OpenTURNS and HPC within SALOME platform

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

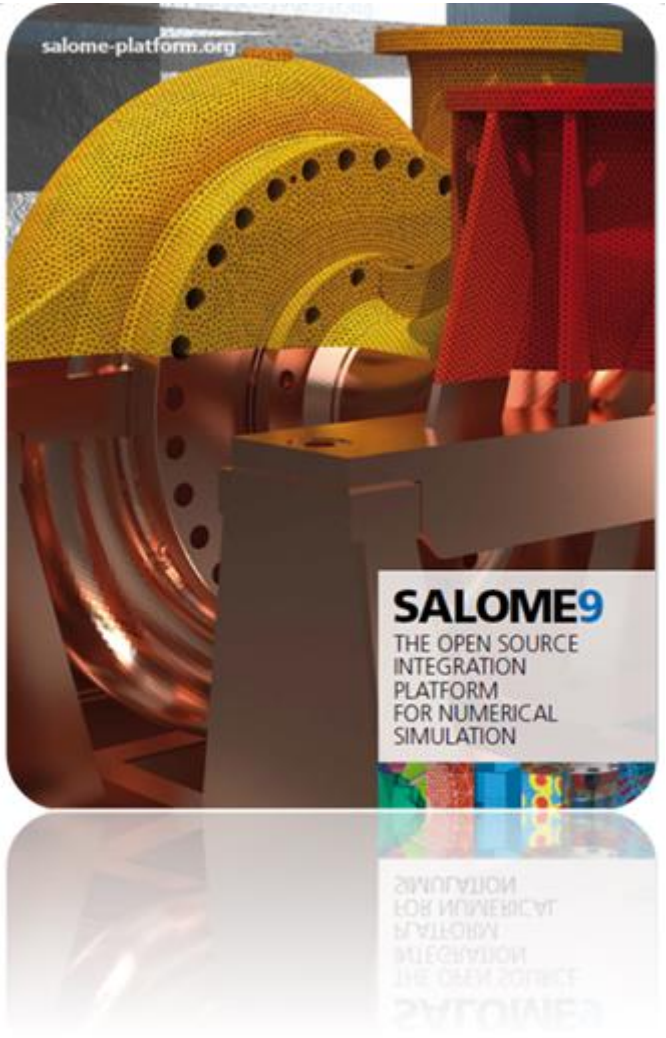
Prace Advanced Training Center
May 29th 2019

OUTLINE

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

Presentation of Salome (1/5)

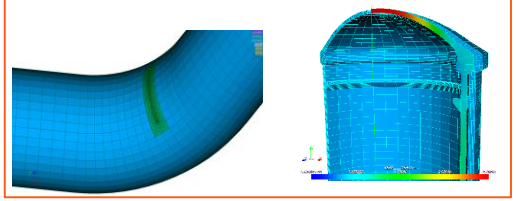
- **What's Salome ?**
  - Modular simulation platform
  - An open framework to build domain specific solutions
- **Who is developing Salome ?**
  - EDF, CEA and OpenCascade partnership



Presentation of Salome (2/5)

- **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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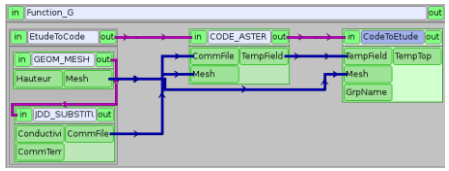
Computation scheduling
(workflow, distribution)



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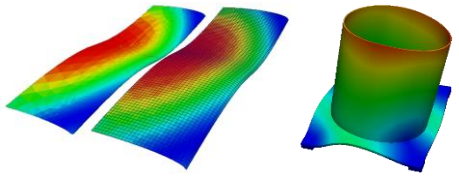
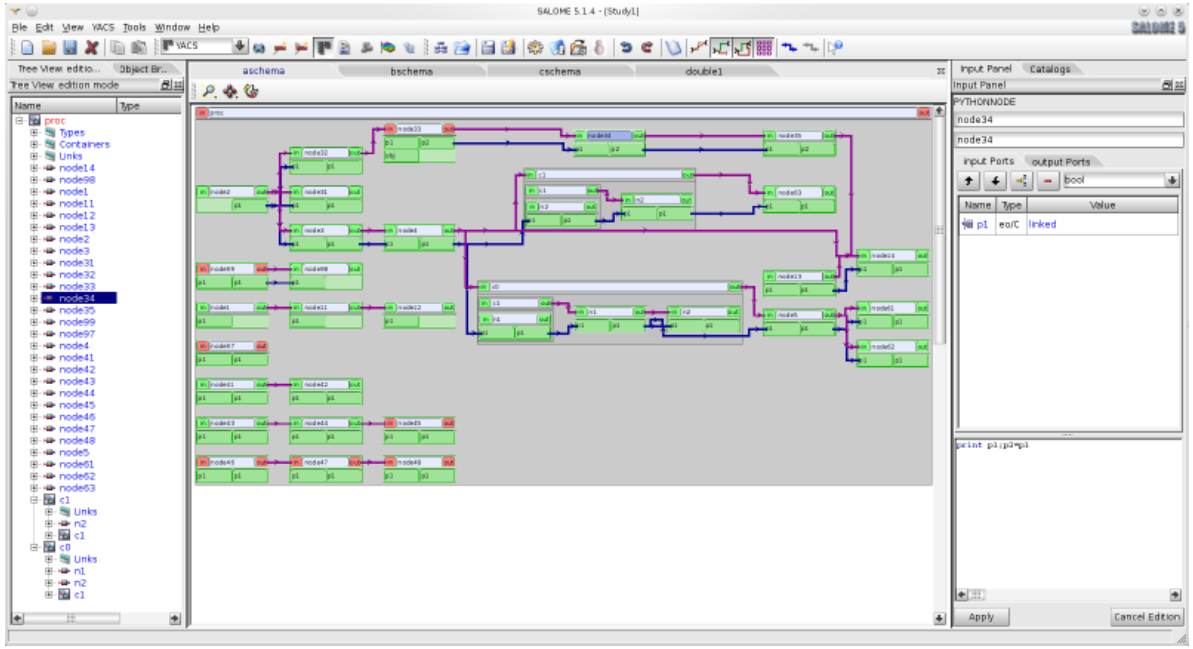
Complex data processing
(fields, matrix, etc)



= SALOME Platform

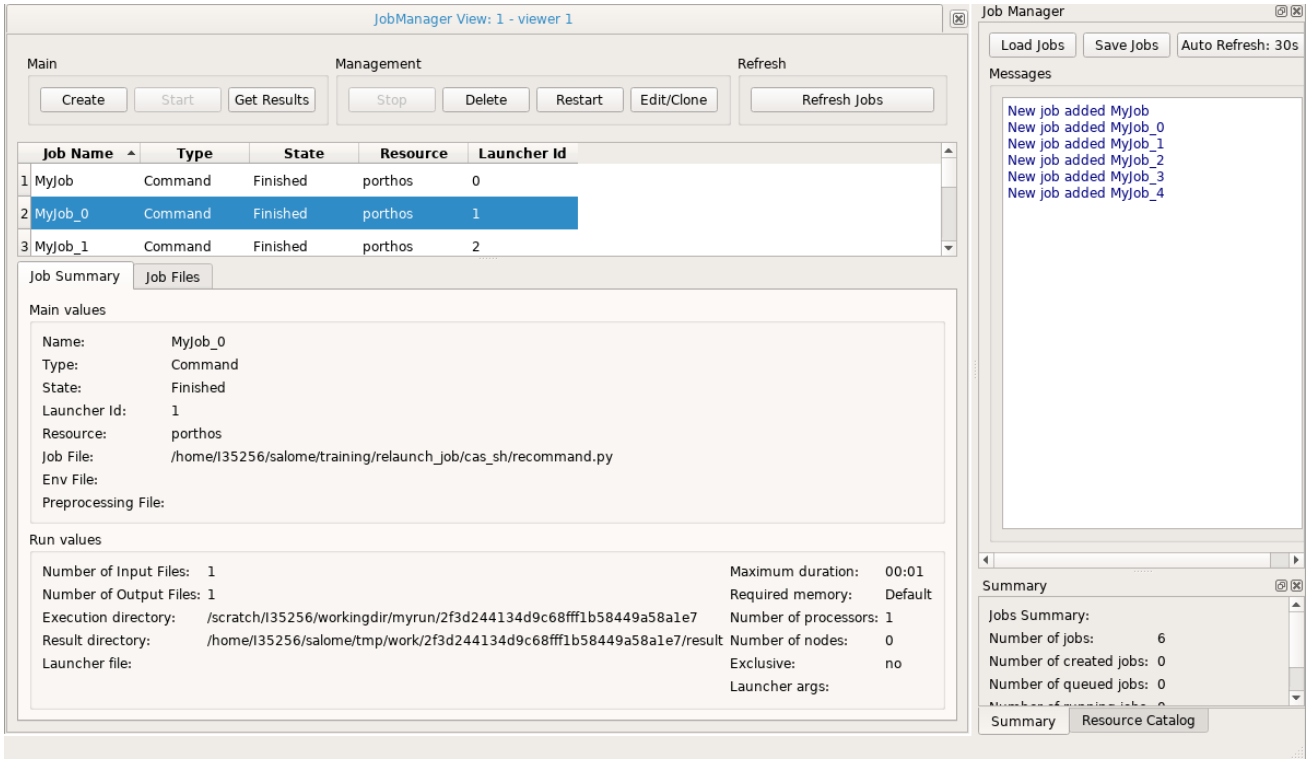
Presentation of Salome (3/5)

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



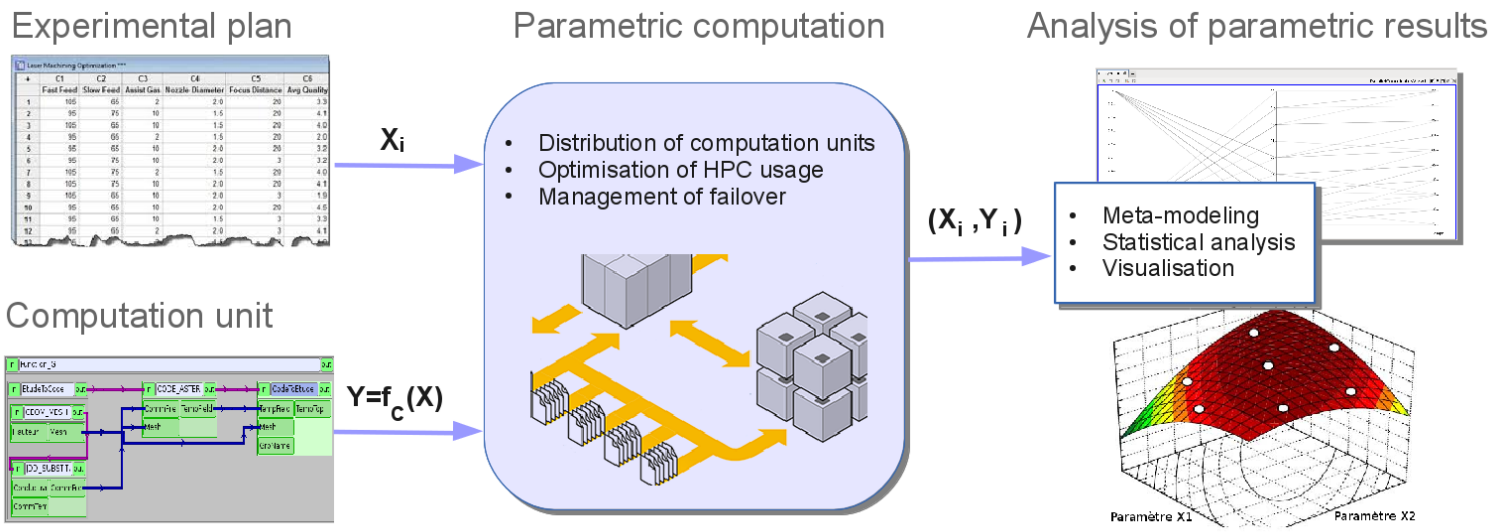
Presentation of Salome (4/5)

- **Presentation of JOBMANAGER**
  - 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



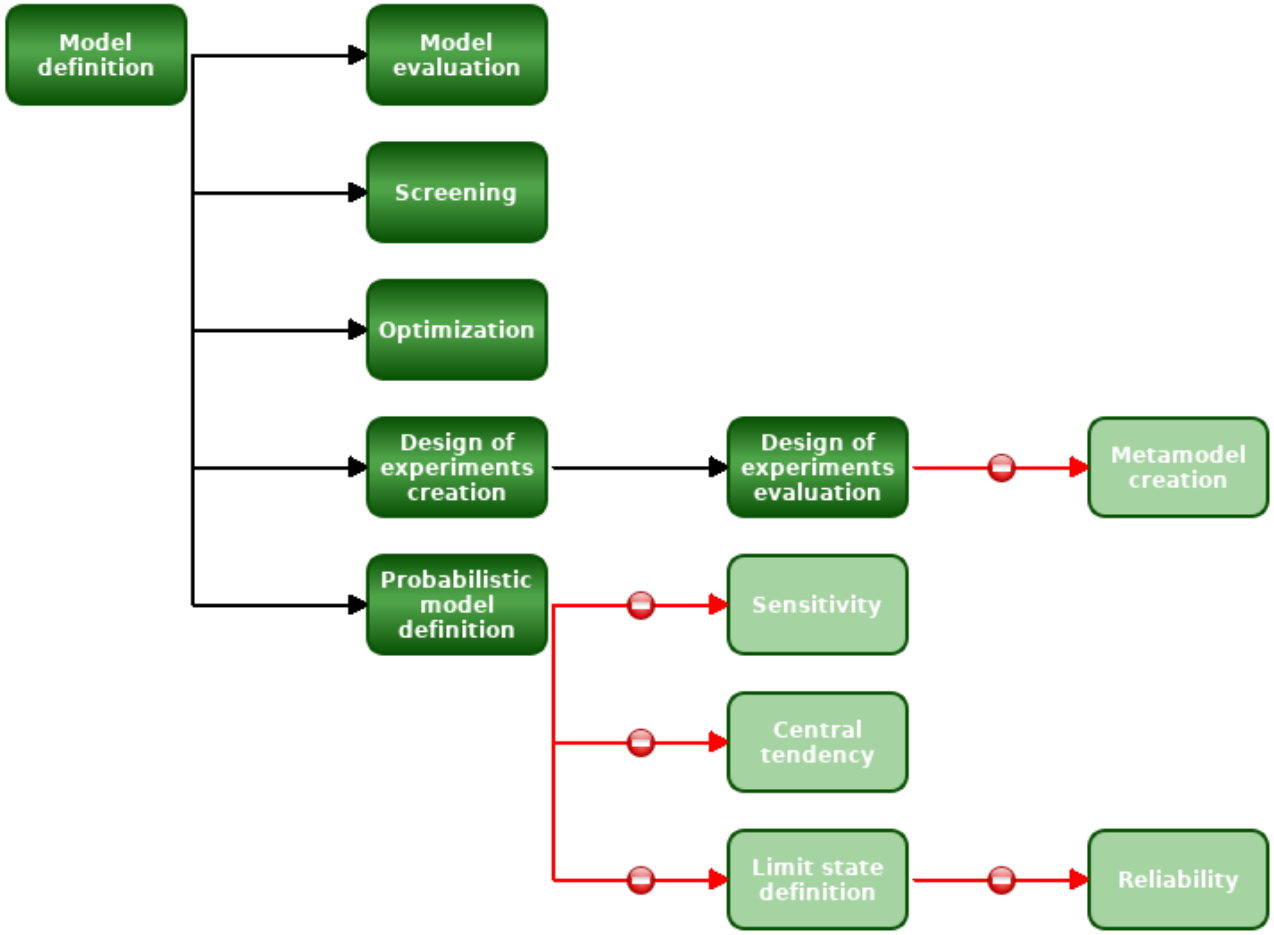
Presentation of Salome (5/5)

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



OpenTURNS Graphical User Interface (1/5)

- **Goal of OpenTURNS GUI**
  - Guide the user in a homogeneous environment through the roadmap defined by the global methodology of treatment of uncertainties



OpenTURNS Graphical User Interface (2/5)

- **OpenTURNS GUI is more than a simple GUI !**
  - OpenTURNS GUI is based on a high level object model (study workflow)
  - 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 a customized salome module

OpenTURNS Graphical User Interface (3/5)

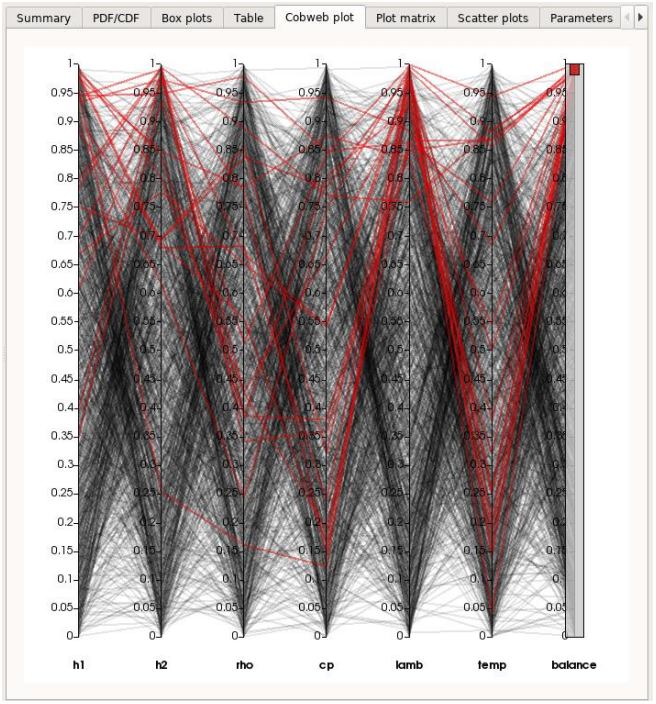
- **Two complementary ways to pilot OpenTURNS GUI : Python and widgets**
- **The design of OpenTURNS GUI allows a strong relationship between Python scripting and graphical interface (Model/View paradigm).**
  - Actions you perform on gui can be mapped into a Python representation.
  - Load python script 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 evaluations
- **Salome features used by OpenTURNS GUI:**
  - Manage a catalog of available resources
  - Make the evaluations parallel and distributed
  - Communicate with the batch manager
    - Define the job parameters
    - Submit and keep track of a job
  - Define the execution environment
    - Define a working directory
    - Copy data from the local workstation to the remote cluster
  - Fetch the results

OpenTURNS Graphical User Interface (5/5)

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

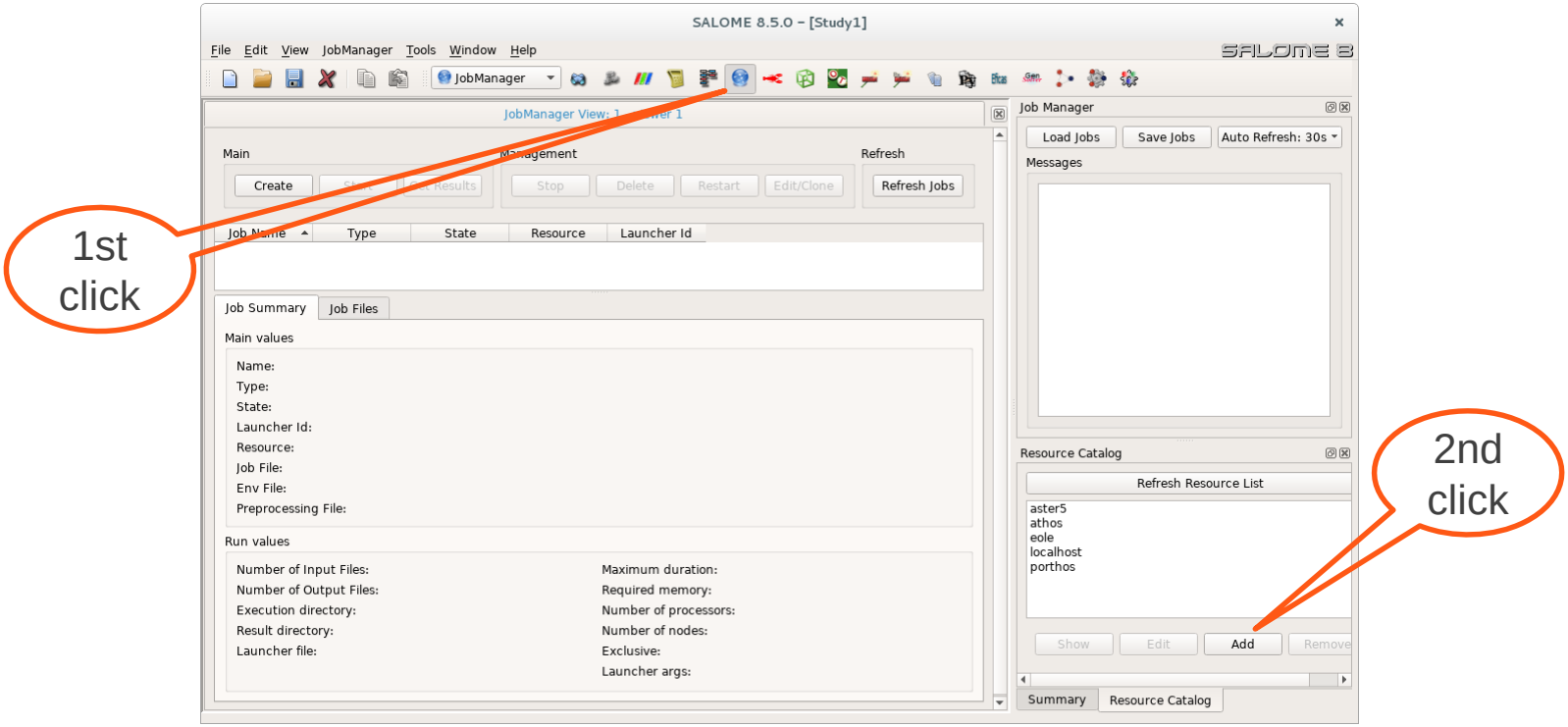


A STUDY STEP BY STEP

- Install and configure Salome
- Define the function to be studied
- Create a model (YACS or python models in the GUI)
- Define the laws of input parameters
- Choose the type of study (central tendency, etc.)
- Choose the execution parameters
- Run the study and wait for results
- Analyse the results

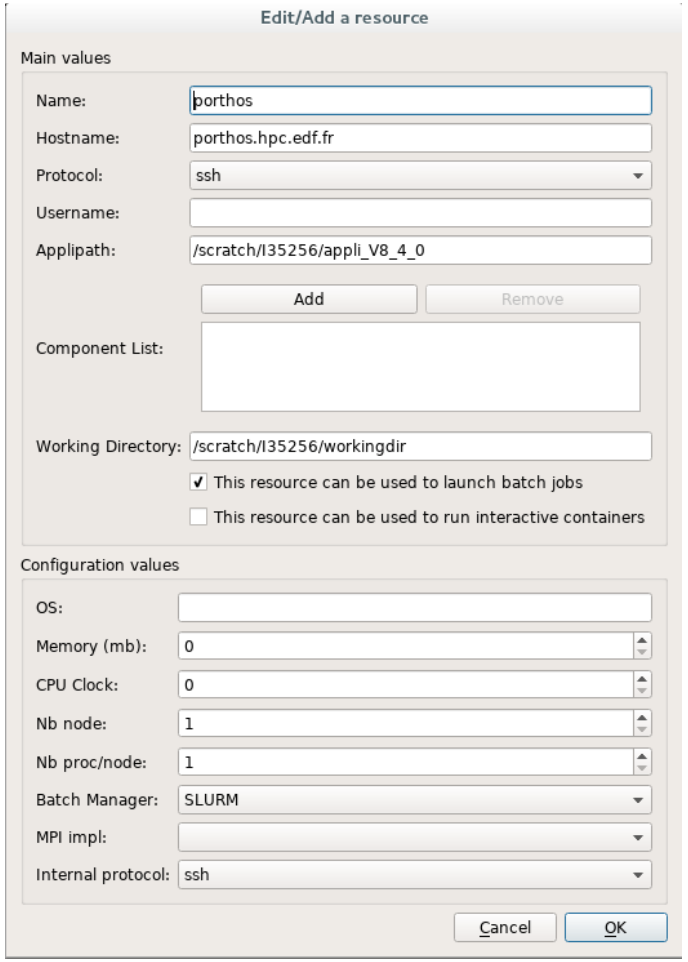
Install and configure Salome

- **Installation steps**
  - Install Salome on your personal computer
    - https://www.salome-platform.org/contributions/edf_products
  - 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)



Configure available resources

- **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
  - Main parameters:
    - Name
    - IP adresse
    - User name
    - Path to Salome installation
    - Batch manager



Define the function to be studied

- **Identify uncertain parameters – inputs and outputs of your study**
- **Use the python language**
  - Input parameters must be only float variables
  - Return statement must contain only float variables
  - The name of the function should be “_exec”
- **The python function should:**
  - Generate the input files for the solver based on the input parameters
    - Create a specific working directory for each execution of the function
  - Launch the solver
  - Retrieve the results from the output files of the solver
- **Test your function**

Example of a study function

- **Syrthes : thermal radiation solver**

Heat exchange computation with SYRTHES

h1 T1
Face S1

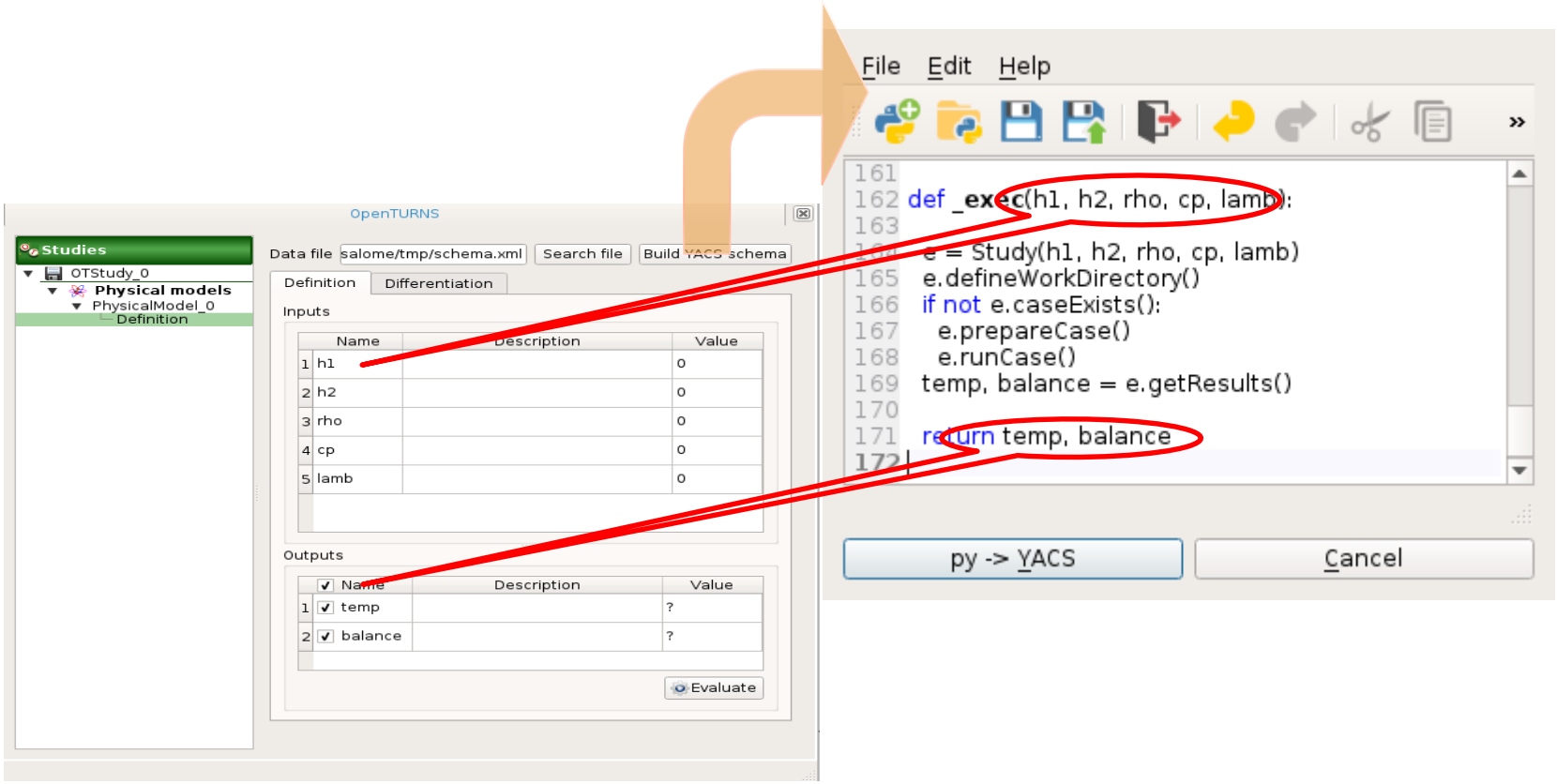
h2 T2
Face S2

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

```
def _exec(h1, h2, rho, cp, lamb):
  e = Study(h1, h2, rho, cp, lamb)
  e.defineWorkDirectory()
  if not e.caseExists():
    e.prepareCase()
    e.runCase()
  temp, balance = e.getResults()
  return temp, balance
```

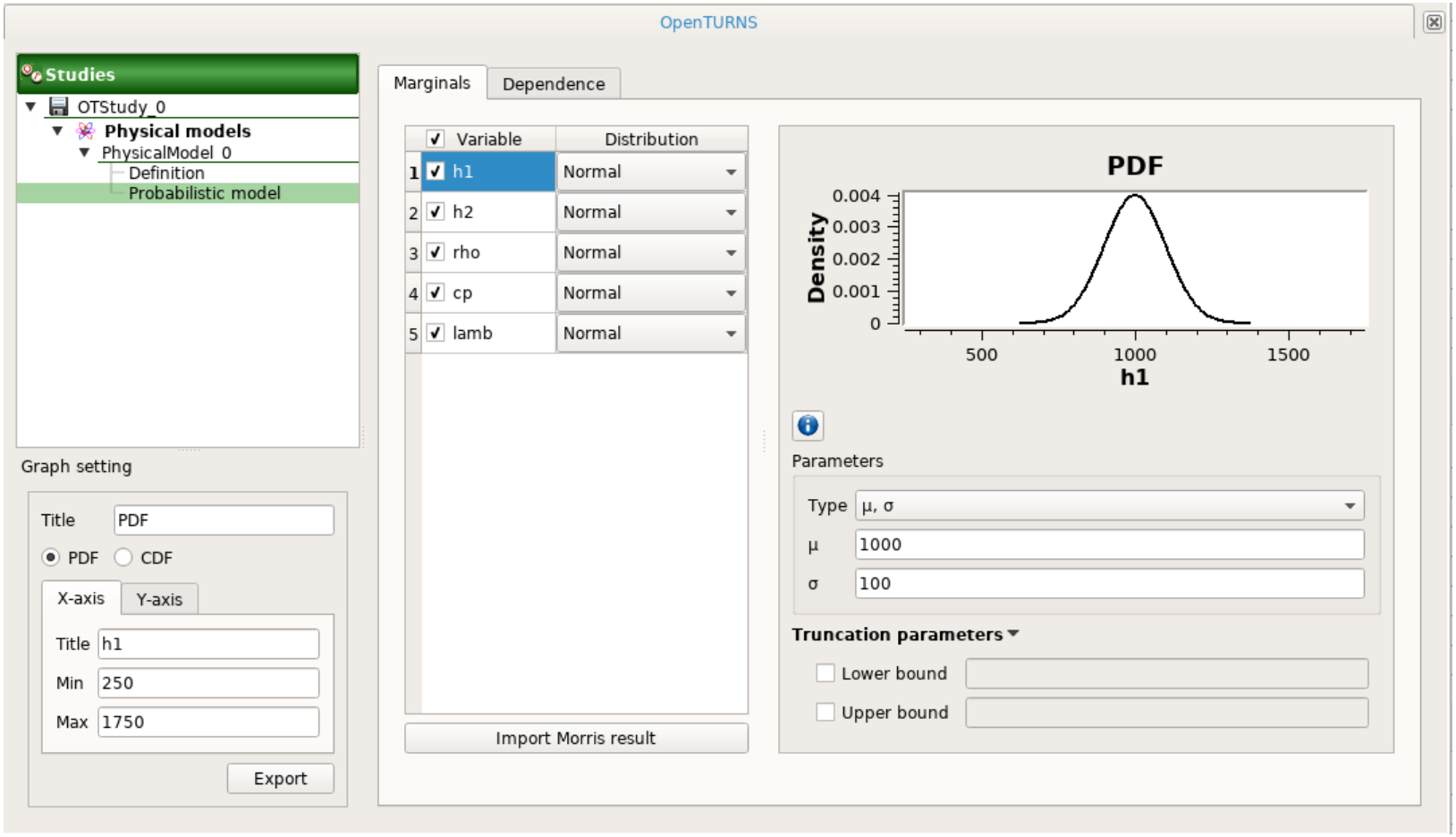
Create a model

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

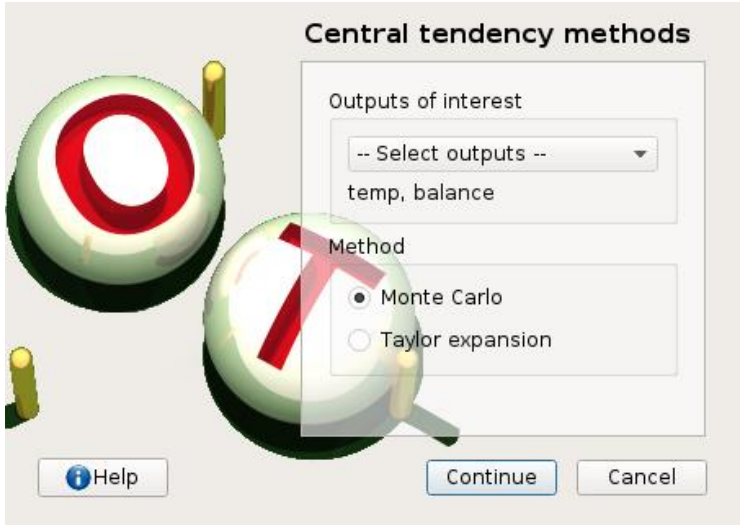


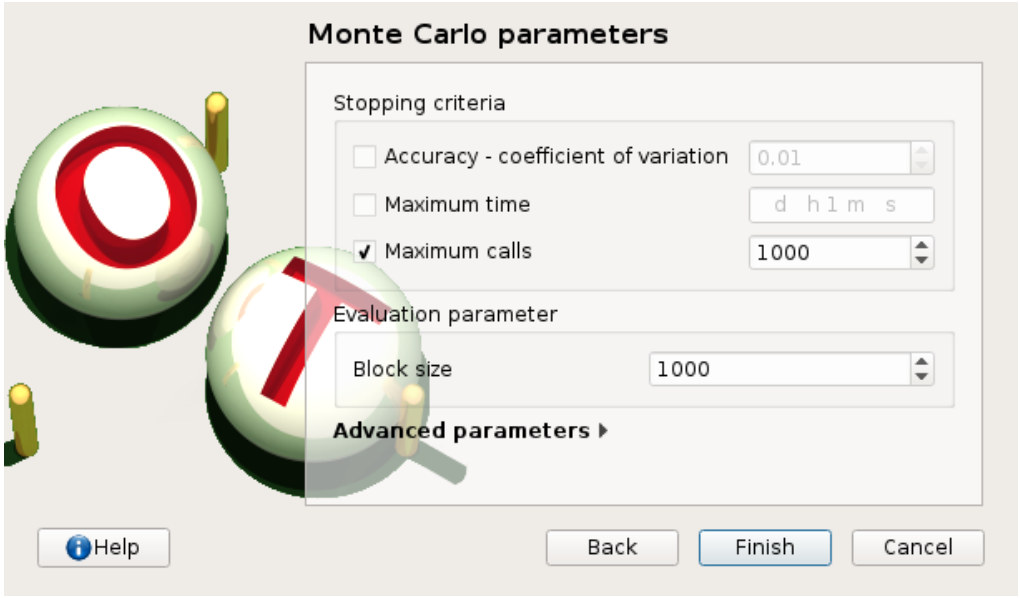
Define the laws of input parameters

- **Probabilistic model**
- **User design of experiments**



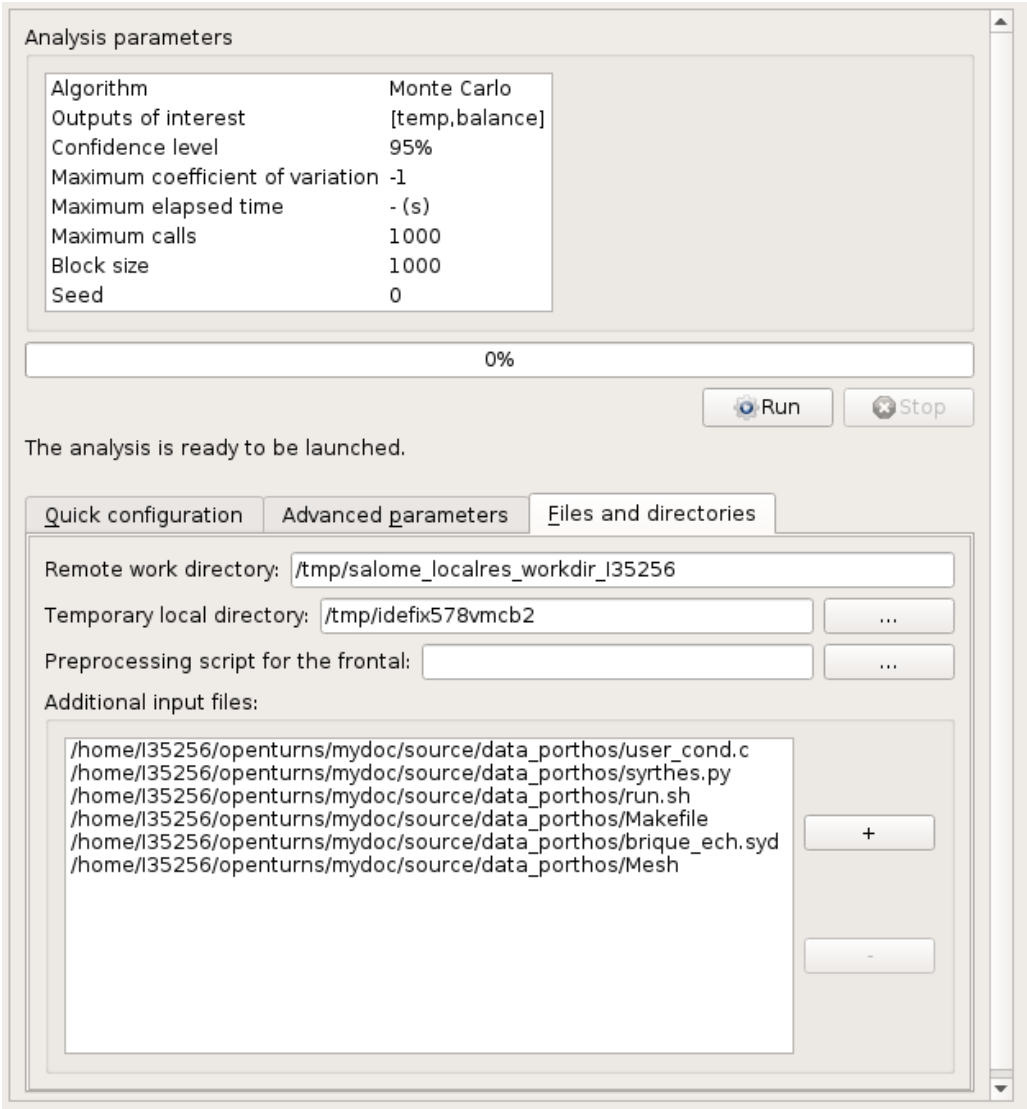
Choose the type of study





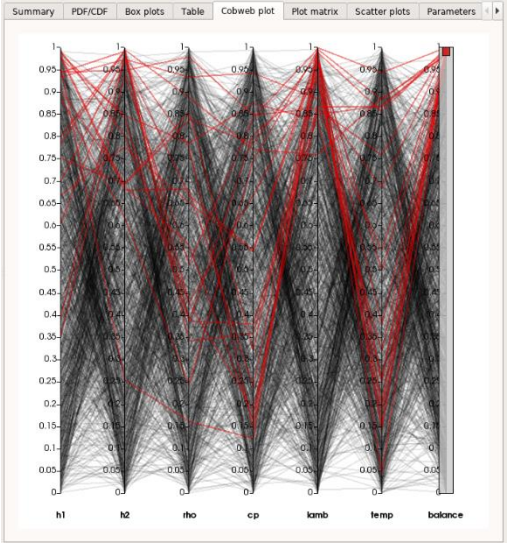
Run the study and wait for results

- **Choose**
  - Computing resource
  - Job parameters
    - Number of nodes
    - Time to execute
    - Etc.
  - Remote working directory
  - Local files to be copied to the remote working directory



Result analysis tools

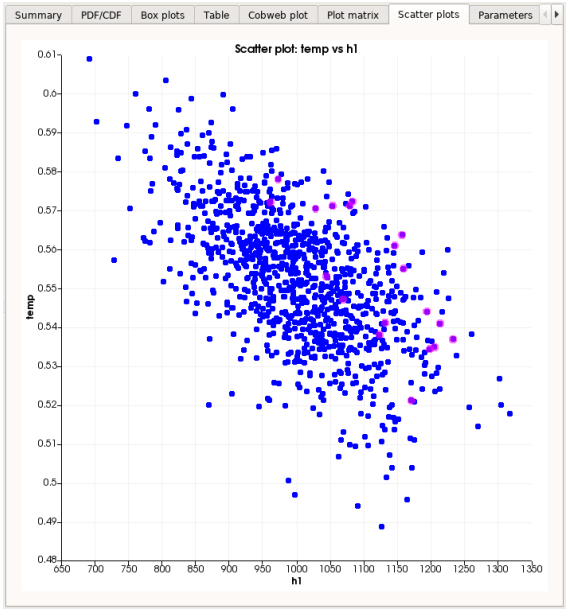
- **Box plots, Cobweb plot, Plot matrix, Scatter plots**

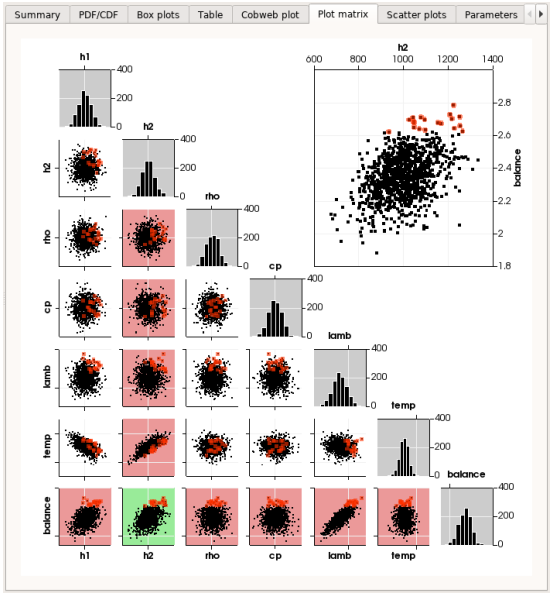


Summary | PDF/CDF | Box plots | **Table** | Cobweb plot | Plot matrix | Scatter plots | Parameters

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 GUI also available stand alone, but without the support for launching on remote resources**

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

Questions?