundaries (vectors and string) and delimiters for two elements (vectors).

Distributing the computations

- simple **fork** processing
- shared-memory distribution: using **pthread**
- split-memory distribution: using **mpirun**



Example of flag format

File Edit Options Buffers Tools Development Help

INPUT FILE with FLAG for the "FLOWREATE" code
\date 2008-04-22 12:55:17

new Implicit_Steady_State sch {
frottement_paroi { @Rw@ @R@ }
tinit 0.0
tmax 1000000.
nb_pas_dt_max 1500
dt_min @Hu@
dt_max @Hl@
facsec 1000000.
kW @Kw@
information_Tu Champ_Uniforme 1 @Tu@
information_Tl Champ_Uniforme 1 @Tl@
information_L {
precision @L@
}
convergence {
criterion relative_max_du_dt
precision @Rw@
}
-:--- flowrate_input_with_flags.in Top L1 (Fundame
Beginning of buffer

File containing flags

File Edit Options Buffers Tools Development Help

INPUT FILE with FLAG for the "FLOWREATE" code
\date 2008-04-22 12:55:17

new Implicit_Steady_State sch {
frottement_paroi { 0.128927 2004.277098 }
tinit 0.0
tmax 1000000.
nb_pas_dt_max 1500
dt_min 1014.704041
dt_max 764.717904
facsec 1000000.
kW 11766.766463
information_Tu Champ_Uniforme 1 75275.183901
information_Tl Champ_Uniforme 1 72.020029
information_L {
precision 1539.312628
}
convergence {
criterion relative_max_du_dt
precision 0.128927
}
-:--- flowrate_input_with_flags.in<UraneLauncher_1> T

Modified file

Advantage

Allow to keep a complicated input file, as long as its structure does not change

Example of flag format

File Edit Options Buffers Tools Development Help

```
# INPUT FILE with FLAG for the "FLOWRATE" code
# \date 2008-04-22 12:55:17
#
new Implicit_Steady_State sch {
    frottement_paroi { @Rw@ @R@ }
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    information_L {
        precision @L@
    }
    convergence {
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        precision @Rw@
    }
}
----- flowrate_input_with_flags.in Top L1 (Fundame
Beginning of buffer
```

File containing flags

File Edit Options Buffers Tools Development Help

```
# INPUT FILE with FLAG for the "FLOWRATE" code
# \date 2008-04-22 12:55:17
#
new Implicit_Steady_State sch {
    frottement_paroi { 0.128927 2004.277098 }
    tinit 0.0
    tmax 1000000.
    nb_pas_dt_max 1500
    dt_min 1014.704041
    dt_max 764.717904
    facsec 1000000.
    kW 11766.766463
    information_Tu Champ_Uniforme 1 75275.183901
    information_Tl Champ_Uniforme 1 72.020029
    information_L {
        precision 1539.312628
    }
    convergence {
        criterion relative_max_du_dt
        precision 0.128927
    }
}
----- flowrate_input_with_flags.in<UranieLauncher_1>
```

Modified file

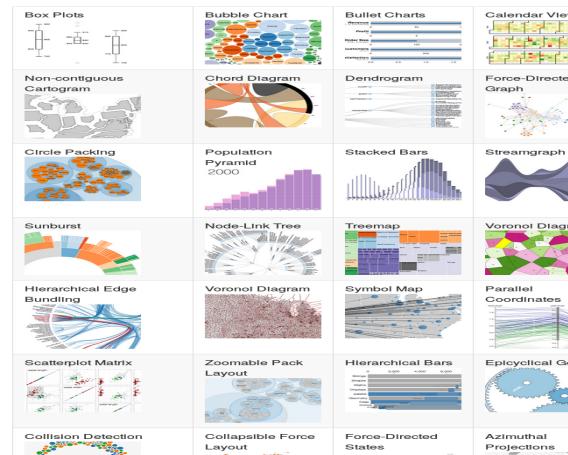
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Communication with other platforms

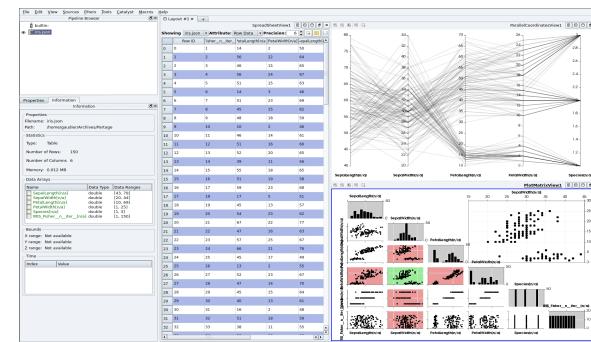
Use standard input/output language to import/export data and models, to help communicate with other platforms (XML, PMML, JSON...)

```
{
  "_metadata" : {
    "table_name" : "IRIS_Fisher",
    "table_description" : "Fisher Iris Data Set",
    "short_names" : [
      "SepalLength", "SepalWidth",
      "PetalLength", "PetalWidth", "Species" ],
    "date" : "Thu Mar 17 11:40:48 2016"
  }
  "items" : [ {
    "PetalLength" : 14, "PetalWidth" : 2,
    "SepalLength" : 50, "SepalWidth" : 33, "Species" : 1
  }, "items" : { ...
}
```



Import/Export data in Json format in order to :

- Benefit the features of [D3 \(D3js.org\)](http://d3js.org)
 - Interactive visualisation into a browser
 - Several available graphics (Cobweb, Sun-Burst, Treemap,...)
- Visualize the same data file in [ParaView / Paraview](#) module of [Salomé](#)
- Proposal as a common format for data with [OpenTURNS](#)



A glimpse at the main modules

The sampler module

Used to generate the design-of-experiments, basis of many analysis.
Some methods can deal with correlation as well.

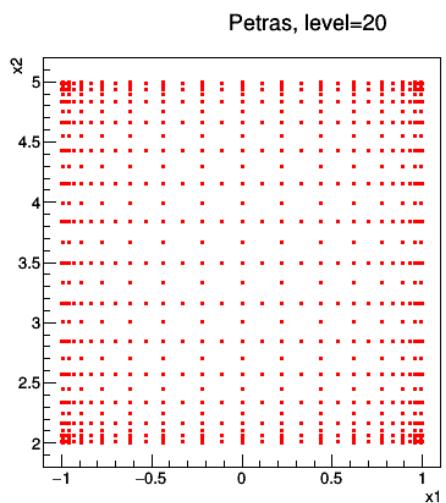
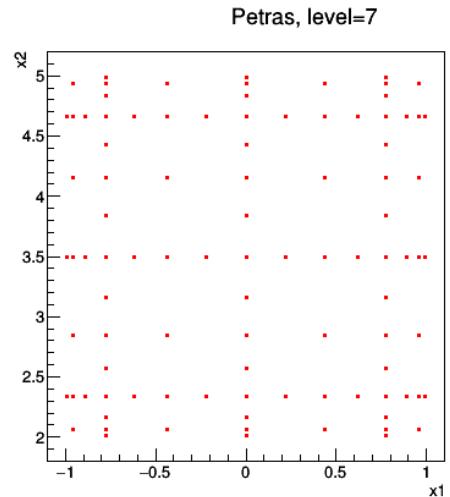
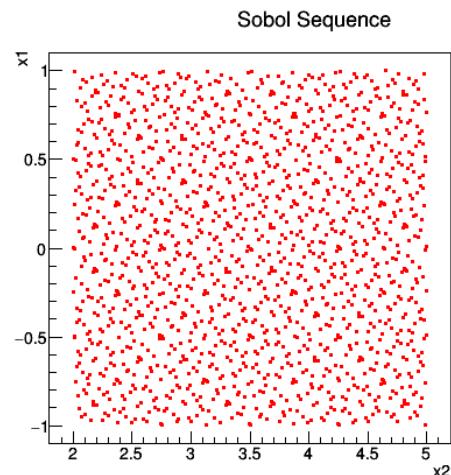
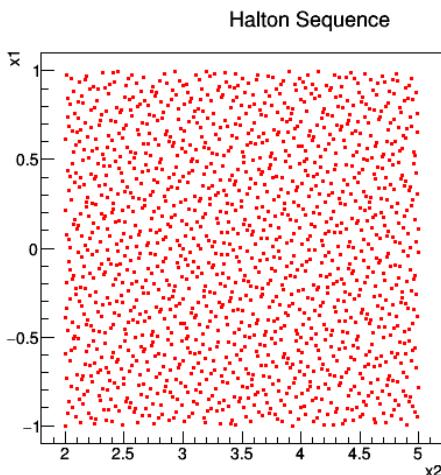
Two main categories

■ Stochastic designs:

- Simple Random Sampling (SRS)
- Latin Hypercube Sampling (LHS)
- One-At-a-Time Sampling (OAT)
- Archimedean copulas
- Random fields...

■ Deterministic designs:

- Regular quasi Monte-Carlo: Halton/Sobol sequence
- Sparse grid sampling: Petras
- Space filling design



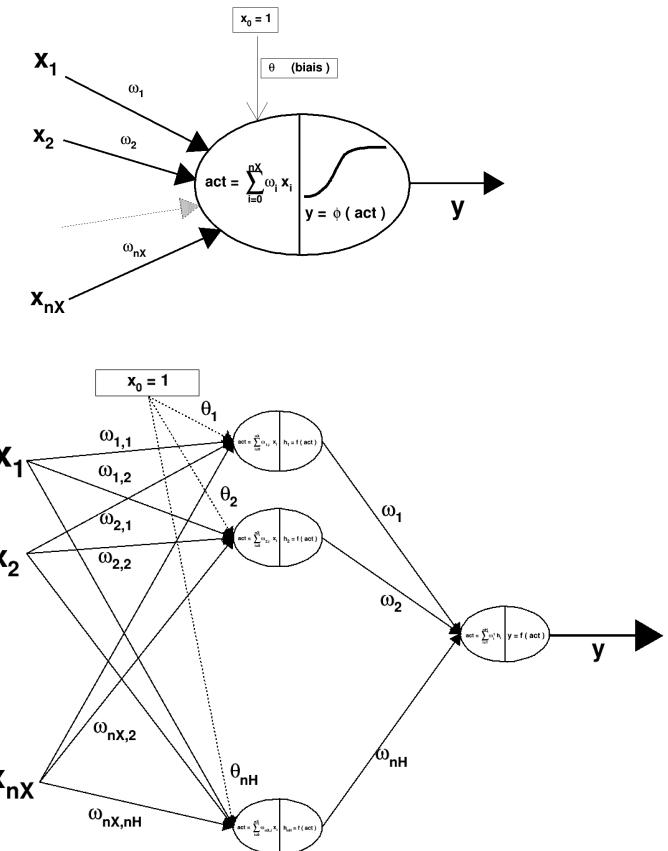
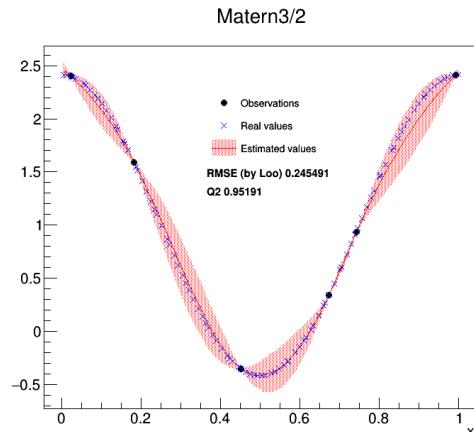
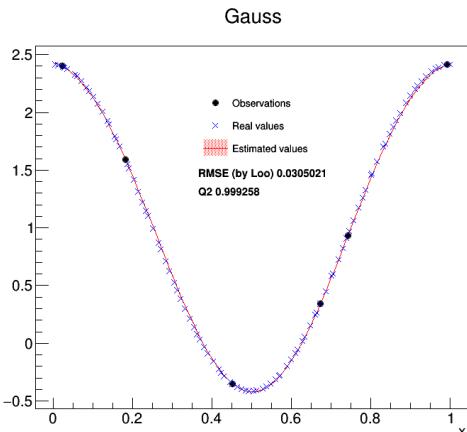
The modeler module

Create a surrogate-model: a numerical model reproducing the behaviour of provided data

Several possible models to be chosen:

- █ Polynomial regressions
- █ Generalised linear models
- █ k-nearest neighbours
- █ Artificial Neural Networks (ANN/MLP)
- █ Chaos Polynomial + ANISP
- █ Kriging

→ Models can be exported in different format (C++, fortran, PMML) in order to be re-used later on.



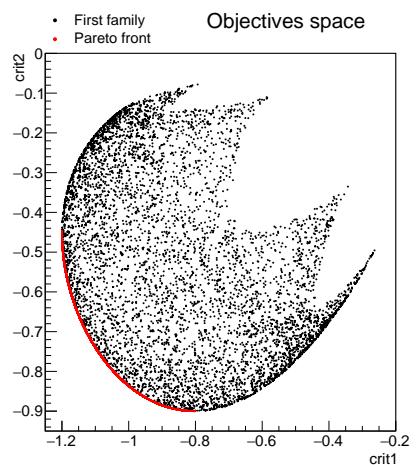
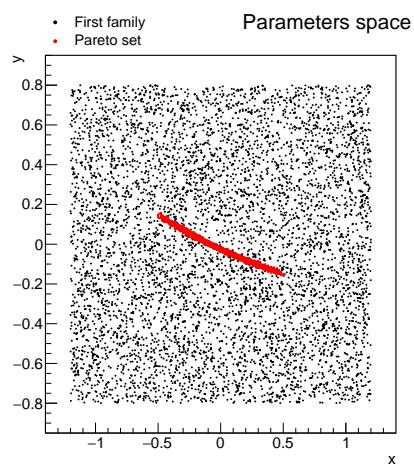
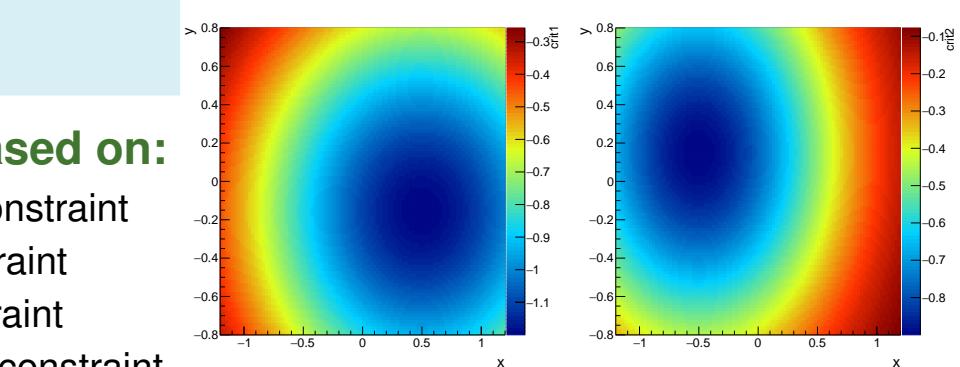
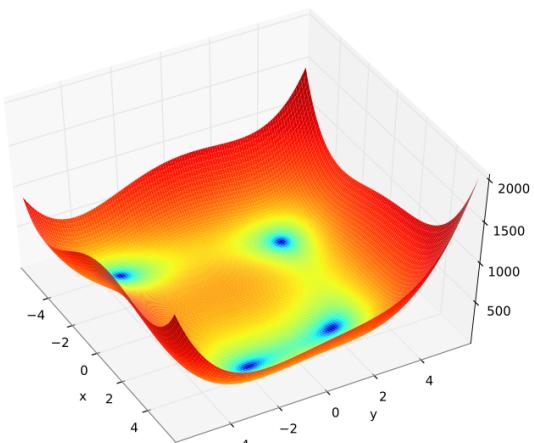
Optimizer module

Dealing with optimisation problem usually means:

- Single Objective (SO) or Multi Objectives (MO) to be minimised
- parameters that have an impact on objective
- possible constraint on these parameters

Many possible implementation for this, based on:

- **Minuit**: ROOT's SO optimisation library without constraint
- **Opt++**: SO optimisation library with/without constraint
- **NLOpt**: SO optimisation library with/without constraint
- **Vizir**: CEA's MO optimisation library with/without constraint, based on stochastic algorithms (e.g. genetic algorithms)

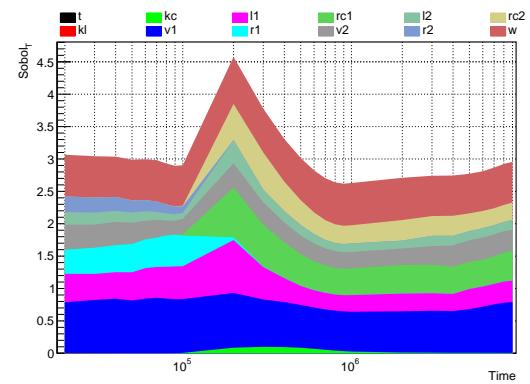
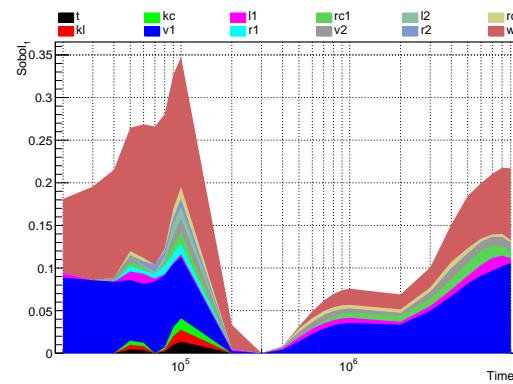
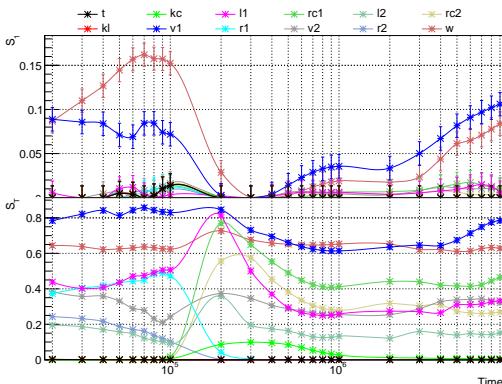


Sensitivity module

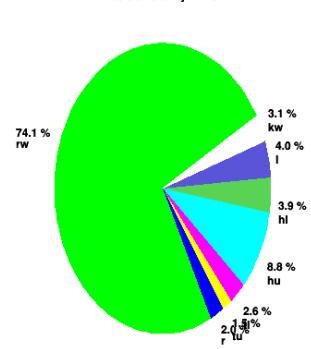
Tools to evaluate the sensitivity of the outputs of a code/function to its inputs.

Several kinds of methods available:

- Local: finite differences ($\frac{\delta Y_i}{\delta X_j}(x_0)$)
- Regression:
 - Pearson (values)
 - Spearman (ranks)
- Screening: OAT, Morris...
- Sobol indexes:
 - FAST (Fourier Amplitude Sensitivity Test)
 - RBD (Random Balance Design)
 - Sobol/Saltelli Methods

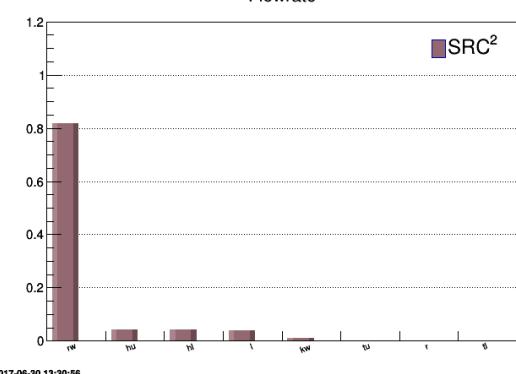


First Sensitivity Index



2017-06-30 13:19:32

Flowrate



Eyes-on: a simple example

emacs@jbpc

- + ×

File Edit Options Buffers Tools C++ Help

Save Undo Cut Copy Find

```

void OneKrigingOnly()
{
    /*Reading a database (y vs x1) from a simple function.
    Informations are stored in the TDataServer object*/
    TDataServer *tdsObs = new TDataServer("tdsObs", "observations"); --- Uranie v3.7/0 --- Developed with ROOT (5.34/23) by Fabrice Gaudier
    tdsObs->fileDataRead("utf-1D-train.dat");
    /*Defining a kriging model with the training database
     by defining a certain number of options */
    TGPBuilder *gpb = new TGPBuilder(tdsObs, "x1", "y", "maternII");
    //Find the best possible parameters by optimisation
    gpb->findOptimalParameters("ML", 20, "BFGS", 100);
    //Build the best obtained kriging model.
    TKriging *kg = gpb->buildGP();

    /*Reading now a test basis (constructed with the same dummy function)
    This is mostly for x-check and illustration purposes*/
    TDataServer *tdsEstim = new TDataServer("tdstest", "base de test");
    tdsEstim->fileDataRead("utf-1D-test.dat");

    //Applying the kriging on the test basis => launching the model on every points
    TLauncher2 *lkrig = new TL launcher2(tdsEstim, kg, "x1", "yEstim:vEstim");
    lkrig->solverLoop();

    //Plotting the results
    gROOT->LoadMacro("PlottingKriging.C");
    PlottingKriging(tdsObs, tdsEstim);
}

----- OneKrigingOnly.C All L1 (C++/l Abbrev)
Loading cc-langs...done

```

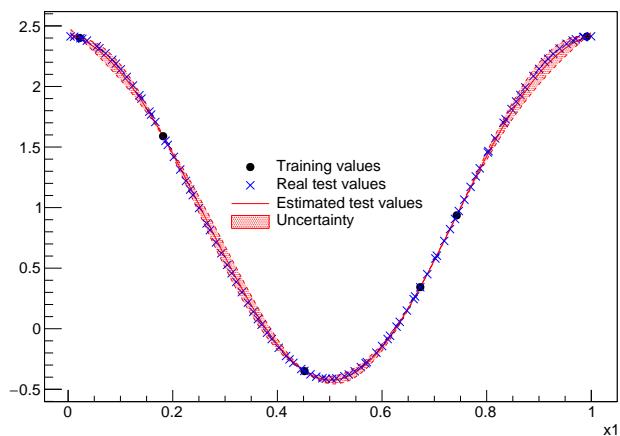
called by

(mar.10mai 0:37)-(blanchard@jbpc:...ipts/modeler)-(1%) root OneKrigingOnly.C
root [0]
Processing /home/blanchard/.root_logon...
Processing OneKrigingOnly.C...
Urane v3.7/0 --- Developed with ROOT (5.34/23) by Fabrice Gaudier
Copyright (C) 2013 CEA/DEN
Version : v3.7/0 - Date : Thu Jul 23, 2015
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TGPBuilder::findOptimalParameters: starting screening procedure (20 evaluations)
TGPBuilder::findOptimalParameters: starting optimisation procedure (BFGS algorithm
!.....!.....
Info in <TCanvas::MakeDefCanvas>: created default TCanvas with name c1
root [2] ■

gives

Kriging example



Plans for the future



Technical improvements

- Parallelise the EGO estimation
- Porting more methods on GPU (kNN and ANN so far)

Methodological improvements

- Combine Hamiltonian Markov-chain and ANN
- Get new sensitivity indexes (Shapeley)
- Bayesian calibration (through MCMC algorithms in non linear settings)
- Improve many-criteria algorithms from VIZIR

Feel free to test the platform

The code is available here: <http://sourceforge.net/projects/uranie>

- All documentations are embedded in the archive
- We give 2-3 formation sessions a year
 - Dedicated session also on specific modules once every 18 month (roughly)
- Can contact us at support-uranie@cea.fr

More information can be found in our recent paper (published in EPJ-N):
<https://doi.org/10.1051/epjn/2018050>

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