

PERSALYS, the graphical interface of OpenTURNS

M. Baudin ¹ T. Delage ¹ A. Dumas ² A. Dutfoy ¹
G. Garcia ² A. Geay ¹ O. Mircescu ¹ J. Pelamatti ¹
F. Robin ¹ J. Schueller ² T. Yalamas ²

¹EDF R&D. 6, quai Watier, 78401, Chatou Cedex - France, michael.baudin@edf.fr

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

June 10th 2022, OpenTURNS User's day



Contents

Overview

What's new?

What's next?

Bring Uncertainty Methodology to Engineers

- ▶ Partnership started in 2015
 - ▶ EDF R&D wanted to maximize the use of OpenTURNS® by its engineer/researcher (and improve an existing GUI) → develop a GUI to make more easy to use
 - ▶ Phimeca had already developed an "OpenTURNS GUI" (PhimecaSoft®) which satisfies some needs of EDF R&D but not all.
 - ▶ EDF R&D and Phimeca decided to start a specific partnership in order to develop a new GUI based on OpenTURNS® and "Salome Tools": Paraview, Yacs, ...

Some expectations regarding the GUI

- ▶ As easy to use as possible and, when it is possible, a GUI which can guide the user
- ▶ Possibility to use it inside Salome Platform to
 - ▶ Use supercomputing resources (e.g. Gaïa, 3 052 Tflops peak, 41 000 cores)
 - ▶ Connect to EDF numerical code users (Code_Aster for example)
- ▶ Take benefit from the advanced visualization capability from Paraview
- ▶ Drive the GUI from a python script usable in an "expert" mode

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), physical model with vector input and vector output or 1D Fields, central tendency, sensitivity analysis, probability estimate, metamodeling (polynomial chaos, kriging), screening (Morris), optimization, design of experiments
 - ▶ Generic (not dedicated to a specific application)
 - ▶ GUI language : English, French

Summary

- ▶ Partners : EDF, Phimeca
- ▶ Licence : LGPL
- ▶ Schedule : new release twice a year
- ▶ Availability :
 - ▶ Stand-alone version : for free on demand on www.persalys.fr
Commercialization by Phimeca consists in providing support and/or developing customized versions
 - ▶ SALOME_EDF in the "CONTRIBUTIONS" section since 2018 on <https://www.salome-platform.org>

Ergonomics - Sample cleaning wizard

- ▶ NaN/Inf are detected and the user can choose to replace/remove them (user-defined value or statistical moment)

Persalys

File Tools Help

Studies

- Physical models
 - symbolicModel
 - Definition
 - Designs of experi...
 - fixedDesign
 - Evaluation
 - grid
 - importDesign
 - Evaluation
 - Evaluation
 - evaluation1
 - Screening
 - aMorris
 - Optimization
 - optim
 - Calibration
 - observations
 - calibration
 - pythonModel
 - Definition
 - Designs of experi...
 - onePointDesign
 - twoPointsDesign
 - couplingModel
 - Definition
 - Data models
 - fixedDataModel
 - Definition
 - importDataModel
 - Definition

Data model

Data file: data.csv

The sample contains invalid values

Variables

Variable	x_0	x_1	x_2	x_3
Type	Input	Output	Input	Input

Sample

Size: 201

Row ID	x_0	x_1	x_2	x_3
189	-0.0176004631063	-0.82724900267	0.236397085634	0.734540813069
190	0.22312730662	-1.45401848455	-0.940404048177	1.27675284978
191	-0.160861593363	-1.06006266482	0.141830304929	-0.537890691297
192	-0.0874317578983	0.305523284047	0.874539469433	-0.510192937938
193	0.432141985042	2.32684296655	0.994601801252	0.957529759332
194	-2.43156578393	0.974395311646	0.353721233187	-0.476528044143
195	1.06175096388	0.536460327235	0.917410053005	0.350824156653
196	-1.02075953077	-0.188416722485	0.463183535654	-0.24272794184
197	-3.06051410955	-0.51221264559	-0.46336917612	-0.198204386583
198	-0.12799819632	0.297934354645	-0.108813312559	2.5172092907
199	0.262321682364	0.0278401295732	-0.322081459382	3.71341153146
200	nan	0	0	inf

Data Cleaning

Variable	x_0	x_2	x_3	x_1
Mean	-0,0143208	0,081108	0,0507527	0,568041
Median	-0,0210107	0,1199	0,11353	0,416581
Number of NaN/Inf (%)	0,497512	0	0	0,497512
Replacing value	0	0	0	0

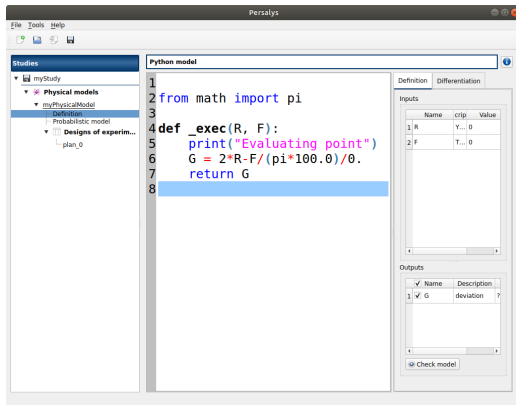
☐ Mean
☐ Median
☐ User value
☒ Remove

Help

Finish Cancel

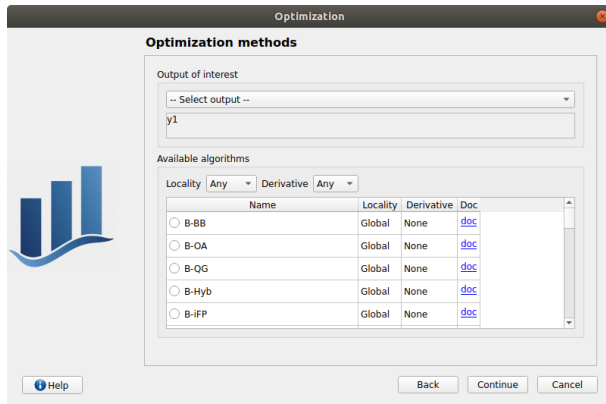
Ergonomics - Python editor overhaul

- Syntax highlighting and zooming in/out with ctrl+mouse-wheel



Ergonomics - Optimization algorithms filters

- ▶ Algorithms are filtered based on the problem definition (bounds, need for derivative)
- ▶ Link to algorithm documentation directly accessible

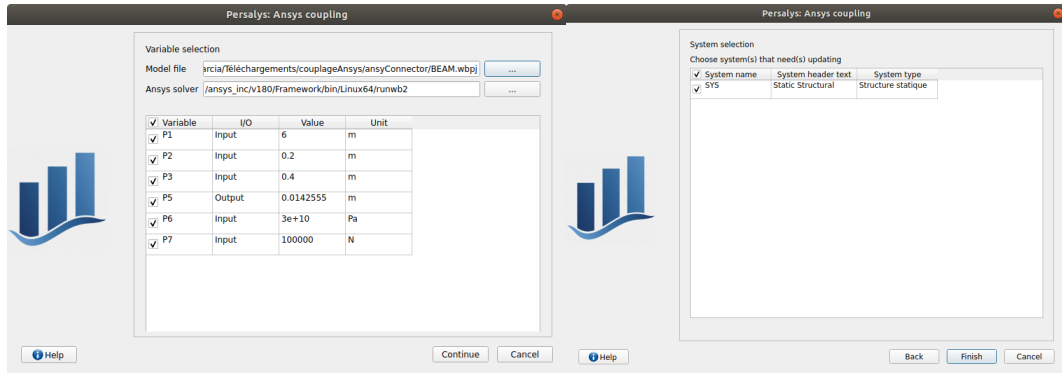


Ergonomics - DoE duration estimation - CSV import/export

- ▶ Estimated DoE duration based on single evaluation
- ▶ CSV support improvements
 - ▶ Numerical and column separator combinations are tested before importing data
 - ▶ The user can choose numerical and column separator before exporting data

Coupling - Ansys coupling wizard (1)

- ▶ Creating a coupling model can be tricky and/or tedious (command, resource, templates...)
- ▶ Added a wizard which helps the user to pre-fill the coupling model information
 - ▶ The user specifies the workbench project and the blocks the will need updating
 - ▶ The wizard looks for the Ansys solver based on project version



Persalys: Ansys coupling

Variable selection

Model file: ...

Ansys solver: ...

<input checked="" type="checkbox"/> Variable	I/O	Value	Unit
<input checked="" type="checkbox"/> P1	Input	6	m
<input checked="" type="checkbox"/> P2	Input	0.2	m
<input checked="" type="checkbox"/> P3	Input	0.4	m
<input checked="" type="checkbox"/> P5	Output	0.0142555	m
<input checked="" type="checkbox"/> P6	Input	3e+10	Pa
<input checked="" type="checkbox"/> P7	Input	100000	N

Help Continue Cancel

Persalys: Ansys coupling

System selection

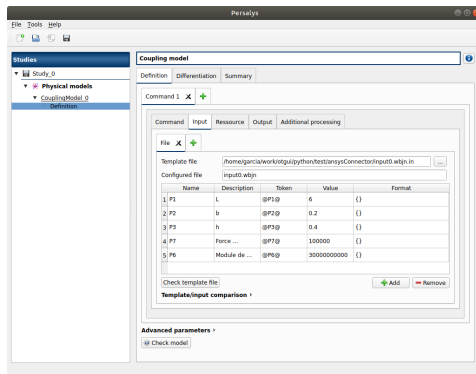
Choose system(s) that need(s) updating

<input checked="" type="checkbox"/> System name	System header text	System type
<input checked="" type="checkbox"/> SYS	Static Structural	Structure statique

Back Finish Cancel

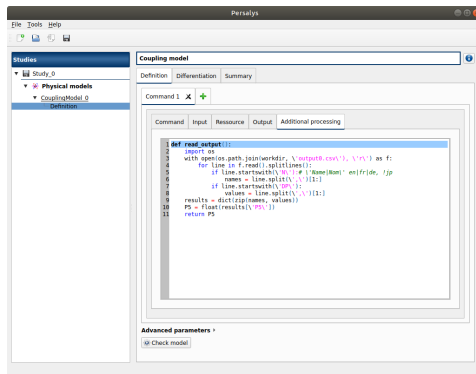
Coupling - Ansys coupling wizard (2)

- Input template file automatically generated based on variables selected by the user



Coupling - Ansys coupling wizard (3)

- Post processing step to account for Ansys output variables



Coupling - Ansys coupling wizard (4)

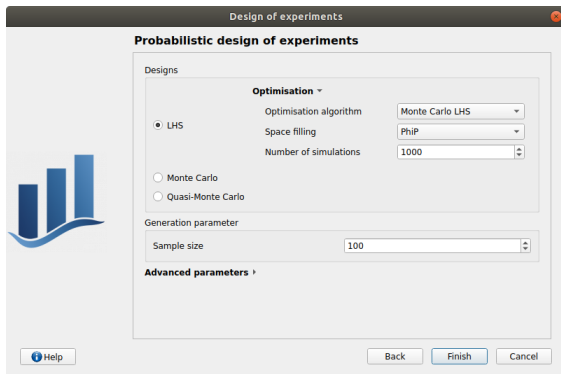
- ▶ Semi-automatic coupling model generation (everything is still modifiable by the user)
- ▶ Benefits from coupling model cache
 - ▶ Already ran evaluation are skipped
 - ▶ Failed points can be reran by editing the cache file

Features - HDF5 support

- ▶ OpenTURNS updates allow to use XMLH5StorageManager
- ▶ Floats and integers are stored in HDF5 datasets (zip-like binary file)
- ▶ Speeds up studies writing/reading
- ▶ Saves up disk-space

Features - Aggregated Sobol' Indices - Optimized LHS

- ▶ Aggregated Sobol' Indices are now available for sensitivity analysis
- ▶ Optimizations for LHS : Simulated-annealing / Monte Carlo LHS available along with space filling algorithms



Field data (functional outputs)

- ▶ 1D fields : better visualisation of large data sets
- ▶ Import and analysis of field data sets
- ▶ Handling of multi-dimensional fields (**long term developments**)

Handling of missing & corrupted data

- ▶ More robust identification of missing data
- ▶ Alternative substitution methods
- ▶ Better interactivity with data tables

Linear regression implementation

- ▶ Regression on polynomial bases of degrees 1 and 2
- ▶ Optimal bases selection (step-wise method)
- ▶ Validation & results analysis (e.g., Cook distance, leverage)

Exportation of surrogate models

- ▶ Possibility of exporting the surrogate models created in Persalys in a python-compatible format easily usable in other scripts

Optimization

- ▶ Handling of equality and inequality constraints
- ▶ Implementation of heuristic (evolutionary) optimization algorithms
- ▶ Possibility of solving multi-objective optimization problems

Kriging

- ▶ Possibility of performing multi-start optimization when training the model

Ergonomic improvements

- ▶ Paraview : better visualisation and interactivity
- ▶ Physical models : numerical differentiation parametrization made more visible

Computation on servers

- ▶ Possibility of stop and restart analyses, even when performed on servers
- ▶ Better handling of error logs

The end

Thanks !

Questions ?