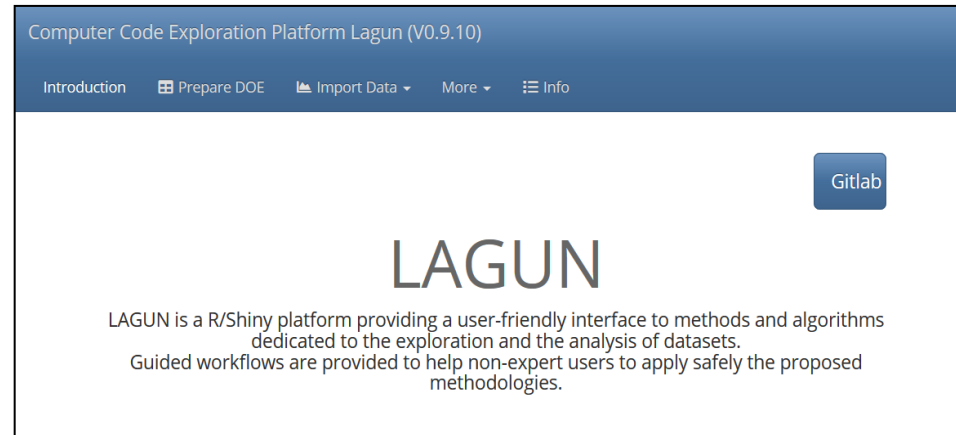


# Lagun

an open-source platform for simulation data exploration and optimization



S. Da Veiga



C. Bénard  
A. El Bachiri  
T. Gonon



M. Menz  
D. Sinoquet



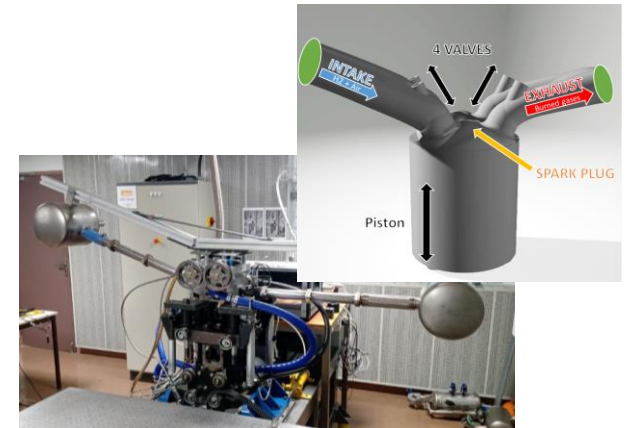
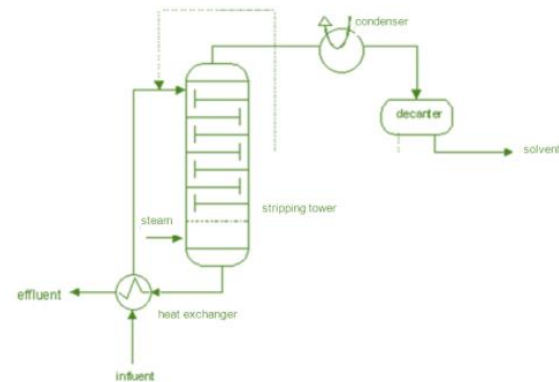
D. Chazalviel



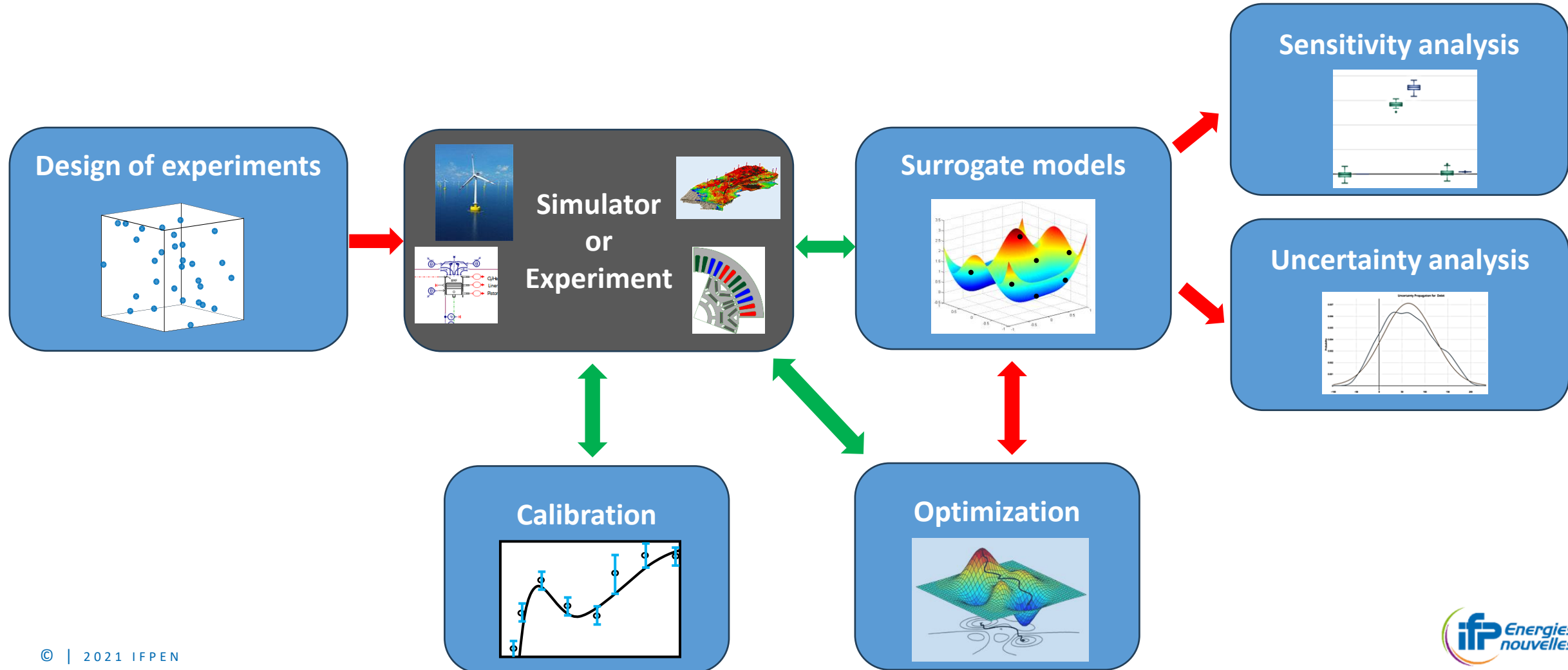
Acknowledgements to **anr**<sup>®</sup> agence nationale de la recherche for grant (IFPEN/TAD)

# LAGUN : APPLICATION CONTEXT

- Lagun : software platform for exploration of complex system data
  - **Very expensive** data generation process
  - Few observations available (1 Ko – 1 Mo)
  - Lagun algorithms enable efficient exploration of parameter space using few observations : **smart data**
- Two main use cases
  - Numerical simulation
  - Experimental data

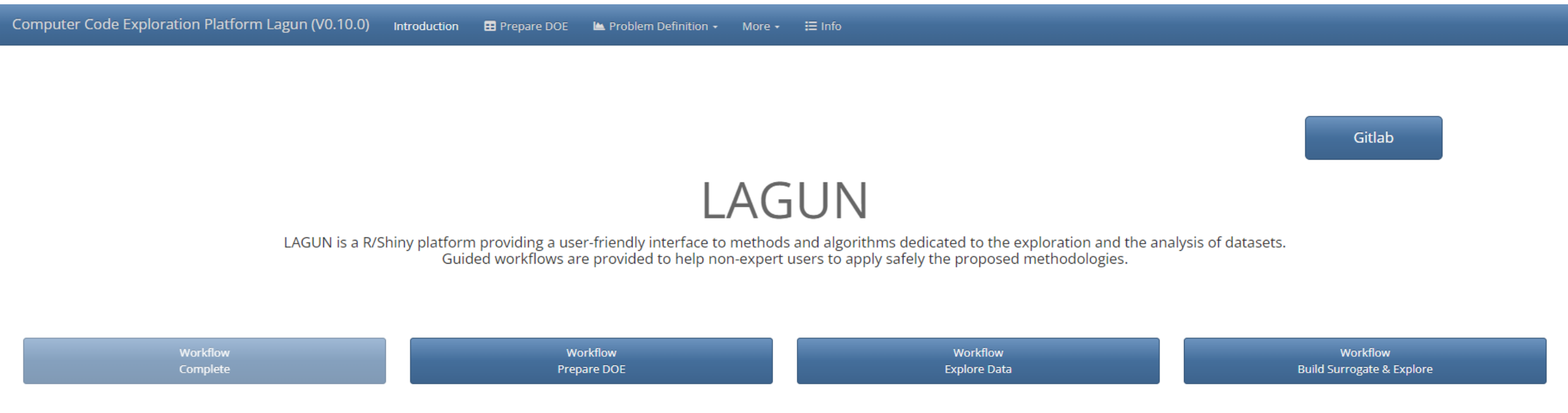


- Improve understanding of a physical system
- Detect influential input variables
- Uncertainty propagation
- Optimization
- Simulator calibration



# LAGUN : SOFTWARE WITH FRIENDLY USER-INTERFACE

- Access via web browser
- State-of-the-art algorithms via R packages
- Simulators running locally or remotely
- Integration of internal R&D results



These tools are commonly used in the numerical uncertainty community (GDR Mascot-Num for example) but are also widely applicable to experimental problems. The main functionalities are the following:

1. Optimized design of experiments  
If you have control on the inputs/parameters on the system which will generate the dataset (numerical simulations, settings of the experiments, ...), you can benefit for a better spatial repartition of the experiments.
2. Visual exploration tools  
When the complete dataset with inputs/parameters and outputs/responses is available, you can load it to perform insightful visual analyses and identify the main trends and the most influential parameters.
3. Going further with surrogate models  
A next common step is to use the dataset to infer a predictive relationship between the inputs/parameters and the outputs. This estimated relationship, the surrogate model, can help push forward the analysis with its ability to predict the responses for any new combination of the inputs. In particular it can be extensively used for uncertainty quantification, sensitivity analysis, deterministic optimization, optimization under uncertainty (robust and reliability based) or more intensive graphical studies.
4. Numerical simulations  
In the special case of numerical simulations, you can benefit from a direct connection between LAGUN and your simulation scripts to perform automatic and sequential optimizations with the surrogate models.

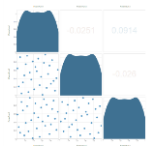
# LAGUN : MAIN FUNCTIONALITIES

- Construction a design of experiments
  - Numeric or categorical variables
- Import data (simulations or experiments)
  - by csv file
  - by connection to external simulator
- Preliminary exploration
  - Interactive visualizations
- Simulation-based optimization
- Simulator calibration
- Learning and validation of metamodels
  - Metamodel types : Lasso, Acosso 1 & 2, Kriging
- Metamodel-based intensive exploration
  - Interactive visualizations
  - Density estimation
  - Uncertainty propagation
  - Sensitivity analysis
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  - Constrained and multi-objective optimization
  - Robust optimization (i.e. under uncertainties)

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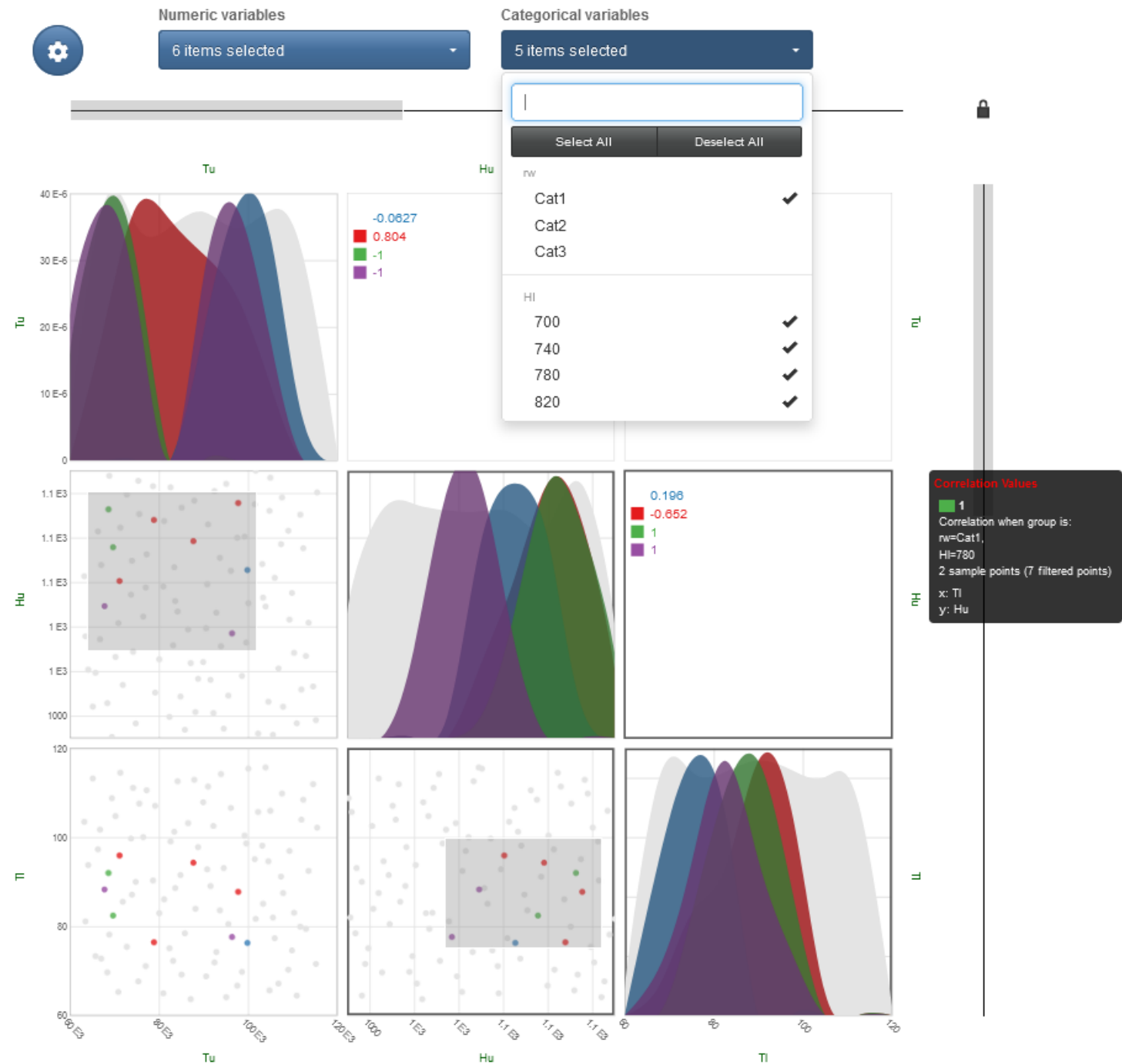
# DESIGN OF EXPERIMENTS

## Define DOE

- Space filling designs
- Numeric / categorical variables

## Visualize and analyze DOE

- Combinations of levels of categorical variables
- Correlations
- Filter data



# LAGUN : MAIN FUNCTIONALITIES

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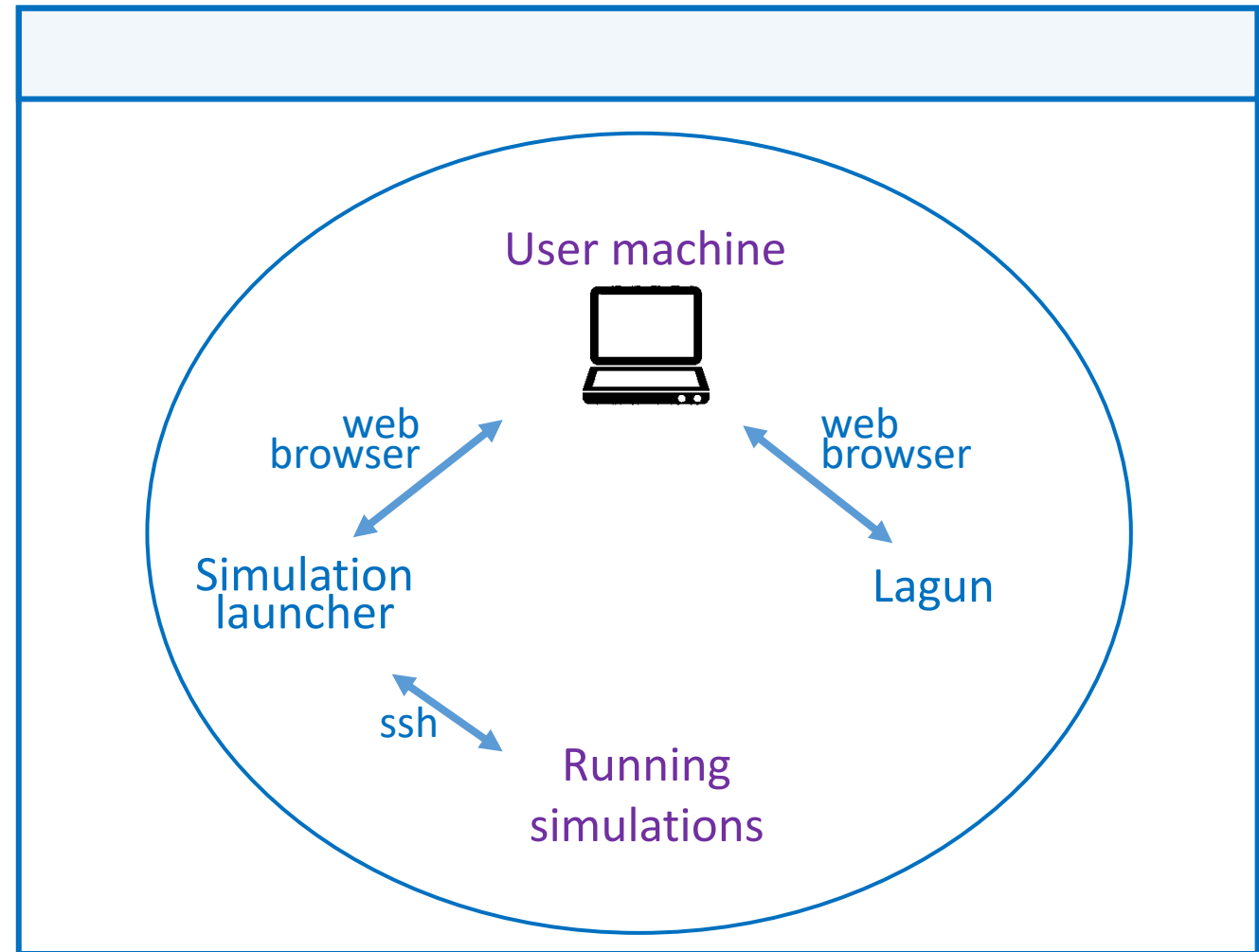


# DATA IMPORT

- Simulations or experiments
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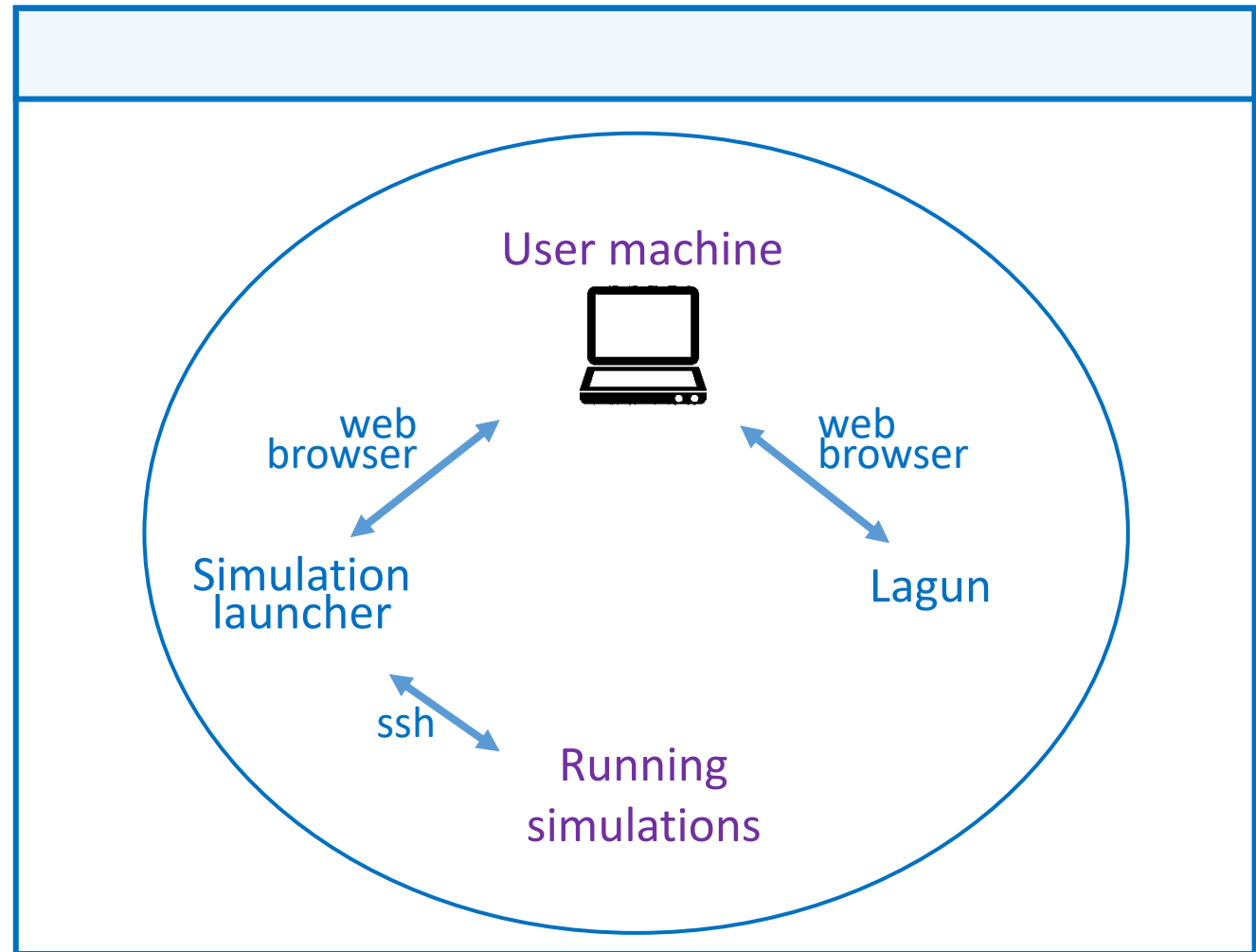
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- **Simulation launcher** : web application that monitors the simulations and connects the user with the simulators



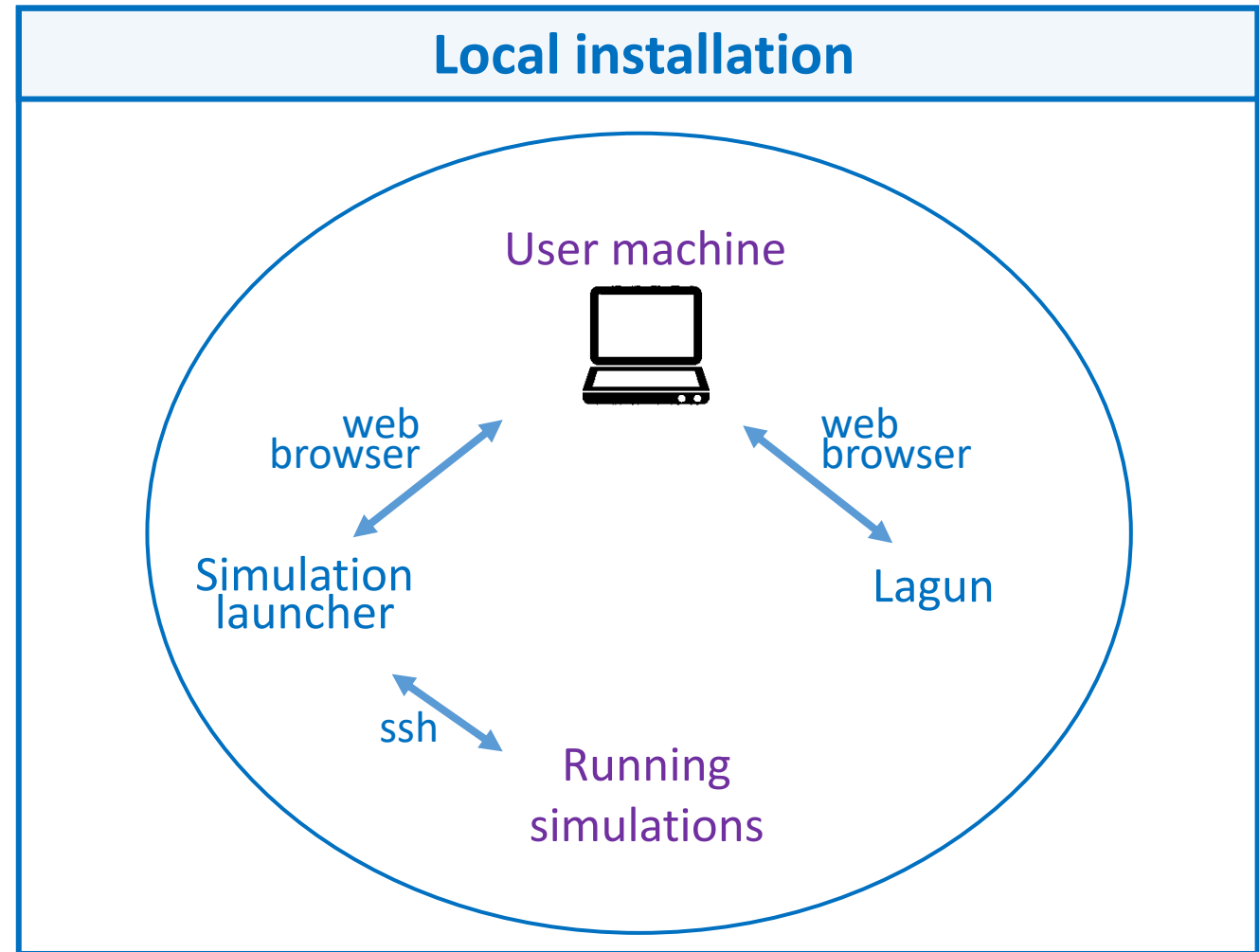
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- Web browser as a support for Lagun and the simulator launcher
  - Lagun / Simulation launcher accessible by all machines sharing the same the network (e.g. IFPEN network)
  - Simulations can be run on Windows or Linux (PC, cluster, ...) locally or remotely



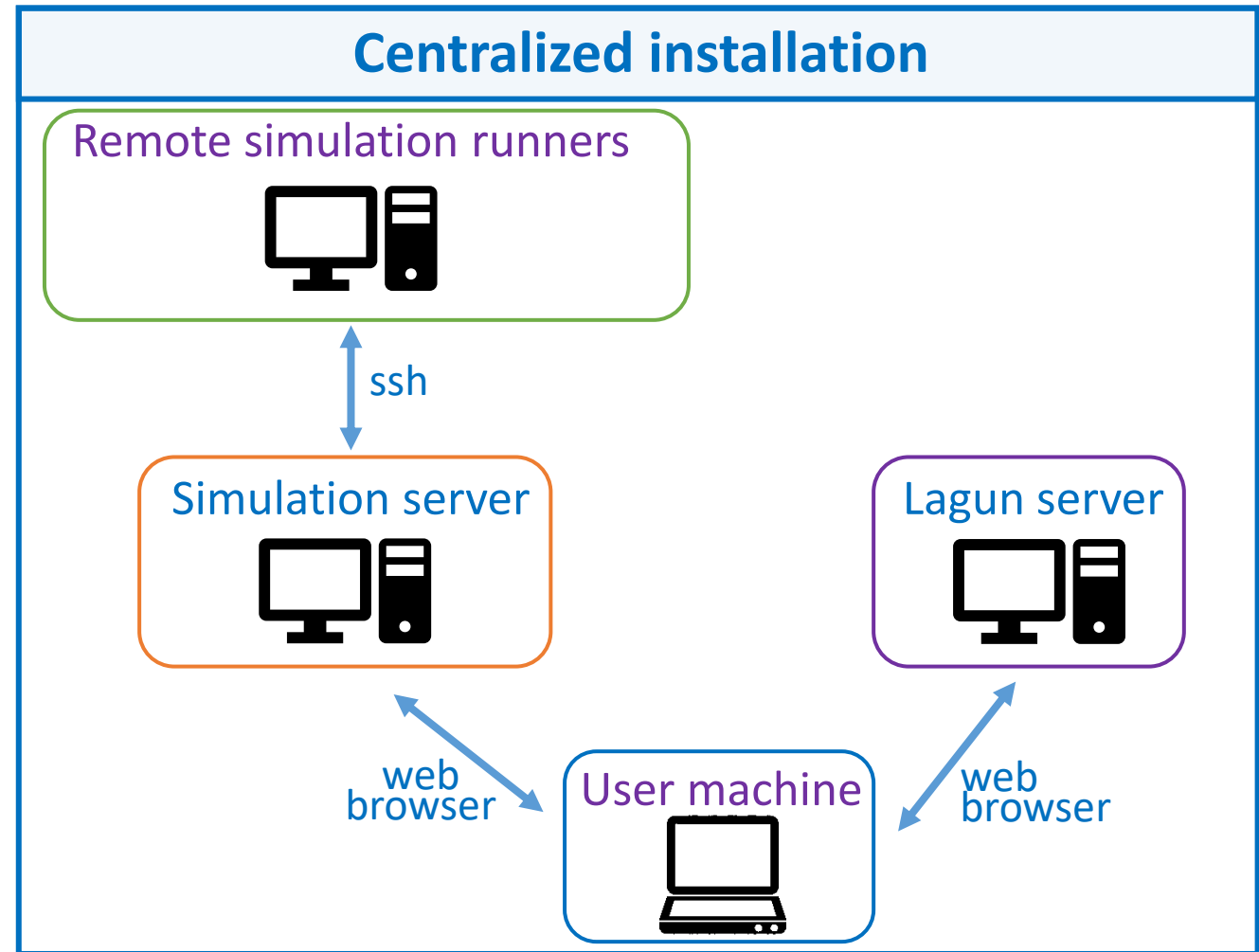
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# SIMULATOR CONNECTION

- **Plug-in of external simulators**  
exe, R or Python scripts, docker images ...
- Simulators share input and output values with Lagun via text files
- Simulator configuration can be shared (via a unique configuration file)
- IFPEN examples:  
Carnot, Abaqus, AMESim, DeepLines, FEMM, Python, R, Matlab scripts ...

Name	<input type="text" value="CarnotExe_Calibration_WMeOH"/>
	This name will be used to identify this simulator.
Description	<input type="text" value="3 inputs + 5 outputs"/>
	This description can be used to add some information describing this simulator.
Executable file	<input type="text" value="D:\Works\lagun\thermoOptimization\CarnotSimulator\InterfaceC.exe"/> <a href="#">Browse</a>
	Full name of the executable simulator file (reference for relative paths is the 'main' execution directory).
Argument	<input type="text" value="Bin_WM"/>
	This string will be sent as argument to the executable simulator file.
Host	<input type="text" value="localhost"/> <a href="#">Edit</a>
	Information about the host used to run simulations
Simultaneous runs	<input type="text" value="4"/>
	Max number of simulations which can be run in parallel.
Input files directory	<input type="text" value="D:\Works\lagun\thermoOptimization\Demo"/> <a href="#">Browse</a>
	Directory where to find the input files of the simulator (reference for relative paths is the 'main' execution directory).
Input files with parameters	<input type="text" value="Bin_WM.DAT"/> <a href="#">Browse</a>
	Specify input files which contain parameters to process.
Input files without parameter	<input type="text" value="fileName1;fileName2"/> <a href="#">Browse</a>
	Specify which input files which don't contain parameters to process.
Results file name	<input type="text" value="Bin_WM_Deviations.csv"/>
	Name of the file containing the results (a 'csv' file located in the simulation directory).
Number of columns of results file	<input type="text" value="5"/>
	Number of columns to be found in 'Results file' (a number for a scalar outputs; or an array of numbers [,] for functional outputs, where each value is the number of columns to be found for a specific functional output; or an array mixing the two previous forms).

# SIMULATOR CONNECTION

## ➤ Monitoring of simulations in LAGUN

possible to preview and analyze the available results (preliminary exploration panel)

Configure simulator

Change Output Groups

Here you can change the outputs types (interest, control, status, constant).

Configure Simulator

Launch Simulations

Stop Simulations

Total 10

Completed 10

Running 0

Waiting 0

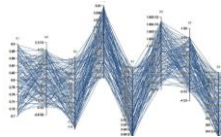
	Info	Status	X1	X2	X3	Output1
1	DOE	Completed	0.05	0.45	0.75	1.37592565247606
2	DOE	Completed	0.15	0.05	0.25	0.166981928271007
3	DOE	Completed	0.25	0.75	0.45	3.50083826427798
4	DOE	Completed	0.35	0.25	0.95	0.799288081567523
5	DOE	Completed	0.45	0.55	0.05	2.34737938097517
6	DOE	Completed	0.55	0.95	0.65	5.16353100666885
7	DOE	Completed	0.65	0.35	0.35	1.42914690809044
8	DOE	Completed	0.75	0.65	0.85	3.28097482913472
9	DOE	Completed	0.85	0.85	0.15	4.70227416874514
10	DOE	Completed	0.95	0.15	0.55	0.977181053103266

Export DOE

# LAGUN : MAIN FUNCTIONALITIES

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# PRELIMINARY EXPLORATION

## ● Pair plots

Choose Outputs

5 items selected

Choose Inputs

4 items selected

Rows

3

Columns

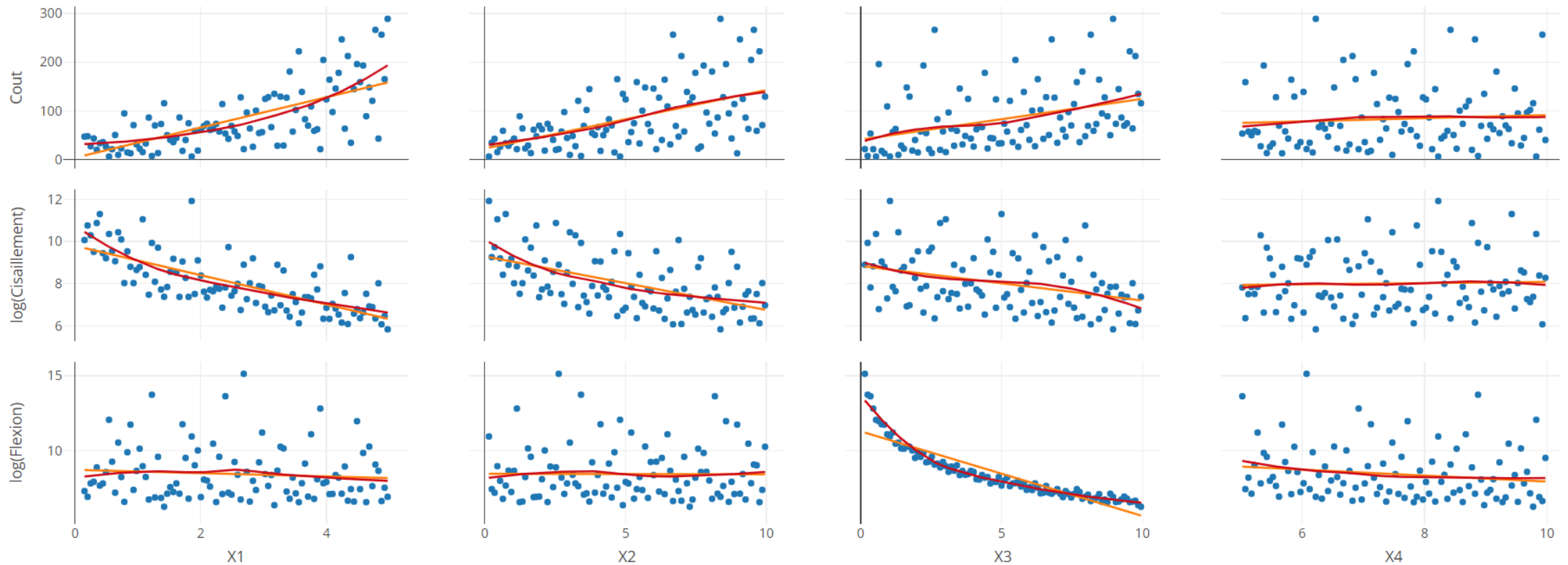
4

«

»

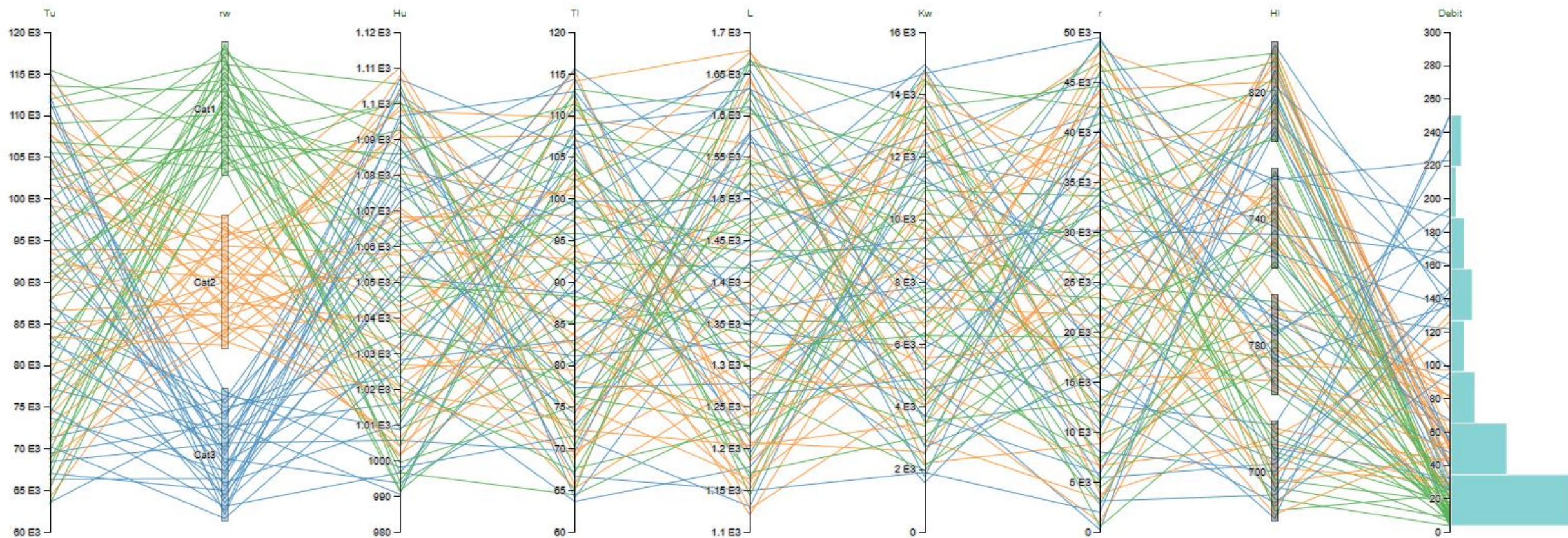
⌵

⌶



# PRELIMINARY EXPLORATION

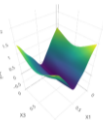
## ● Parallel plot



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# SURROGATE MODELS

Lagun proposes several types of surrogate model built from simulations

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### Build Surrogate Models

Choose Normal/Expert Mode

Normal Mode
Normal Mode
Expert Mode

Train Lasso Model

It is highly recommended to try first this linear model. For some outputs it may be predictive enough and for the others you can check how nonlinear the output may be.

Train Acosso 1

This is the first generalization of the Lasso model; it is additive but nonlinear. If the number of inputs is large you should try it before training a kriging model. Not available for classification.

Train Acosso 2

This model generalizes Acosso 1st order by adding nonlinear interactions between the variables. If the number of inputs is large it may take a long time to compute. Not available for classification.

Train Kriging Model

This model is the most flexible one and can model complex input-outputs relationships. But if the number of inputs is larger than 15-20, its calibration may be hard.

Re-training allowed OFF

Flexibility

Click on a cell in the Q2 table below to display the prediction quality for each output and each metamodel.

Choose Validation

Leave-One-Out

Load Test File

Type	Var	Trend	OF1	OF2	OF3	OF4	OF5	OF6	OF7	OF8	OF9	OFtotal
BestQ2			0.9999	0.9999	0.9997	1	0.9998	1	0.9975	0.9996	1	0.9997
Lasso			0.8243	0.9746	0.6309	0.5845	0.6229	0.9781	0.9054	0.6363	0.9687	0.6787
Acosso1			-0.02494	-0.02548	0.6312	0.9598	0.2822	-0.0254	0.911	0.5869	0.9986	0.5841
Acosso2	All		-0.0238	-0.02548	0.9953	0.9967	0.4209	-0.02524	0.9773	0.9974	0.9997	0.9976
Acosso2	Acosso1		-0.02536	-0.02548	0.6264	0.9993	0.08736	-0.02546	0.9646	0.9973	0.9999	0.8648
Kriging	All	Constant	0.9998	0.9999	0.9997	1	0.9998	1	0.9975	0.9995	1	0.9996
Kriging	All	Linear	0.9999	0.9999	0.9997	1	0.9998	1	0.9975	0.9996	1	0.9997

Select Final Surrogate Models

Additional Simulations to Refine Surrogate Models

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Click on a cell in the Q2 table below to display prediction quality for each output and each r

Type	Var	Trend
<b>BestQ2</b>		
Lasso		
Acosso1		
Acosso2	All	
Acosso2	Acosso1	
Kriging	All	Constant
Kriging	All	Linear

Compare Surrogate(s)

Acosso 1, Acosso 2 with all vars, Kriging 1

Q2 LOO for OF8

Load Test File

	OF7	OF8	OF9	OFtotal
	0.9975	0.9996	1	0.9997
	0.9054	0.6363	0.9687	0.6787
	0.911	0.5869	0.9986	0.5841
	0.9773	0.9974	0.9997	0.9976
	0.9646	0.9973	0.9999	0.8648
	0.9975	0.9995	1	0.9996
	0.9975	0.9996	1	0.9997

Select Final Surrogate Models

Additional Simulations to Refine Surrogate Models

# SURROGATE MODELS

Update the models thanks to new observations

→ improvement criteria used to propose new points to be simulated

Additional Simulations to Refine Surrogate Models

Improvement Criteria

Global Accuracy

Choose Output(s) to Improve

OF3, OF

Number of Additional Simulations

3

Tag DOE Info

Refine Global 1

Generate Additional Simulations

Launch Simulations

Proposed Additional Simulations

Export Additional Simulations

Column visibility

X1X2X3

AllAllAll

Simu1	0.2139892578125	0.9952392578125	0.9927978515625
Simu2	0.9285888671875	0.0130615234375	0.0086669921875
Simu3	0.066650390625	0.999755859375	0.002685546875

Showing 1 to 3 of 3 entries

# LAGUN : MAIN FUNCTIONALITIES

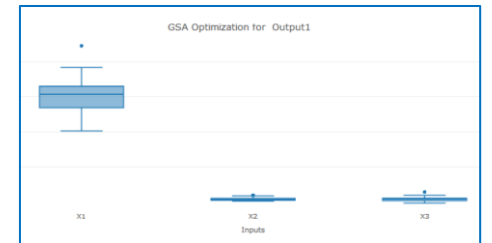
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- Interactive visualizations
- Density estimation
- Uncertainty propagation
- Sensitivity analysis



- Metamodel-based optimization
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  - Robust optimization (i.e. under uncertainties)

# PARALLEL PLOT (METAMODEL-BASED)

Choose Input(s) to Visualize

8 items selected

Choose Output(s) to Visualize

Debit

Visualize Histograms

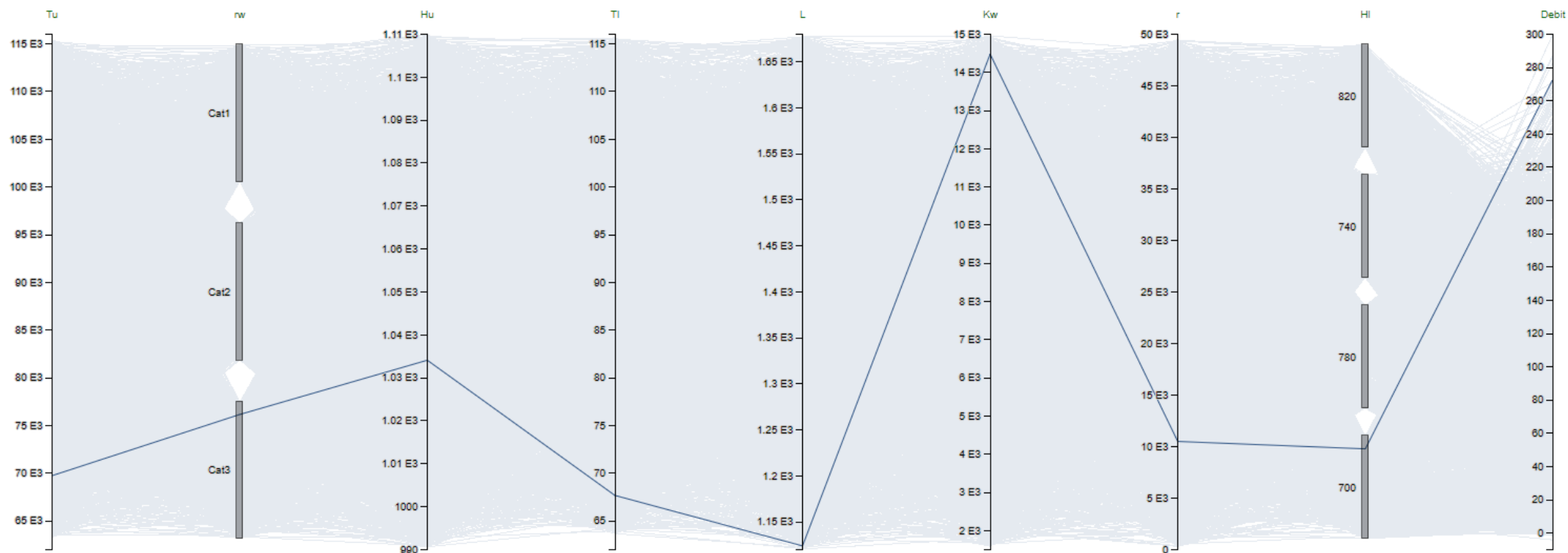
Nothing selected

Manual Bounds

Nothing selected

Sampling  
from File

Refine  
Sampling





# PARALLEL PLOT (METAMODEL-BASED)

Choose Input(s) to Visualize

8 items selected

Choose Output(s) to Visualize

Debit

Visualize Histograms

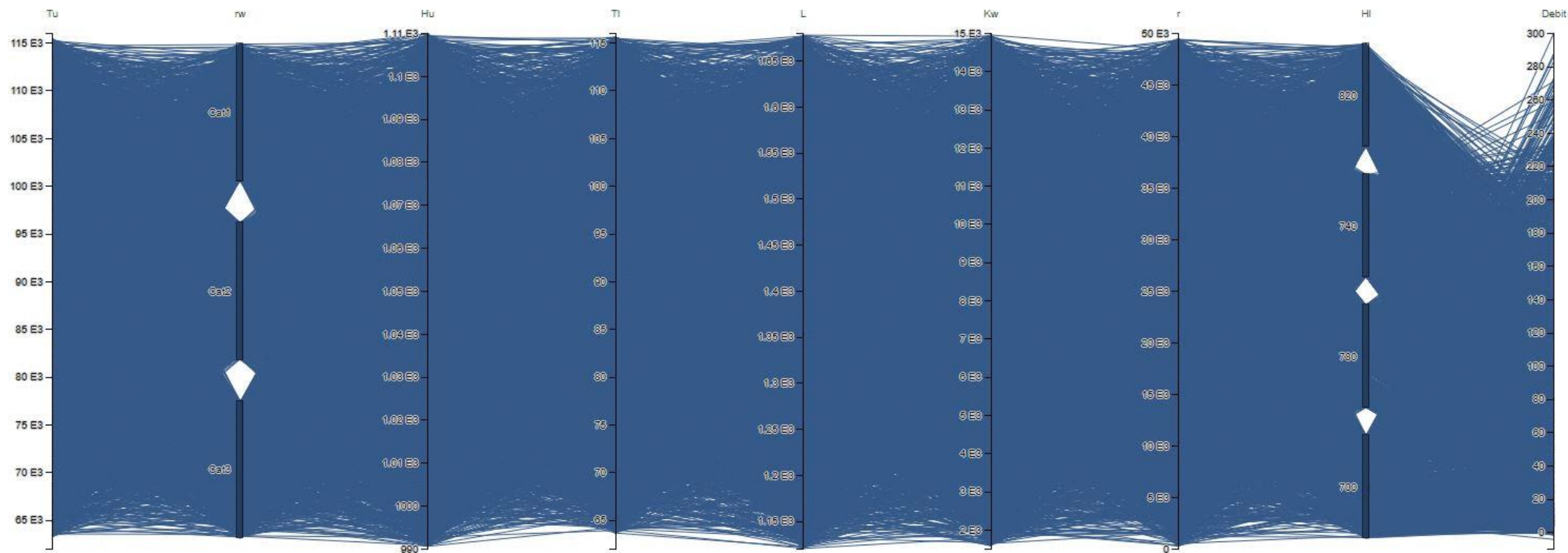
Nothing selected

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from File

Refine  
Sampling



# UNCERTAINTY PROPAGATION (METAMODEL-BASED)

Global Propagation

Probability Estimation

Propagate Uncertainties

Sample Size

10000

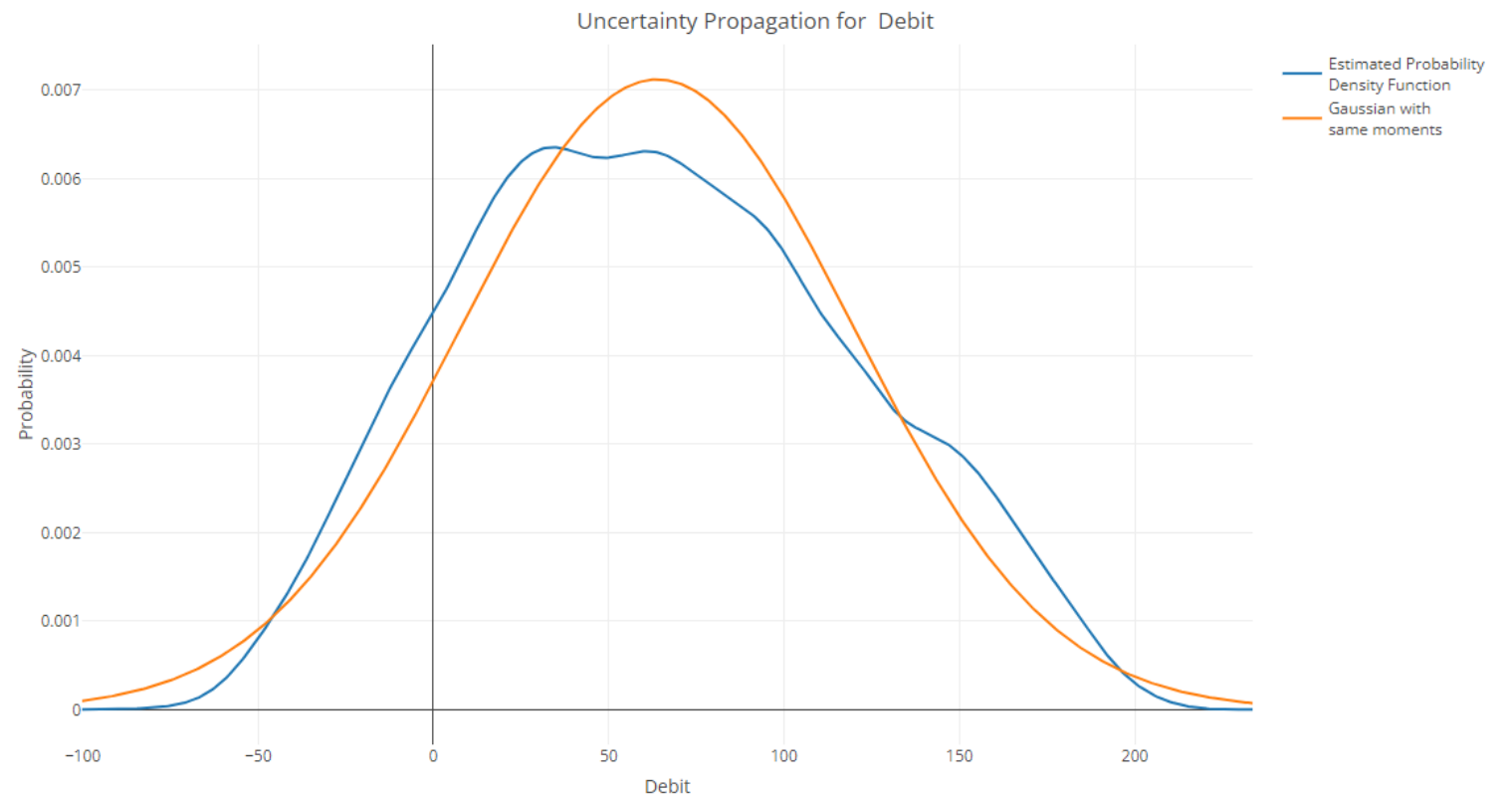
Export UQ propagation

Choose Output to Visualize

Debit

Choose UQ propagation visualization

Probability Distribution Function



# GLOBAL SENSITIVITY ANALYSIS (METAMODEL-BASED)

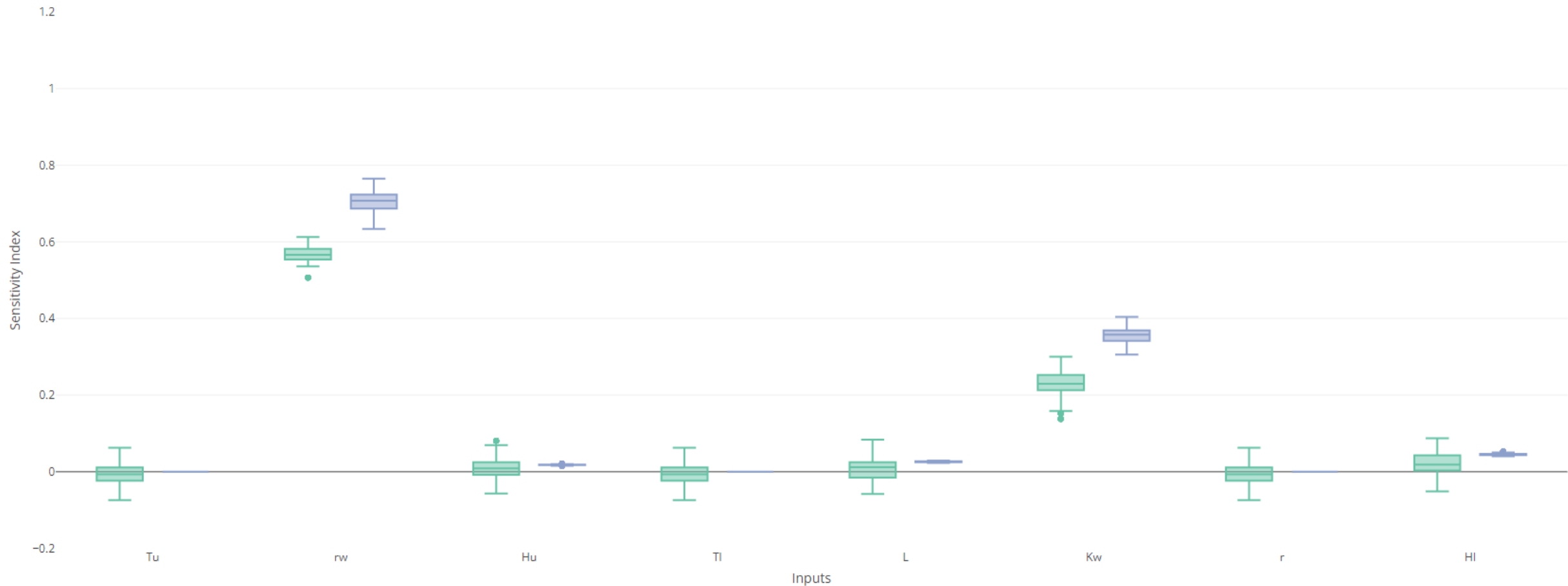
Choose Output to Visualize

Debit

Summary

Reset Sensitivity  
Analysis

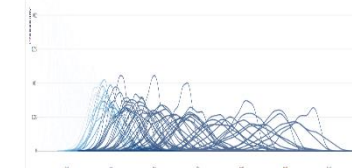
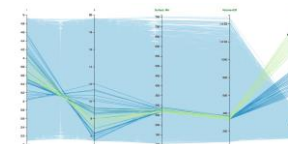
GSA for Debit



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# OPTIMIZATION UNDER UNCERTAINTY (METAMODEL-BASED)

## Solve Problem

Robust Optimization

Select Robust Criterion

Mean

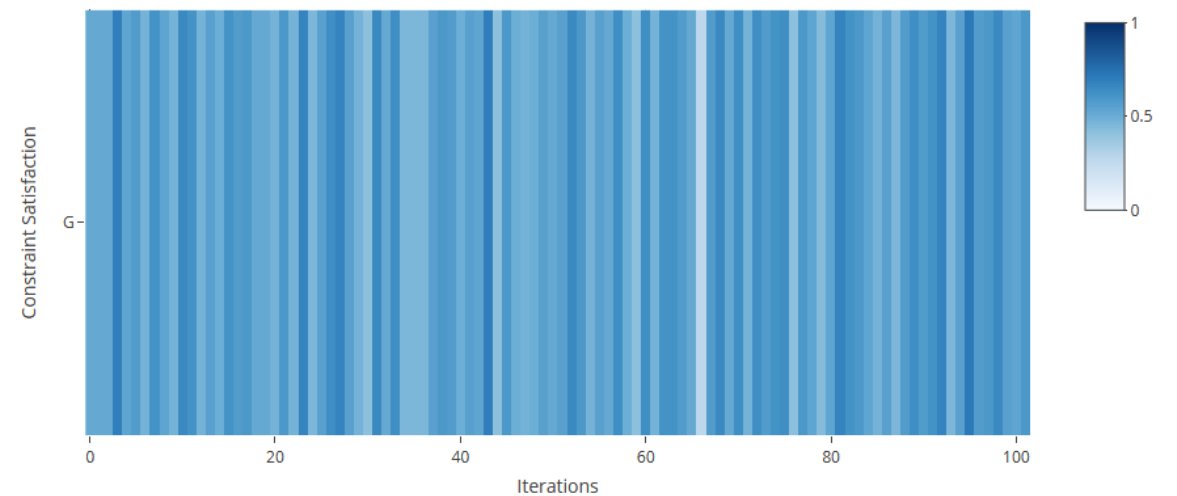
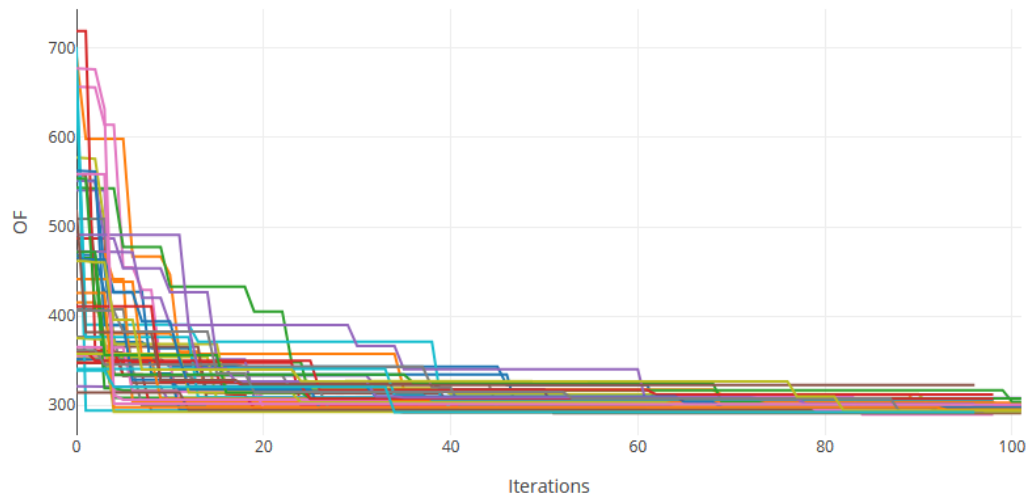
Constraint Probability

0,9

Export Optimization Results

## Graphical Representation

Robust Optimization Results

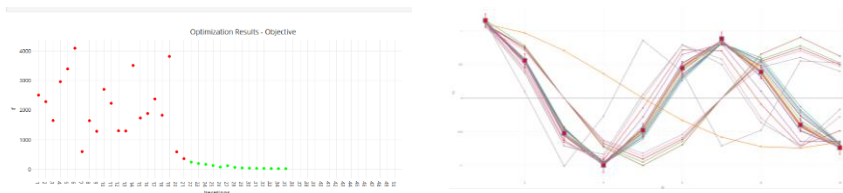


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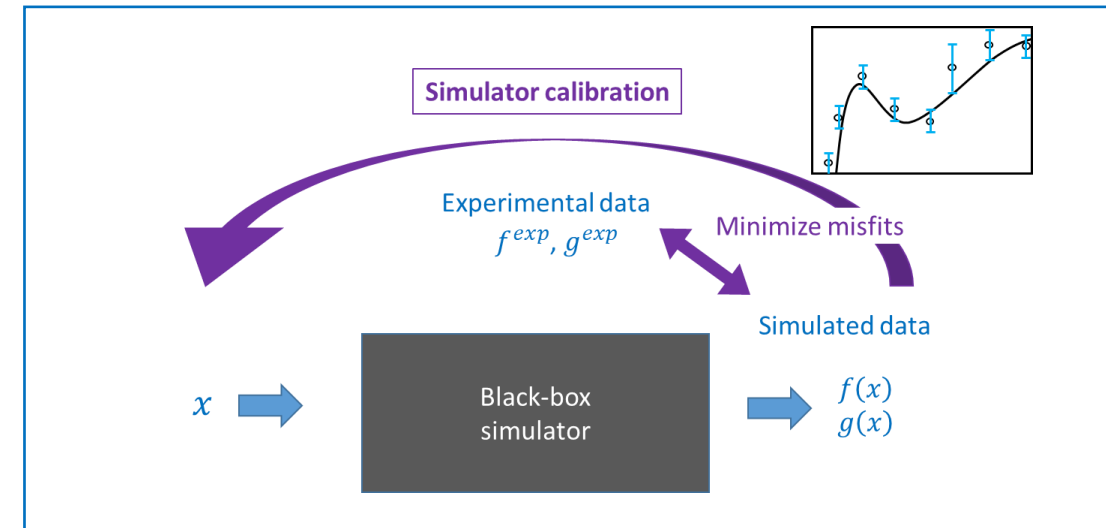
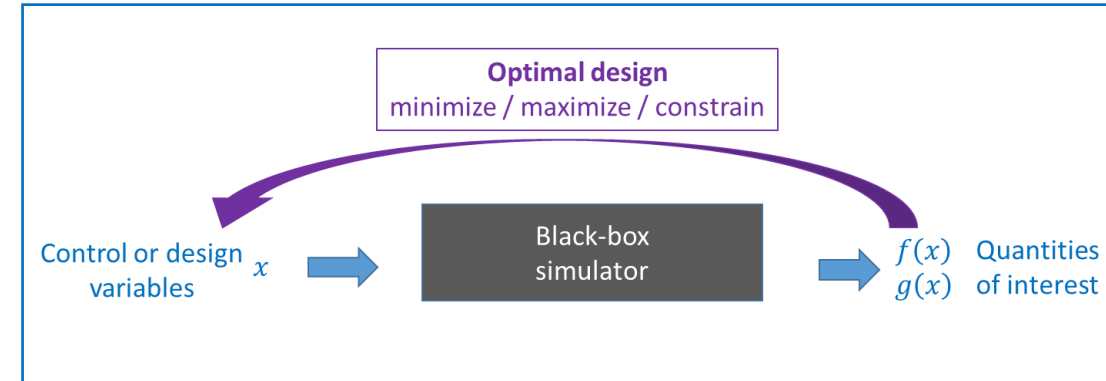
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# DIRECT OPTIMIZATION: SIMULATION-BASED OPTIMIZATION

2 objectives :

- Optimize the simulator outputs
- Calibrate the simulator on experimental data
- Guide to formulate the optimization problem
- List of available optimizers adapted according to the type of optimization problem (*HubOpt inside !*)
- Possibility of connecting the user's preferred optimizer



# DIRECT OPTIMIZATION: SIMULATION-BASED OPTIMIZATION

Launch Optimization

Stop Optimization

Optimization completed

## Monitoring of optimization iterations and simulations

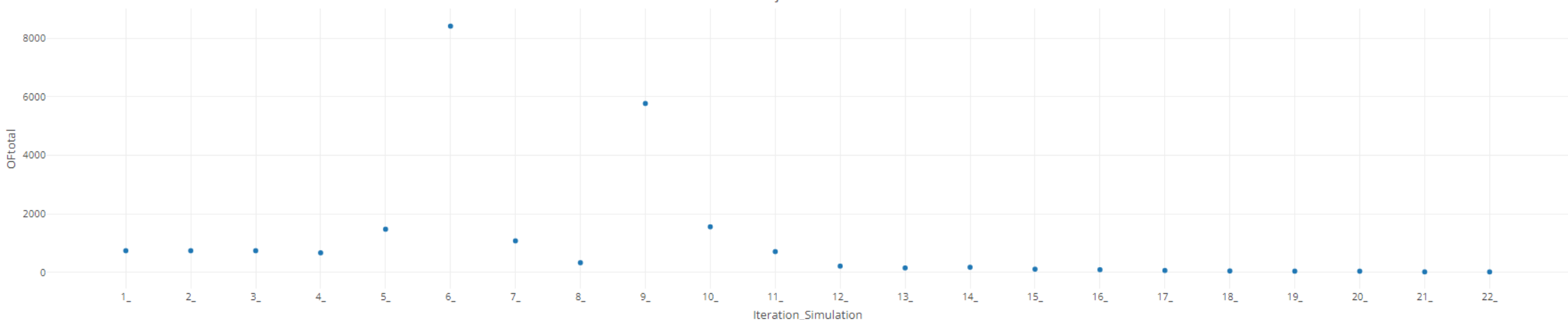
Results Plot

Inputs Plot

ScatterPlotMatrix

Functional plot

Objective



	Directory	Status	X1	X2	X3	Oftotal
12_	run10	ended	1.05	-1.1382	-0.5	209.5279926707984
13_	run11	ended	1.0854	-1.0477	-0.5163	147.6550005503274
14_	run12	ended	1.007	-1.0256	-0.5128	170.507468429605
15_	run13	ended	1.0787	-1.027	-0.4953	104.5667005655024
16_	run14	ended	1.127	-1.0176	-0.4974	87.58735356071631
17_	run15	ended	1.2144	-1.0111	-0.4985	59.8840843175041
18_	run16	ended	1.2686	-1.012	-0.499	43.77223687067989
19_	run17	ended	1.2975	-1.0111	-0.4994	37.35146939556266
20_	run18	ended	1.3462	-1.0022	-0.4987	35.52713769599251



# DIRECT OPTIMIZATION: SIMULATION-BASED OPTIMIZATION

Launch Optimization

Stop Optimization

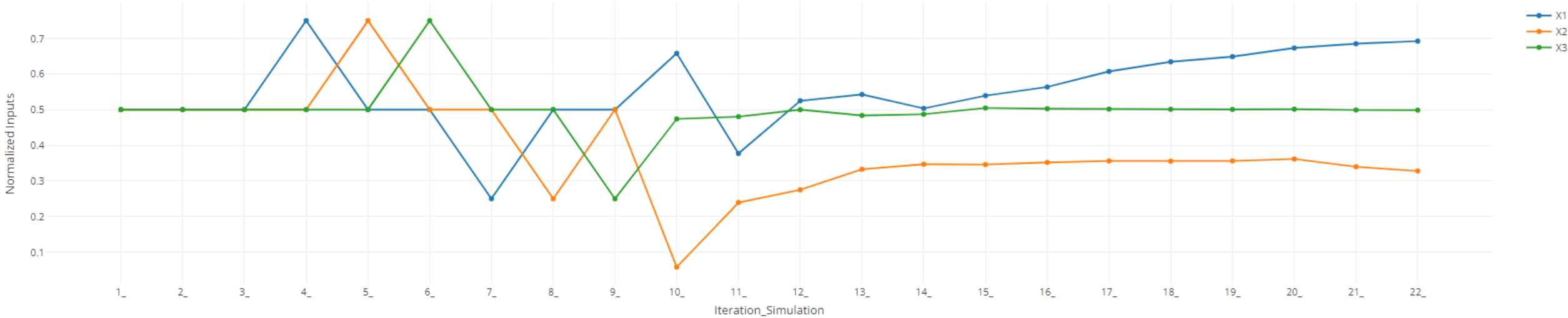
Optimization completed

Results Plot

Inputs Plot

ScatterPlotMatrix

Functional plot



	Directory	Status	X1	X2	X3	OfTotal
12_	run10	ended	1.05	-1.1382	-0.5	209.5279926707984
13_	run11	ended	1.0854	-1.0477	-0.5163	147.6550005503274
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20_	run18	ended	1.3462	-1.0022	-0.4987	35.52713769599251

# DIRECT OPTIMIZATION: SIMULATION-BASED OPTIMIZATION

Launch Optimization

Stop Optimization

Optimization completed

Results Plot

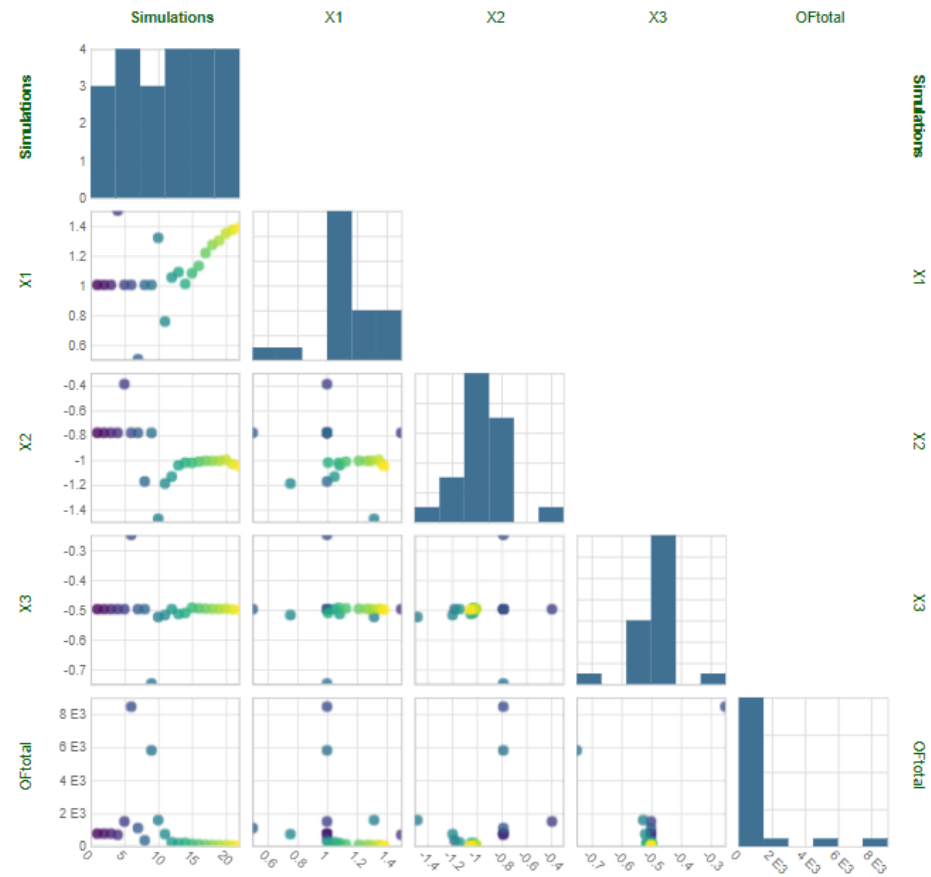
Inputs Plot

ScatterPlotMatrix

Functional plot

Displayed Columns

5 items selected



# DIRECT OPTIMIZATION: SIMULATION-BASED OPTIMIZATION

For simulator calibration

Results Plot

Inputs Plot

ScatterPlotMatrix

Functional plot

Y-axis

Y3

X-axis

t3

Simulation number

45 items selected

Color by

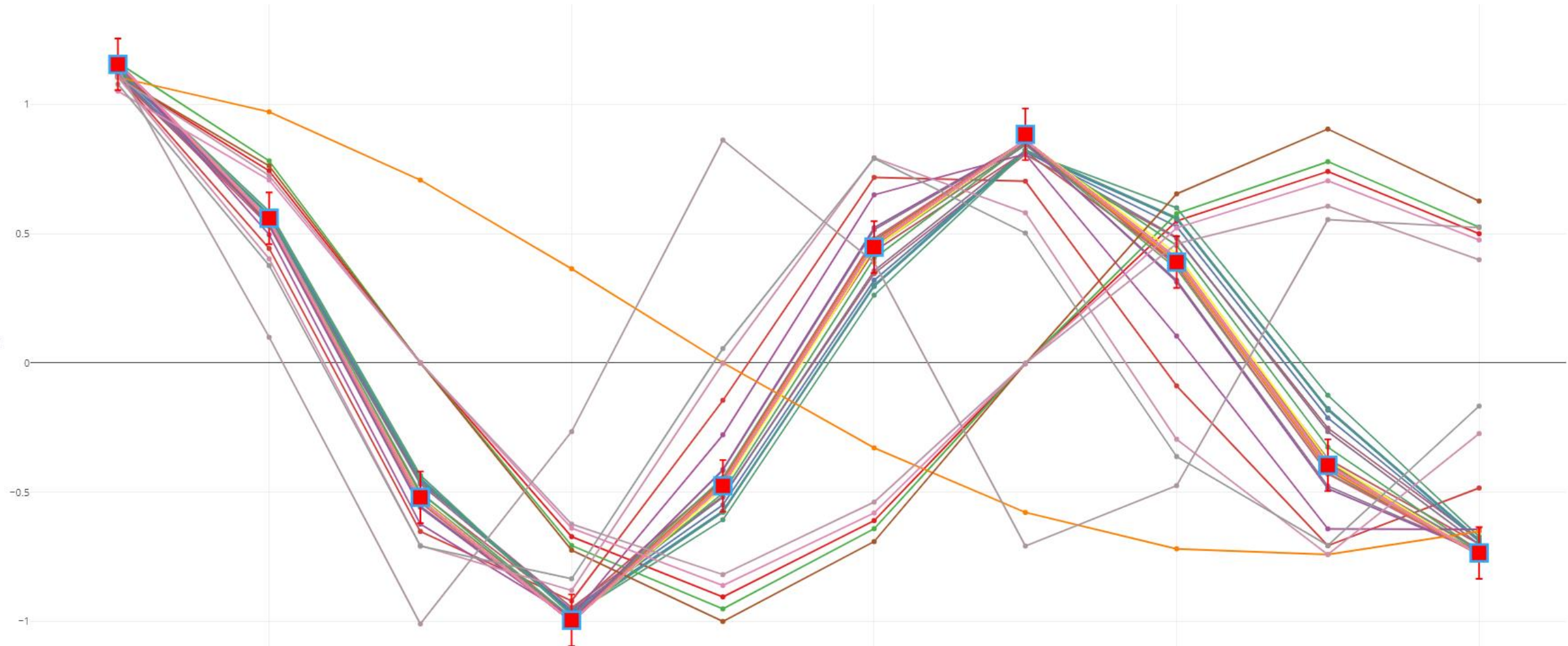
Simulation

ON

Exp  
data

ON

Error  
bars

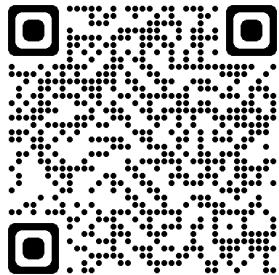


# CONCLUSIONS

- On-going collaboration with Safran Tech for Lagun development
- On-going developments: generic plug-in of metamodels, exports, backups and hot starts, automatic tests, ...

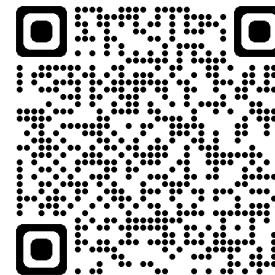
Try Lagun, make suggestions and contribute to platform's development !

Source codes



<https://gitlab.com/drti/lagun>

Docker images of Lagun and of the simulation launcher



[https://ifpen-gitlab.appcollaboratif.fr/detocs/lagun\\_resources](https://ifpen-gitlab.appcollaboratif.fr/detocs/lagun_resources)

Contact : [delphine.sinoquet@ifpen.fr](mailto:delphine.sinoquet@ifpen.fr)