OpenTURNS and HPC within SALOME platform

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HPC and Uncertainty Treatment
Examples with OpenTURNS
EDF – PhiMeca – IMACS -Airbus Group – CEA

Prace Advanced Training Center
May 18th 2018

OUTLINE

1. **Presentation of Salome**
2. **OpenTURNS graphical user interface**
3. **Step by step example**
4. **OpenTURNS graphical user interface distribution and future evolutions**
5. **Examples of OpenTURNS studies with HPC**

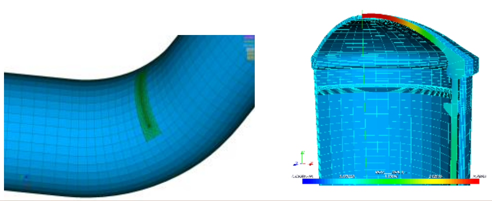
Presentation of Salome (1/8)

- **What's Salome ?**
  - Modular simulation platform
  - An open framework to build domain specific solutions
- **Who is developing Salome ?**
  - EDF, CEA and OpenCascade partnership

Presentation of Salome (2/8)

- **A middleware providing generic tools for numerical simulations**
  - Geometry modelling, meshing, field handling and visualization
  - Data Exchange Model for interoperability between solvers and tools
  - Computation scheduling (YACS)

3D Modelling
(CAD, meshing, visualization)



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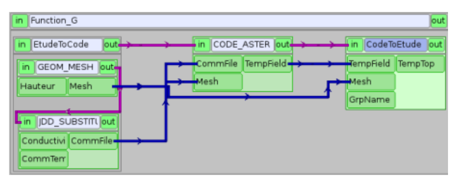
Computation scheduling
(workflow, distribution)



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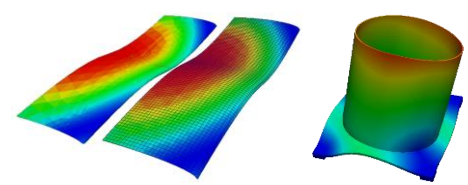
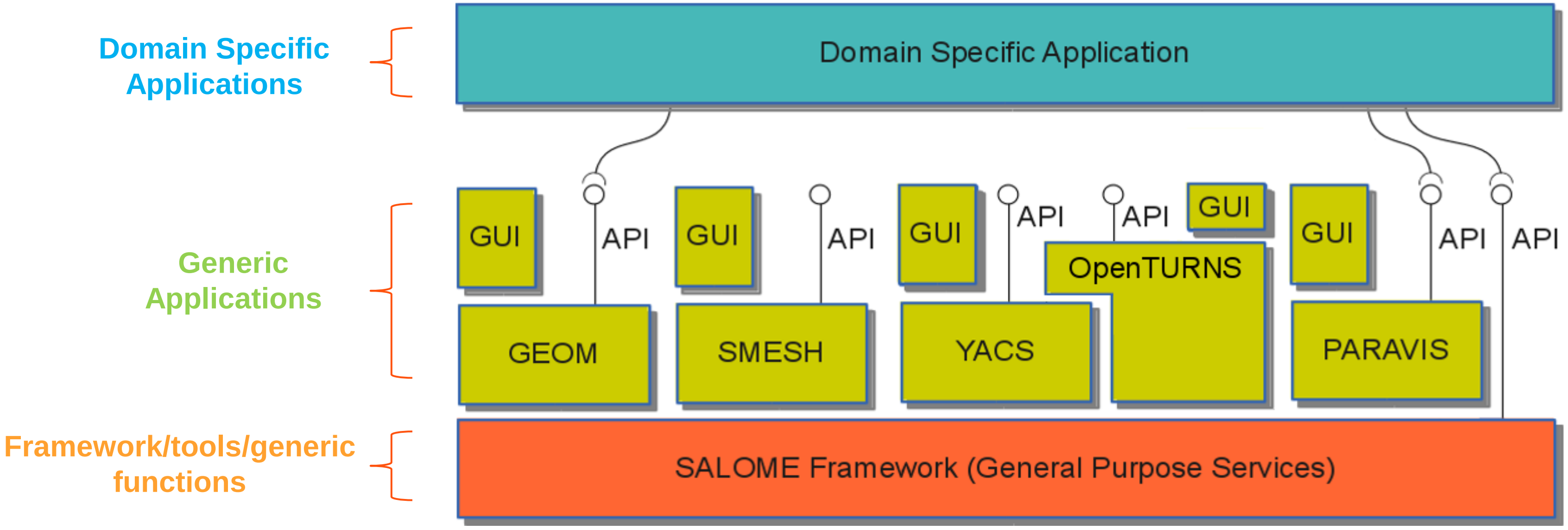
Complex data processing
(fields, matrix, etc)



= SALOME Platform

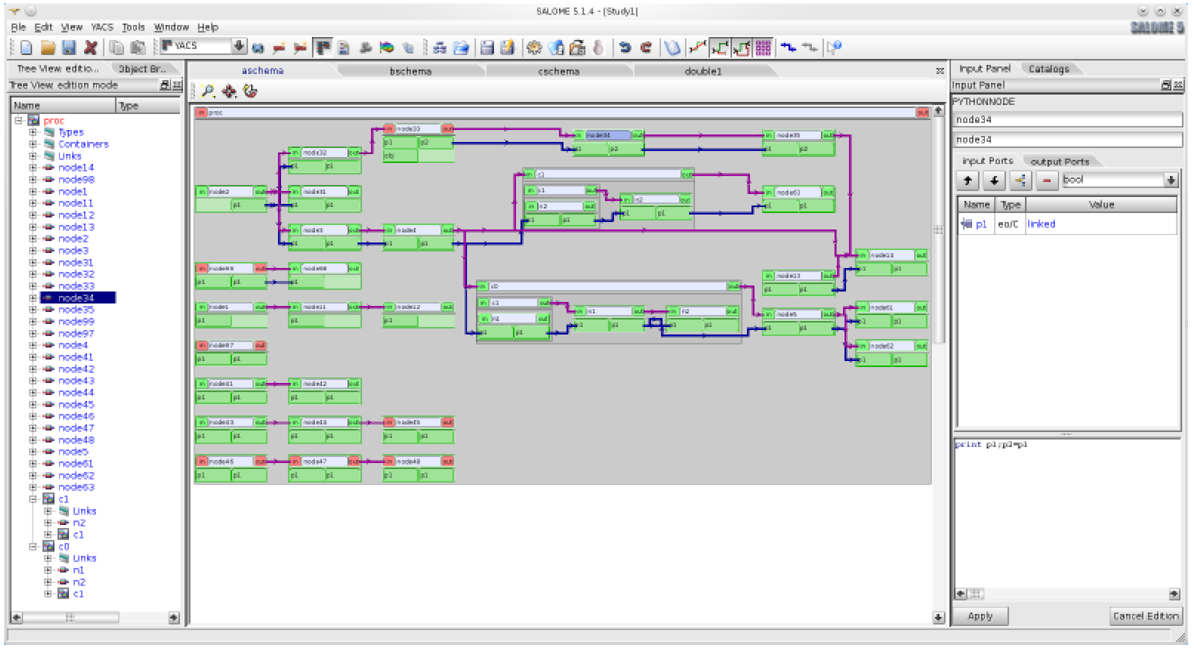
Presentation of Salome (3/8)

- **An open framework to build domain specific solutions**
  - Each module provides :
    - A textual interface for scripting based on Python
    - A graphical interface for interactive usages (C++, Qt, PyQt)
    - A programming interface to build custom applications (API C++ and Python)



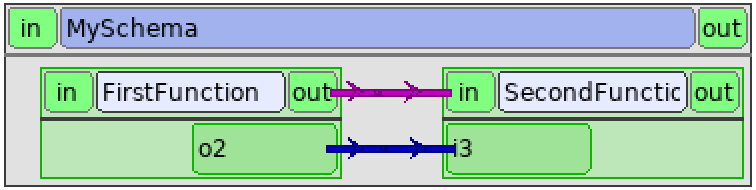
Presentation of Salome (4/8)

- **Presentation of YACS (1/6)**
  - Distribution of computations on multiple resources
  - Parallelism and parametric computation
  - Chaining computation nodes
  - GUI and APIs for Python and C++



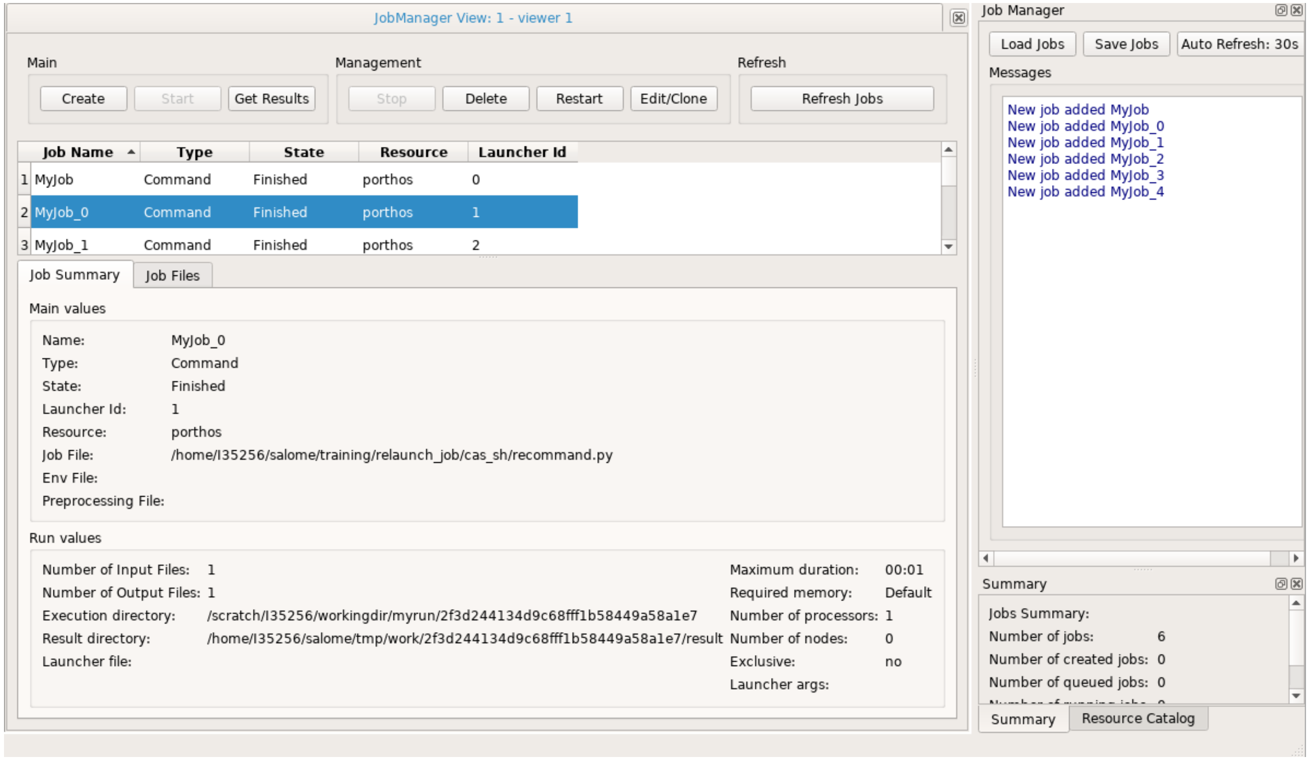
Presentation of Salome (5/8)

- **Presentation of YACS (2/6)**
  - Computation nodes have input and output ports
  - Ports are typed variables (integer, double, string, collections, pyobj or user defined types)
  - Computation nodes have placement constraints
  - Python node: run a python script
  - Salome node: run a function of a Salome component
    - YACSGEN – tool for developing your own SALOME component (C++, python, FORTRAN)
  - Parallel “ForEachLoop”



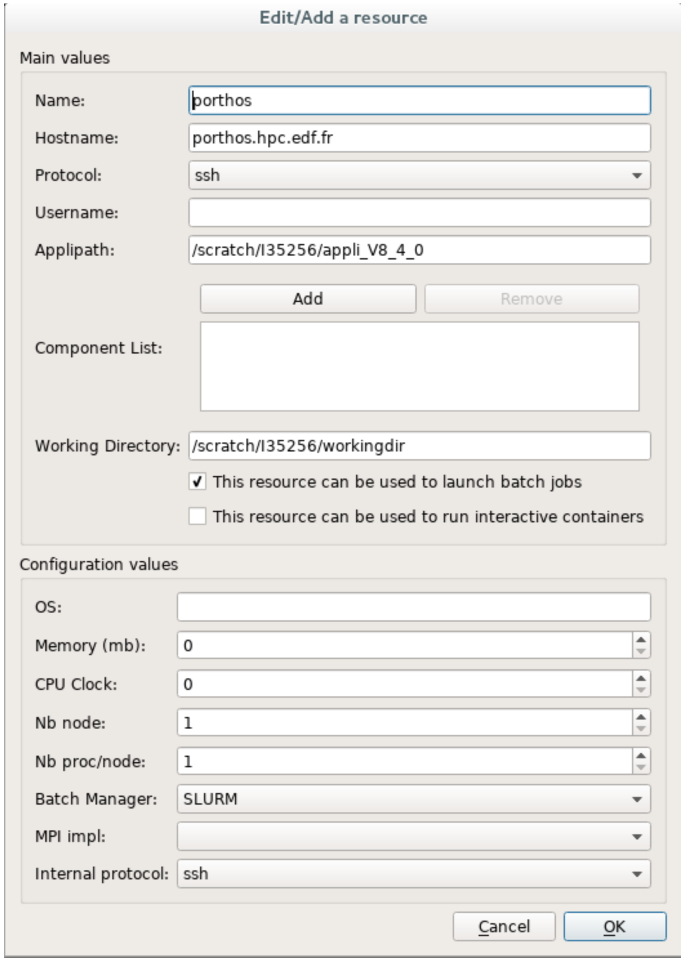
Presentation of Salome (6/8)

- **Presentation of JOBMANAGER (2/6)**
  - Create, launch and monitor jobs on computer clusters
  - Single interface for several batch managers (Slurm, PBS, COORM, OAR, SGE, LSF)
  - GUI and APIs for Python and C++
  - Jobs can run scripts or YACS schemas



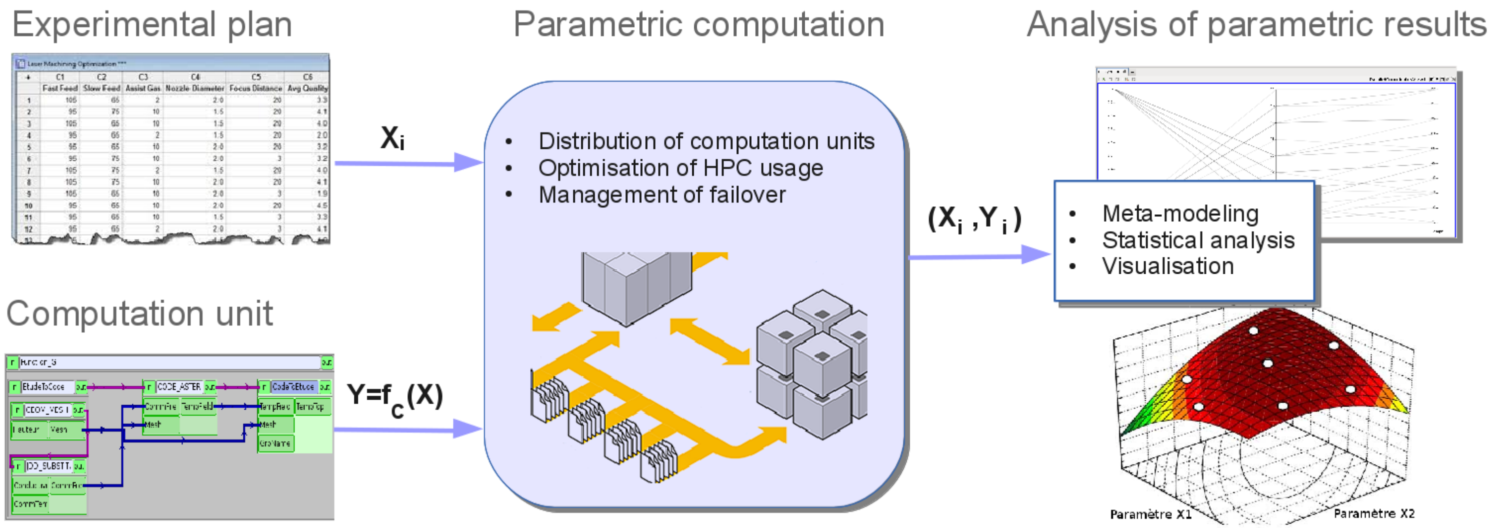
Presentation of Salome (7/8)

- **Salome resources**
  - Salome has to be installed on every machine you want to use
  - You have to declare each installation in your local catalog of resources



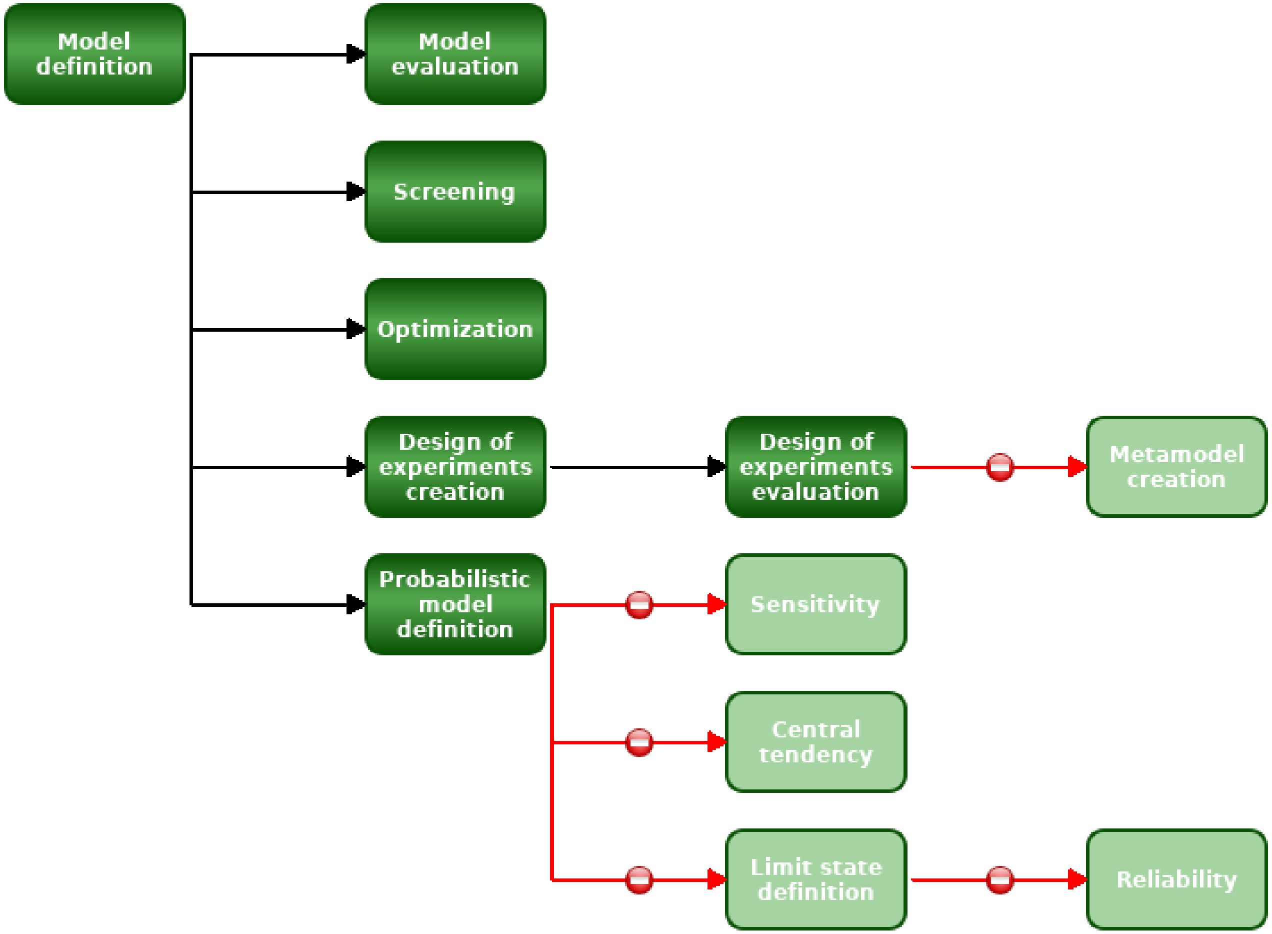
Presentation of Salome (8/8)

- **Parametric layer**
  - Simplified interface for parametric studies
  - Uses YACS and JOBMANAGER



OpenTURNS Graphical User Interface (1/5)

- **Goal of OpenTURNS GUI**
  - Guide user in a homogeneous environment through the roadmap defined by the global methodology of treatment of uncertainties (physical model evaluation and display of result to take decisions…)



OpenTURNS Graphical User Interface (2/5)

- **OpenTURNS GUI is more than a simple GUI !**
  - OpenTURNS GUI is based on a high level object model (Main study, Deterministic study, Probabilistic study, …)
  - OpenTURNS GUI includes a layer over OpenTURNS tools.
  - OpenTURNS GUI has been designed to mix beginners and advanced users

- **How can you use it ?**
  - Standalone binary called otgui
  - In a dedicated salome module
  - Can be used in customized salome module

OpenTURNS Graphical User Interface (3/5)

- **Two complementary ways to pilot OpenTURNS GUI : Python and widgets**
- **The design of OpenTURNS GUI allows a strong relationship between Python scripting and graphical interface (Model/View paradigm).**
  - Actions you perform on gui can be mapped into a Python representation.
  - Load python script and dump python script.
  - Start session with graphical interface then continue with script then…
- **OpenTURNS GUI offers software bricks usable outside a dedicated tool**

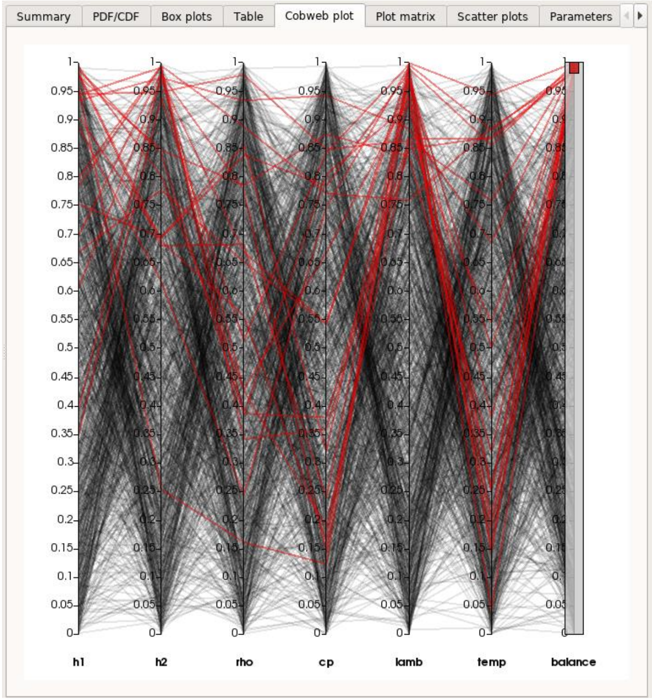
OpenTURNS Graphical User Interface (4/5)

- **OpenTURNS GUI is an excellent target for High Performance Computing (HPC)**
  - A large number of independent computations
- **The usage of distributed resources is very dependent on the context:**
  - Use of a cluster (homogeneous, centralized) / a grid (heterogeneous, decentralized)?
  - Communication protocol with the cluster?
  - Which batch / grid manager?
  - Can we install software on the cluster?
  - Global / local (by node) file system?
  - Execution of OpenTURNS script on the client workstation / on the cluster?
  - Which middleware for the distribution on the cluster?
  - Size of input and output files of the solver code?

→ OpenTURNS GUI uses Salome

OpenTURNS Graphical User Interface (5/5)

- **SALOME software bricks used OpenTURNS GUI**
  - YACS & JOBMANAGER
  - GUI Python console widget
  - PARAVIS widgets



Step by step example (1/6)

- **Goal**
  - Compute an OpenTURNS study of a python function using a computer cluster
- **Prerequisite**
  - Create the python function of a unitary case
  - Input parameters must be only float variables
  - Return statement must contain only float variables
  - Run and test the function outside Salome

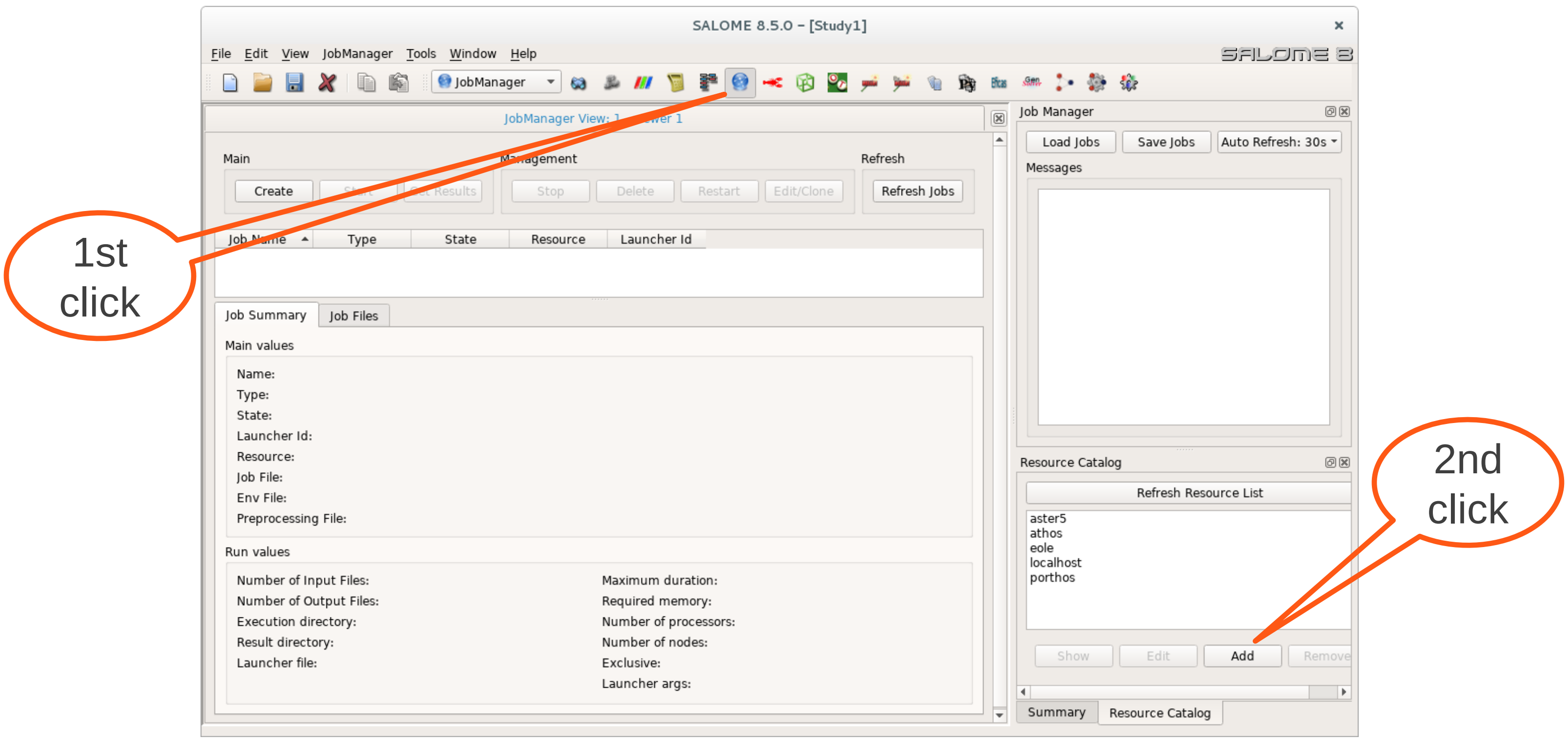
Heat exchange computation with SYRTHES

Heat exchange coefficient: h1, h2
Conductivity: lamb
Density: rho
Heat capacity: cp

```
def _exec(h1, h2, rho, cp, lamb):

    etude=Etude()
    etude.init(h1, h2, rho, cp, lamb)

    #Run the calculation
    etude.launch_calc()

    #Temperature at the probe
    temp = etude.extract_probe(2,2)

    #Balance at 2
    balance = etude.extract_balance(2, 2)

    return temp, balance
```

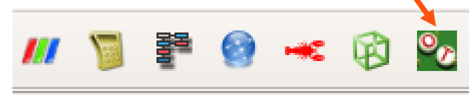
Step by step example (2/6)

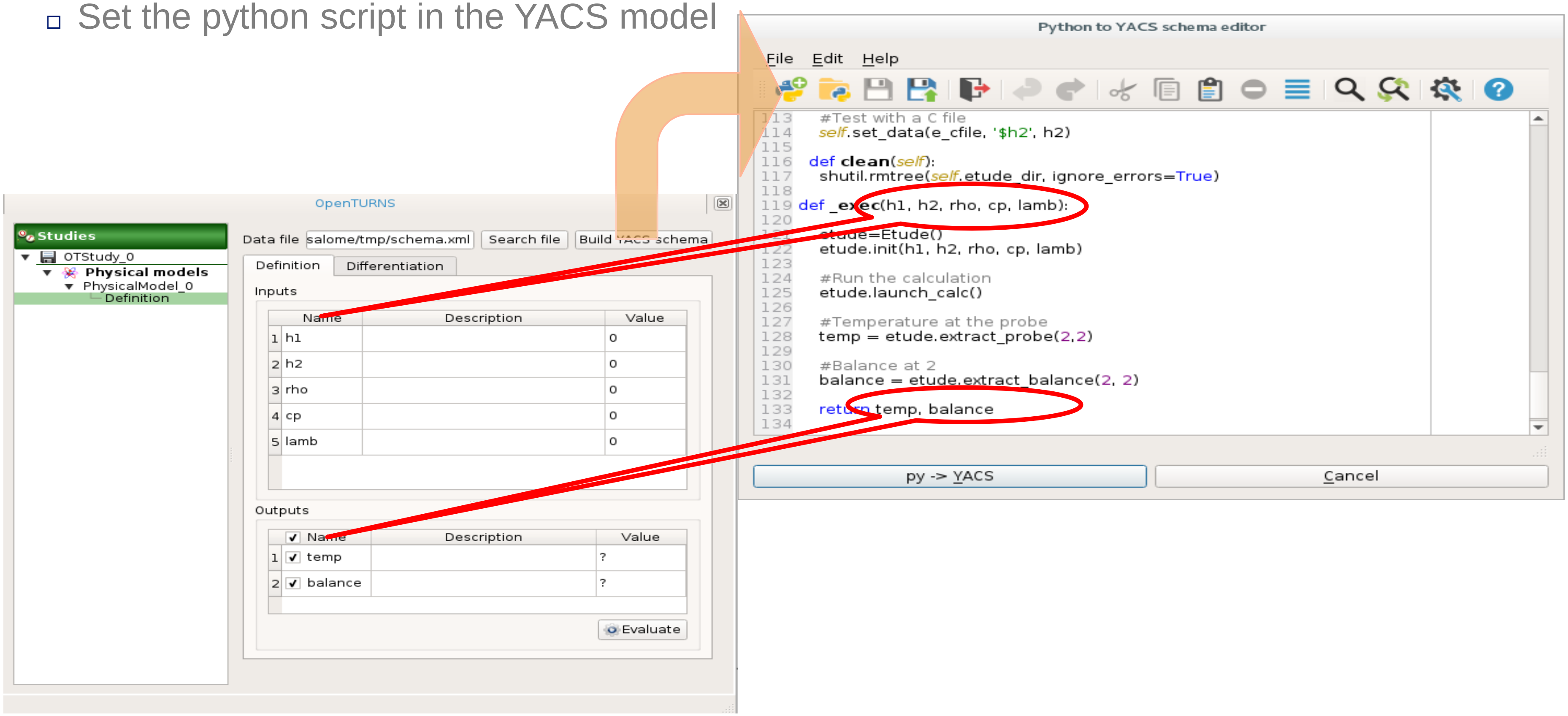
- **Installation steps**
  - Install Salome on your personal computer
  - Install Salome on the remote cluster
  - Make sure you can connect to cluster without typing the password (ssh-copy-id)
  - Declare the cluster installation in your local resource catalog (JOBMANAGER module)



Step by step example (3/6)

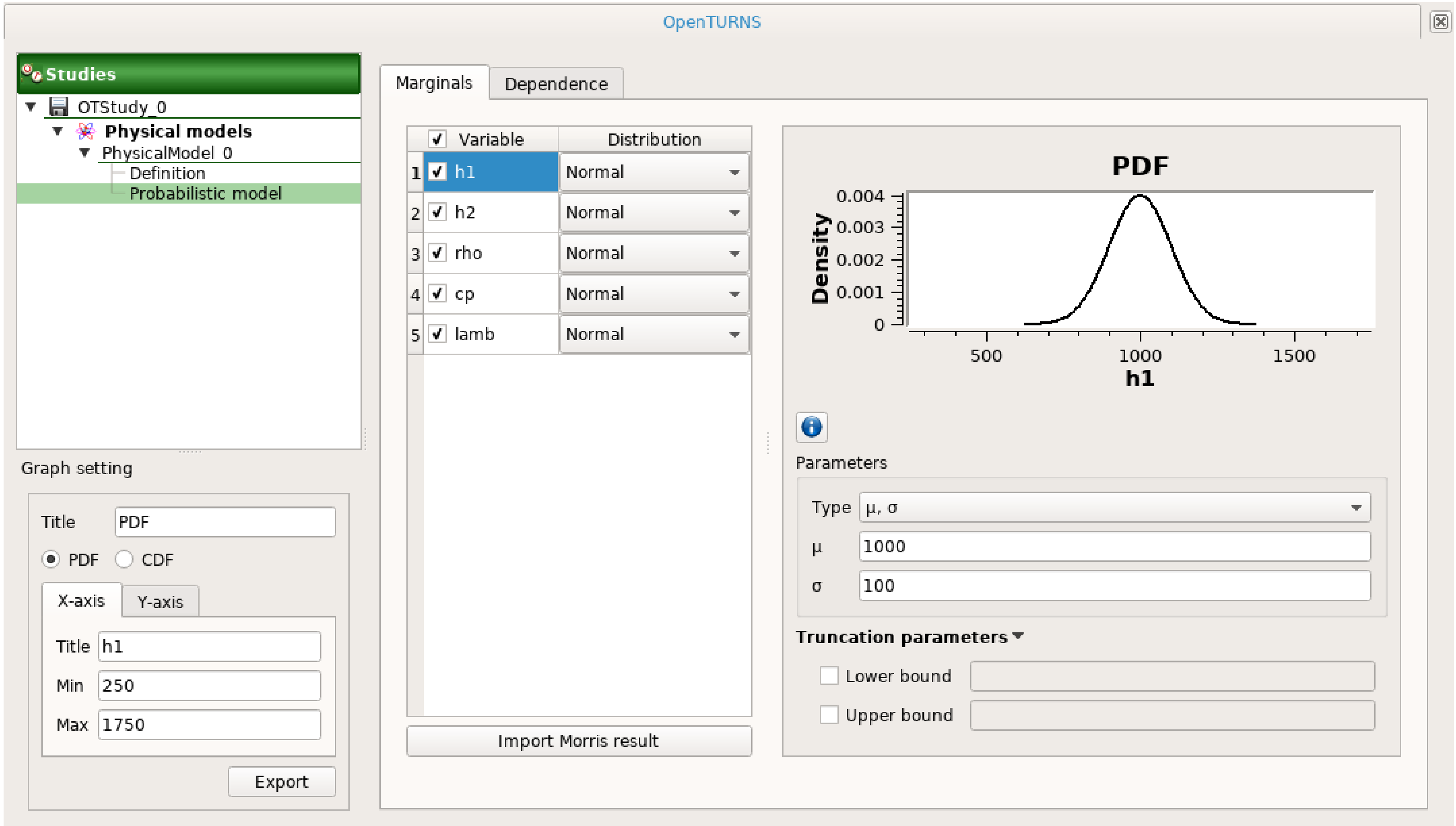
- **OpenTURNS study steps**
  - Open the OpenTURNS module in a Salome session
  - Create a new study with a YACS model
  - Set the python script in the YACS model





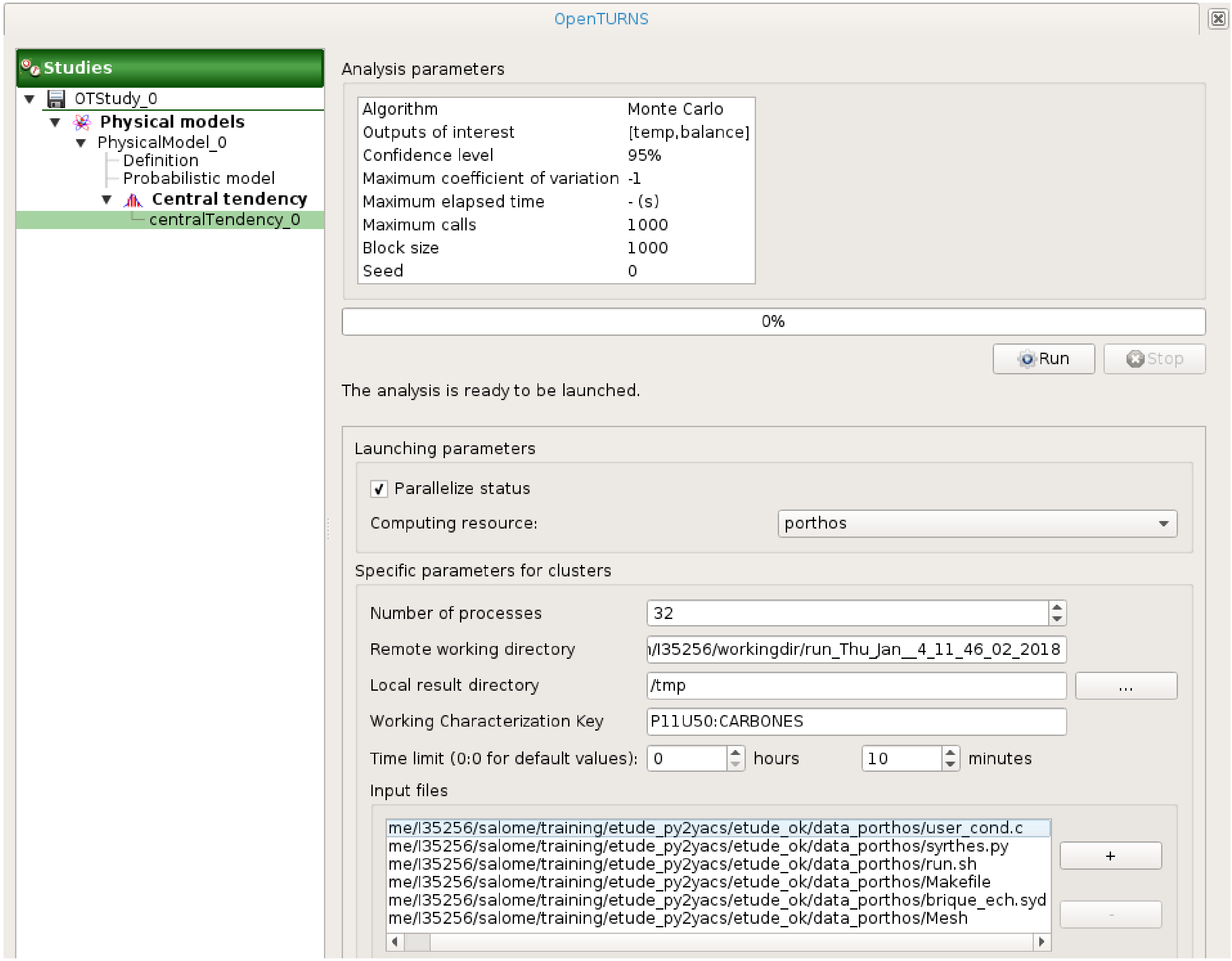
Step by step example (4/6)

- **OpenTURNS study steps**
  - Choose the laws of the input parameters



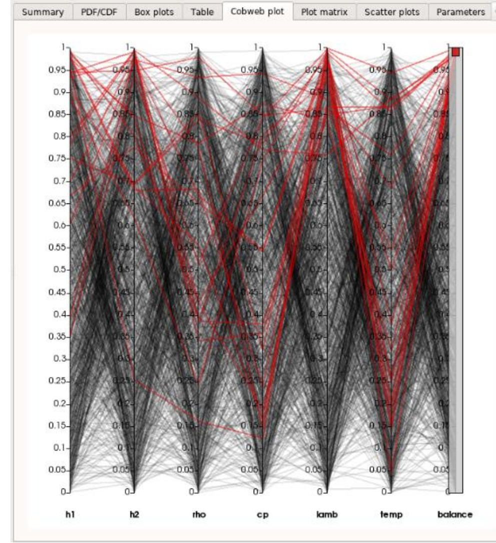
Step by step example (5/6)

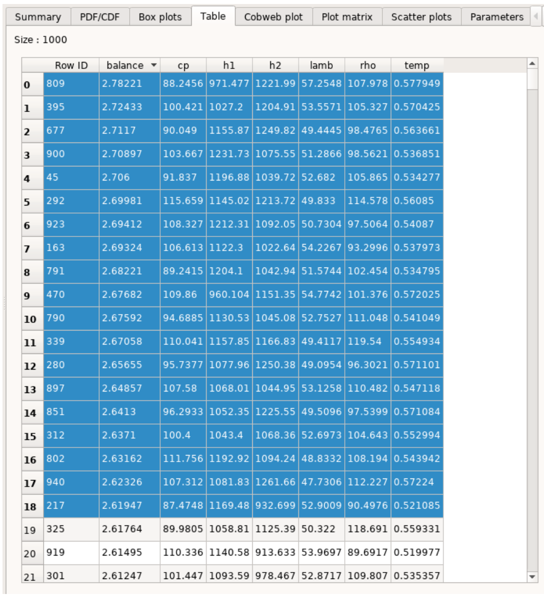
- **OpenTURNS study steps**
  - Launch the computation on the remote cluster



Step by step example (6/6)

- **OpenTURNS study steps**
  - Result analysis
    - Box plots, Cobweb plot, Plot matrix, Scatter plots

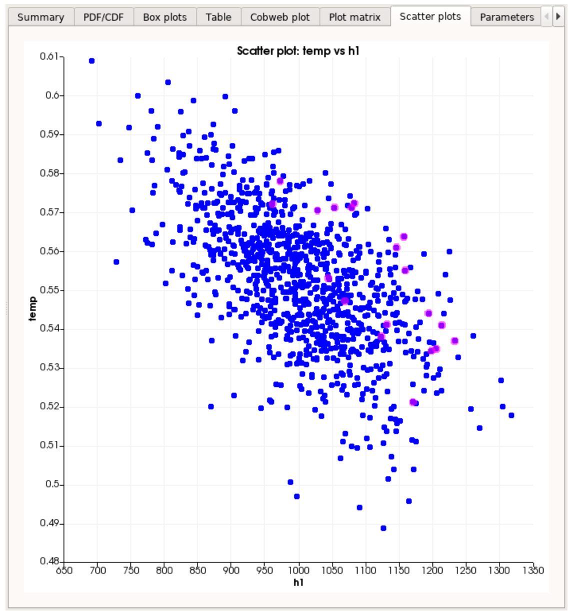


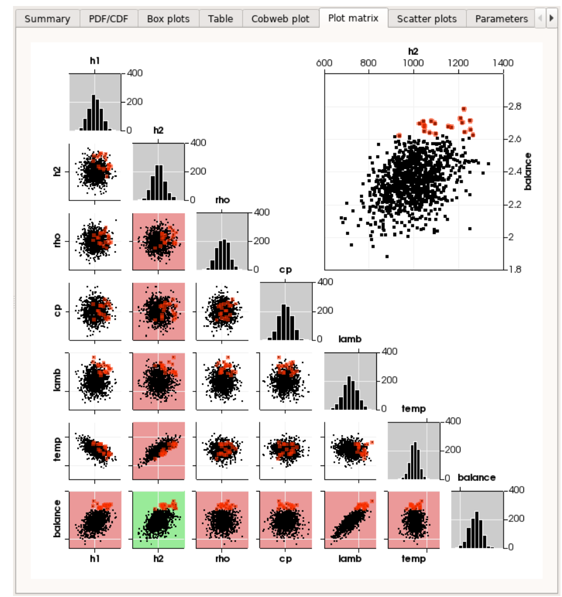


Summary | PDF/CDF | Box plots | Table | Cobweb plot | Plot matrix | Scatter plots | Parameters

Size : 1000

	Row ID	balance	cp	h1	h2	lamb	rho	temp
0	809	2.78221	88.2456	971.477	1221.99	57.2548	107.978	0.577949
1	395	2.72433	100.421	1027.2	1204.91	53.5571	105.327	0.570425
2	677	2.7117	90.049	1155.87	1249.82	49.4445	98.4765	0.563661
3	900	2.70897	103.667	1231.73	1075.55	51.2866	98.5621	0.536851
4	45	2.706	91.837	1196.88	1039.72	52.682	105.865	0.534277
5	292	2.69981	115.659	1145.02	1213.72	49.833	114.578	0.56085
6	923	2.69412	108.327	1212.31	1092.05	50.7304	97.5064	0.54087
7	163	2.69324	106.613	1122.3	1022.64	54.2267	93.2996	0.537973
8	791	2.68221	89.2415	1204.1	1042.94	51.5744	102.454	0.534795
9	470	2.67682	109.86	960.104	1151.35	54.7742	101.376	0.572025
10	790	2.67592	94.6885	1130.53	1045.08	52.7527	111.048	0.541049
11	339	2.67058	110.041	1157.85	1166.83	49.4117	119.54	0.554934
12	280	2.65655	95.7377	1077.96	1250.38	49.0954	96.3021	0.571101
13	897	2.64857	107.58	1068.01	1044.95	53.1258	110.482	0.547118
14	851	2.6413	96.2933	1052.35	1225.55	49.5096	97.5399	0.571084
15	312	2.6371	100.4	1043.4	1068.36	52.6973	104.643	0.552994
16	802	2.63162	111.756	1192.92	1094.24	48.8332	108.194	0.543942
17	940	2.62326	107.312	1081.83	1261.66	47.7306	112.227	0.57224
18	217	2.61947	87.4748	1169.48	932.699	52.9009	90.4976	0.521085
19	325	2.61764	89.9805	1058.81	1125.39	50.322	118.691	0.559331
20	919	2.61495	110.336	1140.58	913.633	53.9697	89.6917	0.519977
21	301	2.61247	101.447	1093.59	978.467	52.8717	109.807	0.535357





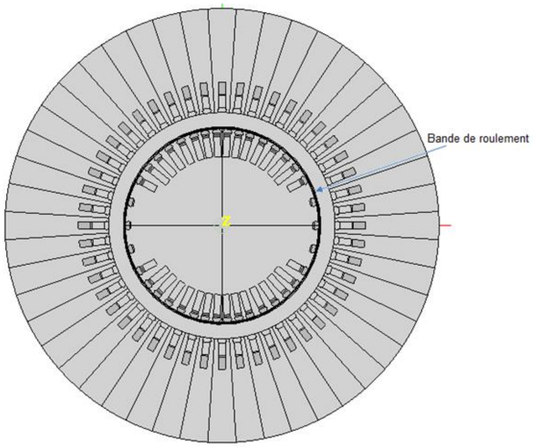
OpenTURNS Graphical User Interface - Distribution and future evolutions (1/2)

- **Distribution of SALOME + OpenTURNS platform**
  - LGPL license for the whole platform (SALOME + OpenTURNS + OPENTURNS GUI)
  - Download SALOME platform with OpenTURNS here:
    - http://www.salome-platform.org/contributions/copy_of_combs

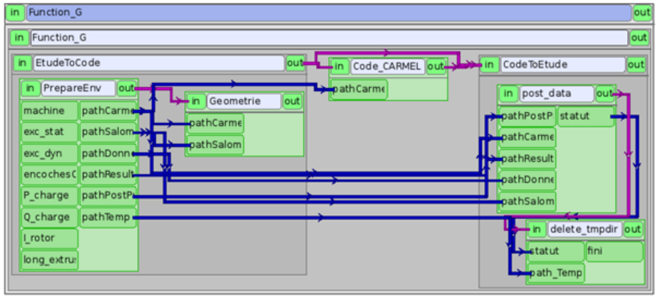
OpenTURNS Graphical User Interface - Distribution and future evolutions (2/2)

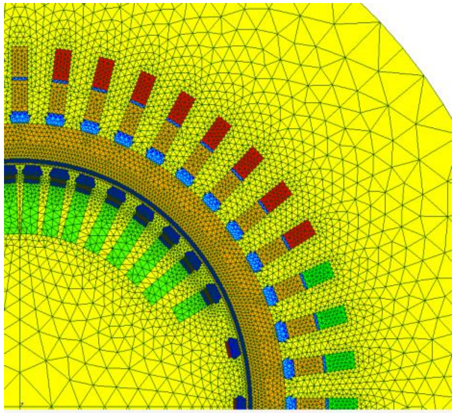
- **Improvements to come**
  - Launch, leave and reconnect to a job
  - Avoid multiple job submissions for one OpenTURNS study
  - Management of a partially executed study
  - Management of failed computations

Examples of OpenTURNS studies with HPC (1/3)



- **Probes in an alternator**
  - Optimization of the position of probes in an alternator to maximize the signal fidelity
  - Solver: CARMEL
  - Elementary calculation: Mesh with ~200000 cells. 92 hours
  - OpenTURNS study: 115 elementary calculations ➔ about 10000 CPU hours

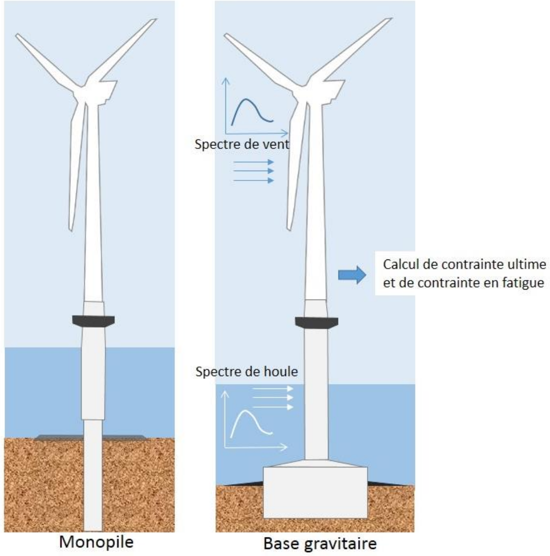




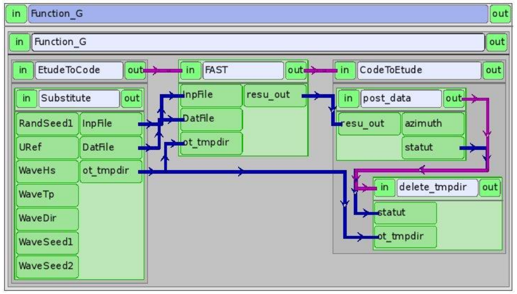
Desquiens 2016

Examples of OpenTURNS studies with HPC (2/3)

- **Offshore wind turbine**
  - Study of lifetime of offshore wind turbine sustaining extreme scenarios in terms of strain.
  - Solver: FAST
  - Elementary calculation: No mesh. ~10 minutes.
  - OpenTURNS study: 10000 elementary calculations ➔ about 17000 CPU hours

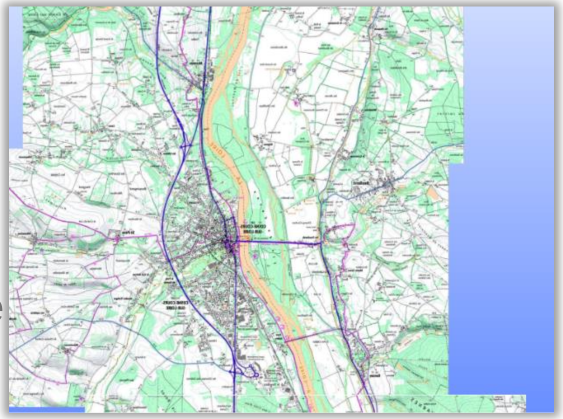


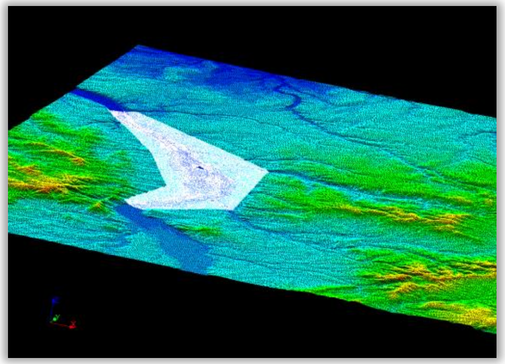
Bousseau 2016

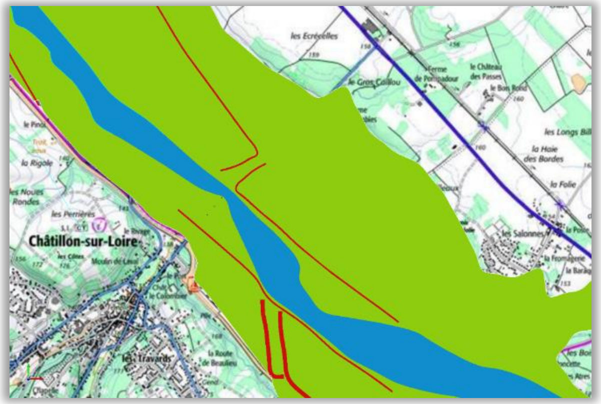


Examples of OpenTURNS studies with HPC (3/3)

- **Evaluation of the environment impact of the flood of a river**
  - Solver: TELEMAC/MASCARET
  - Elementary calculation: Mesh with ~100000 cells. Convergence reached in about ~1-10 hours







Questions?