

# How GEMSEO uses OpenTURNS for multidisciplinary problems

Matthias DE LOZZO on behalf the GEMSEO Team

OpenTURNS Users'Day, Friday 23 June 2023, EDF Lab Saclay



# **IRT Saint Exupéry**

Accelerate science, technology research & transfers to industry

# What is IRT Saint Exupéry?



The IRT Saint Exupery is a collaborative and integrated technological research center bridging the public research to the industrial



#### **Our missions:**

one.

- Promote the French technological research for the benefit of the industry established on the national territory
- Develop the ecosystem for the aeronautics, space and critical systems sectors by providing access to our research projects, technological platforms & expertise.
- Create a link between public and private research in order to facilitate transfer by mobilizing resources from the academic world for the implementation of research in industry.
- Carry out collaborative and integrated research projects based on industrial needs with an upstream contribution from the academic community, supported and financed by the French government and industrial members













**AIRBUS** 



THALES





# IRT Saint Exupéry competences and targets

# 12 competences

**@IRT Saint Exupéry** 

- High voltage energy >
- High Reliability Energy >
  - High density energy >
- Metallic materials and processes >
  - Surfaces / assemblies >
  - Composite materials >
  - Advanced Learning >
  - Al for critical systems >
- **Smart Connectivity and Sensing >** 
  - Systems Engineering >
  - Multi Discipline Optimization >
  - Critical Embedded Systems >

## **4 Technological Axes**

@the service of industrialists



**Advanced** Manufacturing **Technologies** 

**Smart Technologies**  Methods and tools for the development of complex systems

Enable digital and collaborative system engineering Develop and transfer robust multidisciplinary optimization Design efficient & secure hardware and software architectures





Aeronautics



**Space** 



Defence



# Agenda.



1	Multidisciplinary design optimization (MDO)
2	GEMSEO, an open source Python library

- **3 GEMSEO facing uncertainties**
- 4 **GEMSEO** using OpenTURNS
- 5 Roadmap, take home message





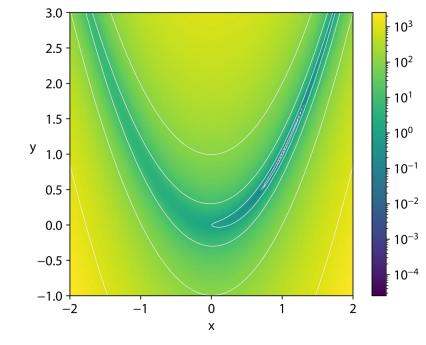
# Minimizing a cost function is an optimization problem.



## **Initial questions**

- Are there constraints?
- Are there local minima?
- Are the variables continuous? discrete? categorical?
- Do I have the gradient?
- Is the evaluation of the function expensive?

• ...



Contour plot of the Rosenbrock function (2D) - Nschloe, CC BY-SA 4.0

# **Final questions**

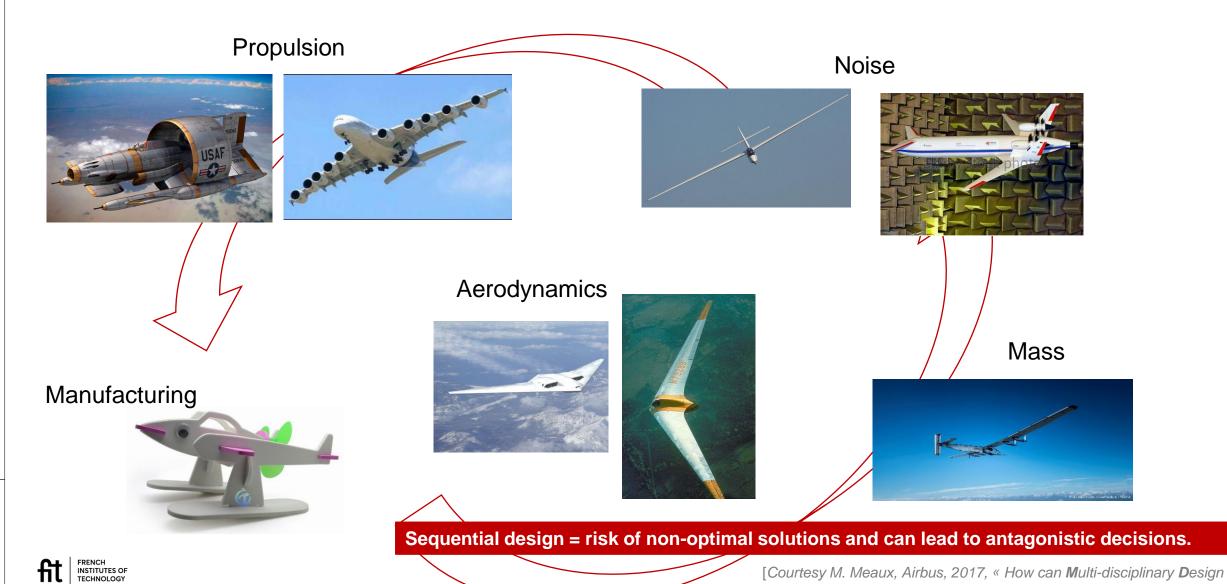
- Which optimizer?
  - and which options?



# Designing a vehicle is multi-disciplinary challenge.



Optimization (MDO) support R&T Portfolio management ?»]

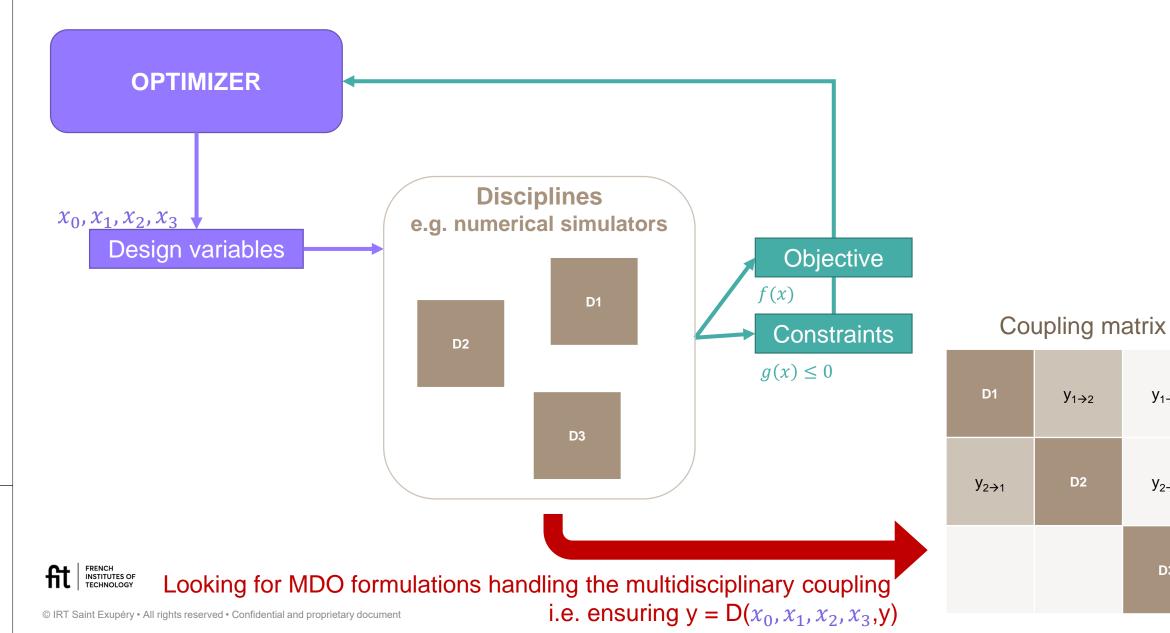




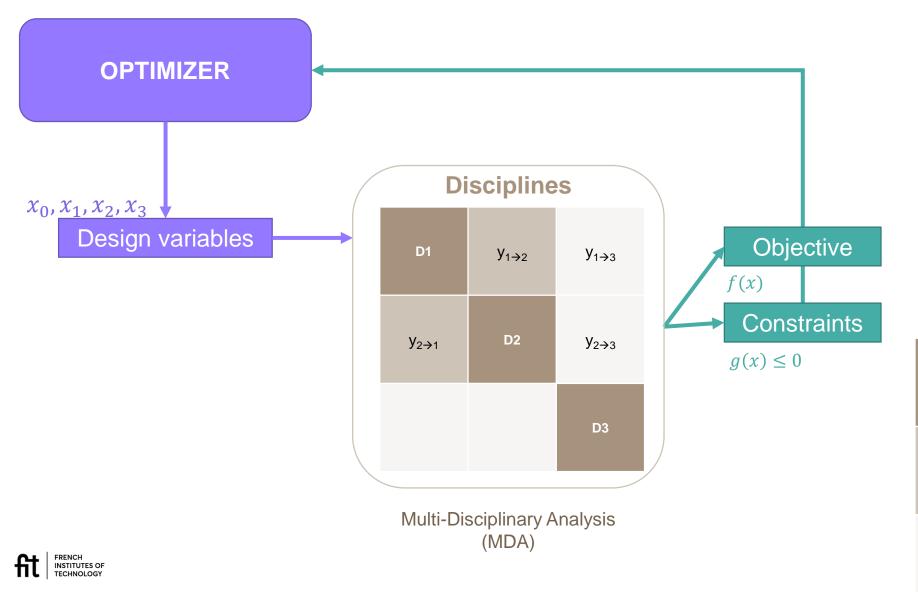
 $y_{1\rightarrow 3}$ 

 $y_{2\rightarrow 3}$ 

D3





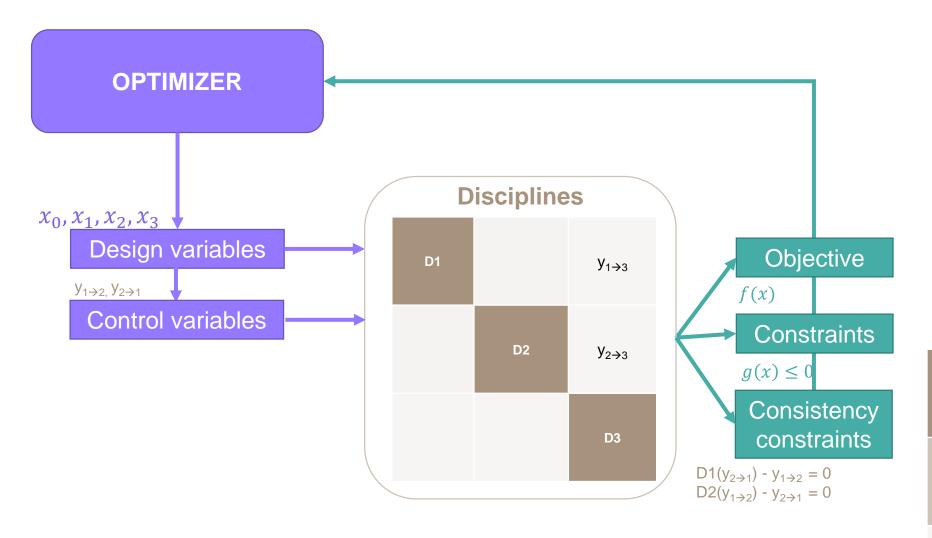


MDF formulation

### Coupling matrix

D1	<b>y</b> <sub>1→2</sub>	y <sub>1→3</sub>
y <sub>2→1</sub>	D2	<b>y</b> <sub>2→3</sub>
		D3



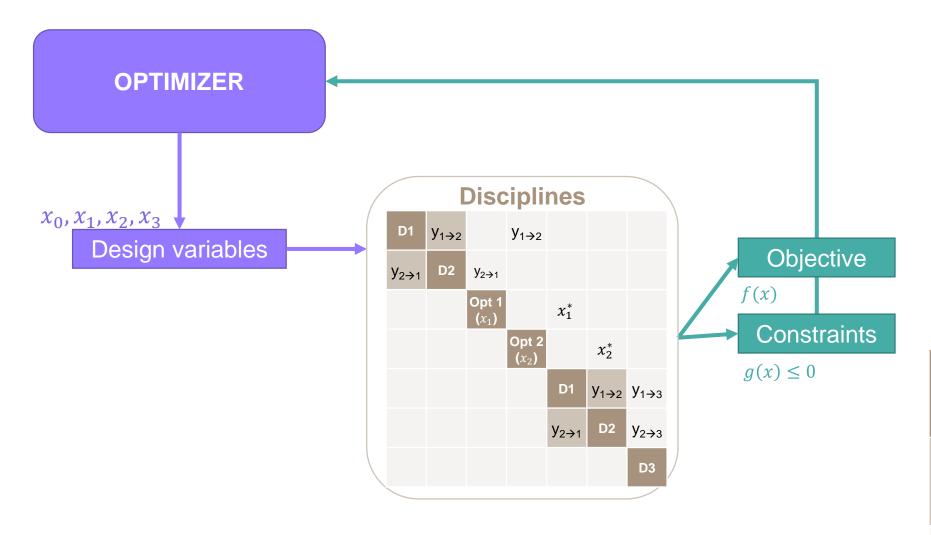


IDF formulation

### Coupling matrix

D1	y <sub>1→2</sub>	y <sub>1→3</sub>
y <sub>2→1</sub>	D2	y <sub>2→3</sub>
		D3





Bi-level formulation

### Coupling matrix



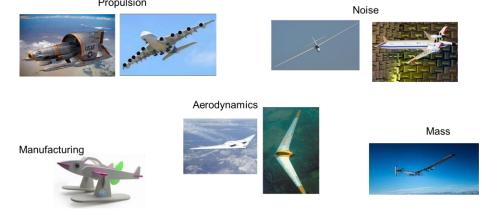
# Designing a vehicle is multi-disciplinary challenge.



## **Initial questions**

- Are there constraints?
- Are there local minima?
- Are the variables continuous? discrete? categorical?
- Do I have the gradient?
- Is the evaluation of the function expensive?

• ...



#### Remind:

An MDO formulation is a mathematical strategy to define the optimization problem(s) to be solved.

### **Final questions**

- Which disciplines?
- Which MDO formulation?
  - and which options?
- Which optimizer(s)?
  - and which options?





# GEMSEO, an open source Python library

# GEMSEO, an open source Python library for MDO and more



created in 2015 at IRT Saint Exupéry within the MDO competence center

Generic Engine for Multidisciplinary Scenarios, Exploration and Optimization









gemseo.org

User guide Notebooks open source

GNU LGPL v3.0

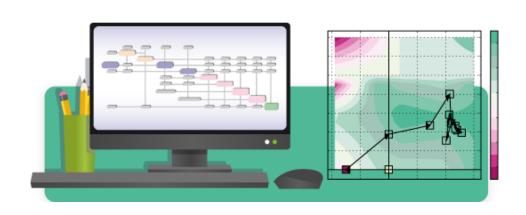
**Python** 

Code quality
Testing
Documentation
CI

#### **Offers**

- Automation of MDO processes based on MDO formulations
- Features: coupling, optimization, design of experiments, visualization, surrogate modeling, machine learning, uncertainty quantification, ...
- Easy to embed in simulation platforms or to use as a standalone software
- Can use tools in Python, Matlab, Excel,
   Scilab, executables, ...





GEMSEO and its plug-ins are on GitLab gitlab.com/gemseo/dev

## **Contributors**





Pierre-Jean Barjhoux



Simone Coniglio



Yann David



Matthias De Lozzo



Antoine Dechaume



Syver Doving Agdestein



Reda El Amri



Vincent Gachelin



François Gallard



Anne Gazaix



Jean-Christophe Giret



Damien Guénot



Selime Gürol



Rémi Lafage



Benoit Pauwels



Arthur Piat



Nicolas Roussouly



Gilberto Ruiz Jimenez



Isabelle Santos



Charlie Vanaret

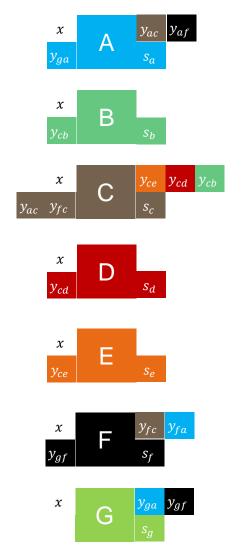


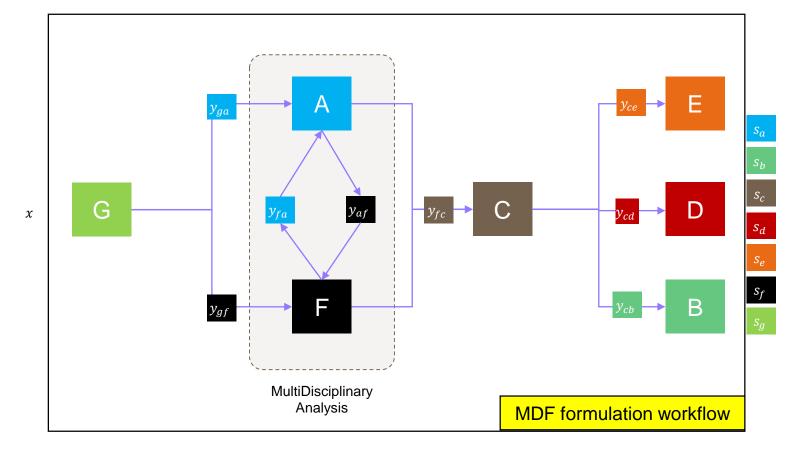
# **GEMSEO** automates the generation of workflows



**1.** The user defines the IO disciplines:

**2.** GEMSEO generates an executable workflow:





→ GEMSEO can generate workflows from thousands of disciplines, which would be very costly to do by hand!

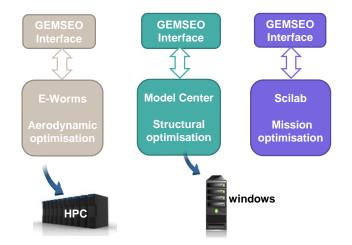
# **GEMSEO** automates the creation of MDO processes



**Define your optimization problem:**  $\min_{x} f(x)$  s.t.  $g(x) \le 3$  and h(x) = 0

Solve the optimization problem with an optimizer, based on this MDO process.

Define your disciplines.



**GEMSEO** saves a lot of programing time by automatically generating MDO processes according to a catalog of MDO formulations.

Hence, GEMSEO reduces maintenance issues and enables to easily reconfigure MDO processes.

Select an MDO formulation (or architecture), i.e. a mathematical rewriting of the optimization problem from the disciplines.

An MDO formulation is

- a mathematical strategy to define the optimization problem(s)
- a template of the MDO process organization,
- problem-independent.

- Optimization problem
- Disciplines
- MDO formulation names and options





MDO process

e.g.





,

#### API

scenario = MDOScenario([•,•,•], "MDF", "f", design\_space) scenario.add\_constraint("h") scenario.add\_constraint("g", "ineq", value=3.) scenario.execute({"algo": "SLSQP", "max\_iter": 100})





# GEMSEO facing uncertainties

# IRT project / VITAL / UQ for composite damage model



VITAL developed VIMS, a platform dedicated to Virtual Testing Integration for Decision Making Support. It uses and develops the UQ part of GEMSEO

# Coupon-level use cases

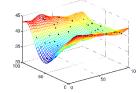




#### **Numerical simulators**







Replace costly simulators

#### **Model exploration**



■ X1 ■ X2 ■ X3 ■ X4

Make a sensitivity analysis to filter out the non-influential parameters



#### **Reliable design**

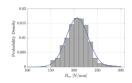


Evaluate a failure probability

e.g. B-value



#### **Uncertainty propagation**



Use probability distributions either data-based or knowledge-based

#### **Model calibration**







Update the model parameters by using data-fitting techniques





J. Camacho Casero, L. Barriere, S. Miot and M. De Lozzo (2021) Virtual testing applied to composite material modelling, SIAM-MS21

# IRT project / R-EVOL / UQ for MDO

SAINT T EXUPÉRY

In an uncertain frame,

we look for the design

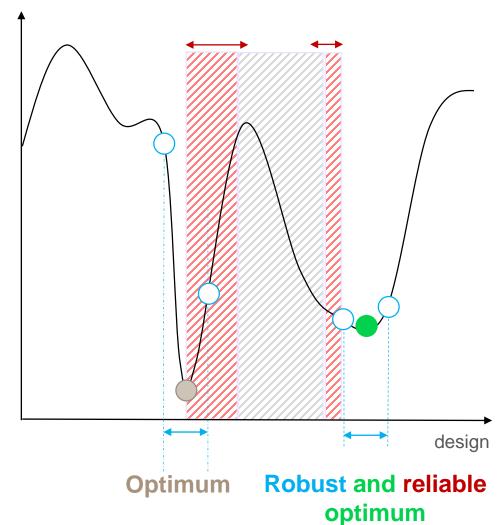
ensuring a mean performance

mean[cost(design,uncertainty)]

whilst satisfying the constraints most of the time.

probability[satisfied\_constraints(design,uncertainty)] > 99%

Design uncertaintyUnfeasible domain

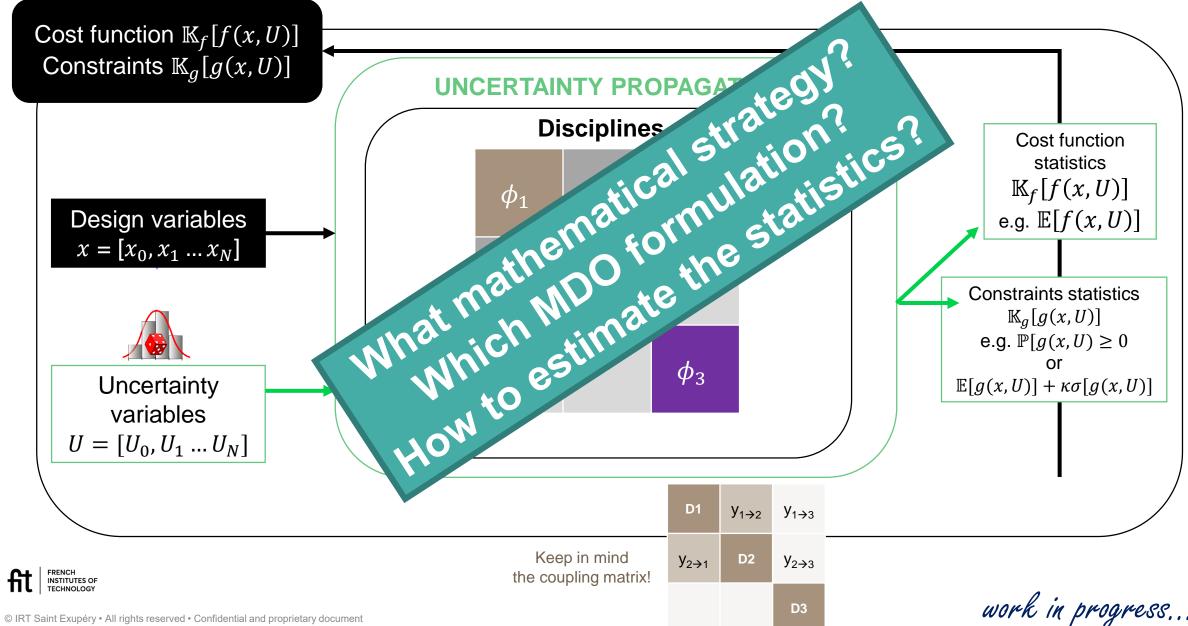


cost function



# IRT project / R-EVOL / UQ for MDO



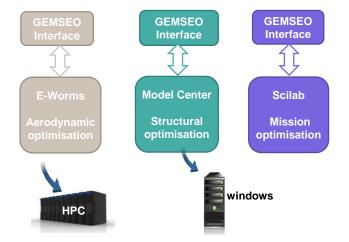


# IRT project / R-EVOL / UQ for MDO / Formulation engine



Define your optimization problem:  $\min_{x} \mathbb{E}[f(x, U)]$  s.t.  $\mathbb{P}[f(x, U) \le 3] \ge 1 - \epsilon_g$  and  $\mathbb{P}[-\epsilon \le h(x, U) \le \epsilon] = 1 - \epsilon_h$ 

Define your disciplines.



Select an MDO formulation (or architecture), i.e. a mathematical rewriting of the optimization problem from the disciplines.

and estimators of statistics

- Optimization problem
- Disciplines
- MDO formulation names and options
- Statistics estimators names and options

Uncertainty-based

MDO formulation engine

MDO process

Solve the optimization problem with an optimizer, based on this MDO process.

#### **API for MDO under uncertainty**

scenario = MDOScenario([•,•,•], "MDF", "f", design\_space, uncertain\_space, "Mean") scenario.add\_constraint("h", "Probability", threshold=1-eps\_h, tolerance=eps) scenario.add\_constraint("g", "Probability", threshold=1-eps\_g, greater=True, constraint\_type="ineq", value=3.) scenario.execute({"algo": "SLSQP", "max\_iter": 100})



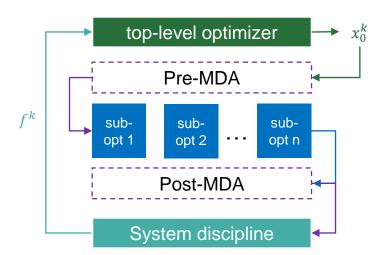
work in progress...

# IRT project / R-EVOL / UQ for MDO / Bi-level formulation



# **Bi-level formulation for MDO** available in GEMSEO

$$\min_{x_0} f(x_0, y_1(x_0, x_1^*(x_0)), ..., y_n(x_0, x_n^*(x_0)))$$
with
$$x_i^*(x_0) \in \operatorname{argmin}_{x_i} f_i(x_0, x_i, y_{-i}(x_0, \mu))$$

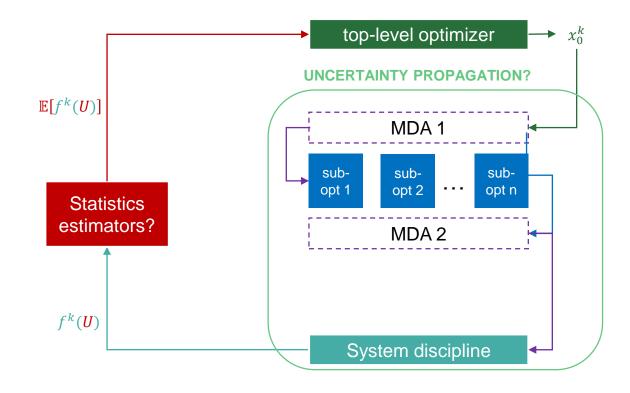


This formulation meets the industria expectations: relying on existing optimizers, validated long ago and on which a great deal of effort has been focused.



# Bi-level formulation for MDO under uncertainty

We want to create an analogous version under uncertainty (PhD thesis of Amine Aziz-Alaoui).



# IRT project / R-EVOL / UQ for MDO A scalable problem to benchmark robust MDO algorithms





A. Aziz-Alaoui, O. Roustant and M. De Lozzo (2023) A scalable benchmark for multidisciplinary optimization. Submitted to Optimization and Engineering.

coupling variable outputted by the i-th discipline

margin  $\mathbb{E} + \kappa \times \mathbb{S}$  or probability  $\mathbb{P}_{\varepsilon}$ 

shared design variable

coupling variables

$$\min_{\mathbf{x} \in [\mathbf{0},\mathbf{1}]} \mathbb{E} \left[ \mathbf{x}_0^T \mathbf{x}_0 + \sum_{1 \le i \le N} \mathbf{Y}_i^T \mathbf{Y}_i \right] \quad \text{s. t.} \quad \mathbb{K} [\mathbf{t}_i(\alpha) - \mathbf{Y}_i] \le 0 \text{ design variable specific to the } i$$

threshold vector

feasibility level

specific to the i-th discipline

where 
$$\mathbf{Y}_i = \mathbf{a}_i - \mathbf{D}_{i,0}\mathbf{x}_0 - \mathbf{D}_{i,i}\mathbf{x}_i + \sum_{1 \le i \le N} \mathbf{C}_{i,j}\mathbf{Y}_j + \mathbf{U}_i$$

random vectors and matrices with coefficients in [0,1]

 $U_i$  can follow any distribution with zero mean and covariance matrix  $\Sigma$ .

We showed that this robust MDO problem reduces to the quadratic optimization (QP) problem

$$\min_{x} \frac{1}{2} x^{T} Q x + c^{T} x + d + \mathbb{E}[U^{T} P^{T} P U]$$

s.t: 
$$Ax \leq b + \text{offset}(\mathbb{K})$$

#### The user can change

- the number of disciplines *N*,
- the dimension of  $x_0, x_1, ..., x_N$ ,
- the dimension of  $y_1, ..., y_N$ ,
- the feasibility level  $\alpha$ ,
- the distribution.

#### The user can compare

- MDO formulations,
- optimization algorithms,
- coupling algorithms,
- estimators of statistics,
- mixtures of that,

	$oldsymbol{\Delta}_{\mathbf{x}}(\%)$	$oldsymbol{\Delta_f}(\%)$	$oldsymbol{\Delta}_{\mathbf{g}}(\%)$
MC	0.370 $(0.176)$	0.592 $(0.127)$	0.877 $(0.278)$
TP	0.093	0.005	0.143

INSTITUTES OF TECHNOLOGY

# IRT project / R-EVOL / UQ for MDO / Statistics estimation → MLMC + polynomial chaos expansion (PCE) + control variate (CV)





M. Reda El Amri, P. Mycek, S. Ricci, M. De Lozzo (2023) Multilevel Surrogate-based Control Variates. Submitted to SIAM JUQ.

We showed that mixing sampling and surrogate modelling reduce the variance of statistics estimators, even with poor-quality surrogate models.

Using multi-level simulators for both sampling and

We proposed an MLMC-MLCV algorithm allocating samples to levels according to the variance reduction.

control-variates can reduce it even further.

# 1 Use surrogate-based CV

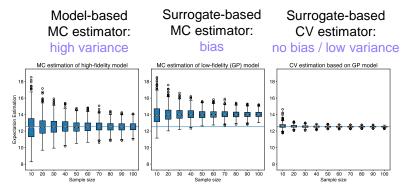


Illustration: stochastic Rosenbrock



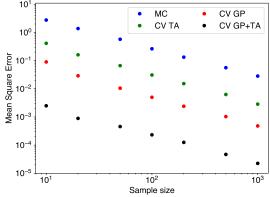


Illustration: stochastic Rosenbrock

# 3 Use multi-level simulators (MLS)

# Require: $n_\ell^{\rm init} > 1$ , $r_\ell > 1$ , surrogate models (depending on the method), and budget $\mathcal{C}$ . 1: Set consumed budget to $\tilde{\mathcal{C}} = 0$ and $\delta n_\ell = n_\ell^{\rm init}$ samples on levels $\ell \leq L$ ; 2: while $\tilde{\mathcal{C}} \leq \mathcal{C}$ do 3: compute $\delta n_\ell$ samples on each level by evaluating $f_\ell$ and the appropriate surrogates; 4: update sample size on each level: $n_\ell \leftarrow n_\ell + \delta n_\ell$ ; 5: update consumed budget: $\tilde{\mathcal{C}} \leftarrow \tilde{\mathcal{C}} + \sum_{\ell=0}^L \delta n_\ell (\mathcal{C}_\ell + \mathcal{C}_{\ell-1})$ ; estimate the optimal CV parameter(s) on each level; 7: compute/update CV estimates for $\hat{T}_\ell^{(\ell)}$ and $\mathcal{V}_\ell^{\rm CV}$ from samples on levels $\ell \leq L$ ; 8: select level $\ell^* = \arg\max_{0 \leq \ell \leq L} \frac{\mathcal{V}_\ell^{\rm CV}}{r_\ell n_\ell^2 (\mathcal{C}_\ell + \mathcal{C}_{\ell-1})}$ ; 9: $\delta n_{\ell^*} \leftarrow \lfloor (r_{\ell^*} - 1) n_{\ell^*} \rfloor$ , $\delta n_{\ell \neq \ell^*} \leftarrow 0$ ; 10: end while 11: return $\hat{\theta}_L^{\rm MLMC-*}$ , the MLMC-\* estimate of $\theta_L$ .

Algorithm 1 Simplified MLMC-\* algorithm inspired by [36].

# 4 Combine MC, MLS and SBCVs

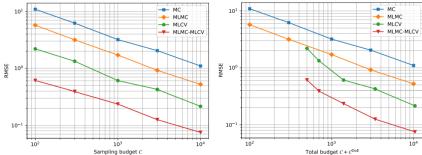
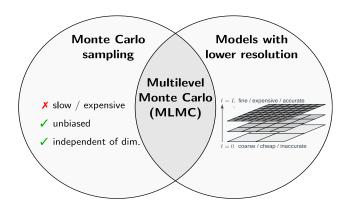


Illustration: heat equation; CV = Polynomial Chaos Expansion with LARS



The is a rich literature on MLMC.



# GEMSEO using OpenTURNS

# Before UQ, GEMSEO allowed the user to ...



- create a DesignSpace
- solve an OptimizationProblem
  - create objective and constraints as MDOFunctions,
  - use an optimization or DOE algorithm from a **DriverLibrary** interfacing an algorithm library callable from Python
  - post-process the results
- solve an MDO problem
  - create **MDODiscipline**s (analytic formula, Python function, executable, ...)
  - select an MDOFormulation (IDF, MDF, BiLevel, ...)
  - use an optimization or DOE algorithm from any **DriverLibrary** callable from Python (e.g. SciPy, NLOPT, pymoo, OpenTURNS, ...)
  - post-process the results
- automatically couple disciplines:
  - create MDODisciplines... and voilà!
- create SurrogateDiscipline from any machine learning or scientific library callable from Python (e.g., SciPy, scikit-learn, ...)

• ...



The user was familiar with the GEMSEO concepts and somehow appreciated its abstract layer that doesn't make it dependent on a single library, but allows it to be extended to a multitude of libraries.

So we started the UQ with an abstract layer independent of OpenTURNS or any other UQ library.



# **Probability distributions**



- Distribution
  - SPDistribution (based on SciPy)
  - OTDistribution (any OpenTURNS distribution)



- OTExponentialDistribution
- OTNormalDistribution
- OTUniformDistribution
- OTTriangularDistribution
- OTComposedDistribution (used copula)

# First option

normal = OTNormalDistribution("x", 1.0, 2.0)

# Second option (direct interface to OpenTURNS)

normal = OTDistribution("x", "normal", (1.0, 2.0))

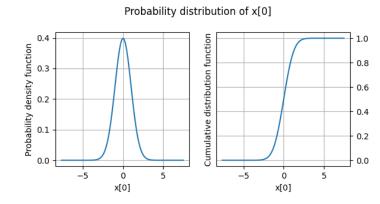
normal.mean

normal.standard\_deviation

normal.support

normal.range

normal.plot()





# **Uncertainty propagation**



- AlgorithmLibrary
  - LinearSolverLibrary
  - DriverLibrary
    - OptimizerLibrary
    - DOELibrary
      - PyDOE
      - CustomDOE (from CSV file or arrays
      - OpenTURNS
        - "OT\_MONTE\_CARLO"
        - "OT FAURE"
        - "OT HALTON"
        - "OT HASELGROVE"
        - "OT\_REVERSE\_HALTON"
        - "OT SOBOL"
        - "OT LHS"
        - "OT OPT LHS"
        - "OT AXIAL"
        - "OT COMPOSITE"
        - "OT FACTORIAL"

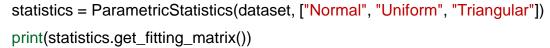
```
# Creation of the uncertain space
uncertain_space = ParameterSpace()
uncertain_space.add_random_variable("x", "OTNormalDistribution", ...)
uncertain_space.add_random_variable("y", "OTTriangularDistribution", ...)
# A scenario creates the OptimizationProblem corresponding to a formulation.
scenario = create scenario(
  disciplines.
  formulation="MDF",
  objective name="foo",
  design_space=uncertain_space,
  scenario_type="DOE".
scenario.add_constraint("bar")
scenario.add observable("baz")
# Use any algorithm name.
scenario.execute({"algo": "OT_OPT_LHS", "n_samples": 30})
scenario.post_process("ScatterPlotMatrix")
dataset = scenario.to_dataset() # A Dataset is an advanced pandas dataframe.
dataset.describe()
```



# **Uncertainty quantification**

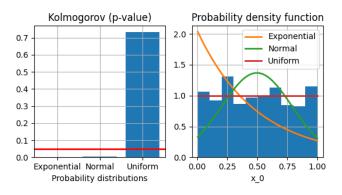


- Dataset-based statistics
  - Methods:
    - compute\_mean
    - compute\_variance
    - compute\_probability
    - •
  - EmpiricalStatistics (pure NumPy / SciPy)
  - ParametricStatistics
    - ot.DistributionFactory
    - ot.FittingTest.{BIC,ChiSquared,Kolmogorov}



Variable	Exponential	Normal	Uniform	Selection
x_0   1.6   x_1   2.   x_2   1.5	502160180879313e-10 82659088382179e-53 5387797946575896e-09	0.005823020521403932 0.8587721484840084 0.0016128012413438864 2.0987474708559965e-10	0.7338504331264553 5.660300987516015e-18 7.748433868335025e-67 7.782983660206643e-152	Uniform Normal Normal

mean = statistics.plot\_criteria("x\_0")



mean = statistics.compute\_mean()





# **Sensitivity analysis**



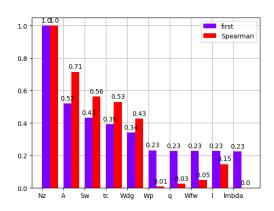


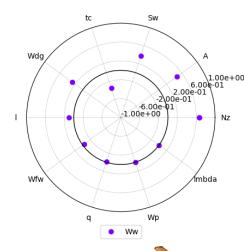
- SensitivityAnalysis
  - MorrisAnalysis
  - CorrelationAnalysis
  - SobolAnalysis

- Methods
  - Visualization (with/without sorting)
    - plot\_bar
    - plot\_radar → higher scalability
    - plot\_field → 1D/2D output
    - plot\_comparison (to be used carefully!)
    - plot → specific to a type of sensitivity analysis
  - sort\_parameters according to main\_method

- Can be applied to
  - 1 discipline
  - 1 multidisciplinary process (disciplines + formulations)















# **Sensitivity analysis – Morris method**



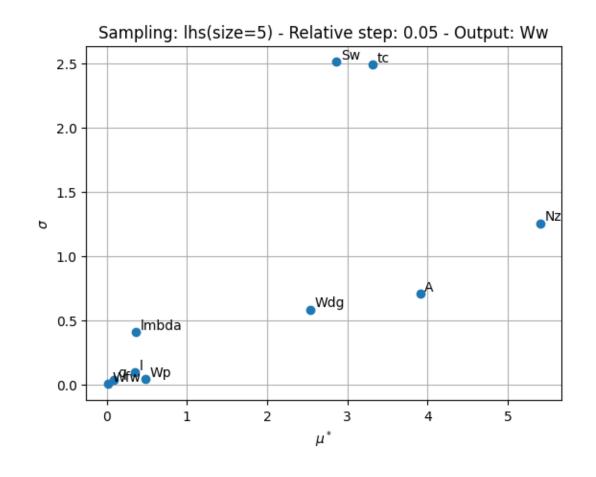
Idea: compare the impact of the uncertain variables on the output based on finite differences (FD)

#### **Properties:**

- $\mu$  = mean of the FD
- $\mu^*$  = mean of the absolute FD
- $\sigma$  = standard deviation of the FD
- min = minimum value of the output
- max = maximum value of the output

### **Options:**

- Step (5%)
- Number of repetitions (5)
- DOE algo (LHS)
- Filter variables in the plot









# **Sensitivity analysis - Correlation coefficients**



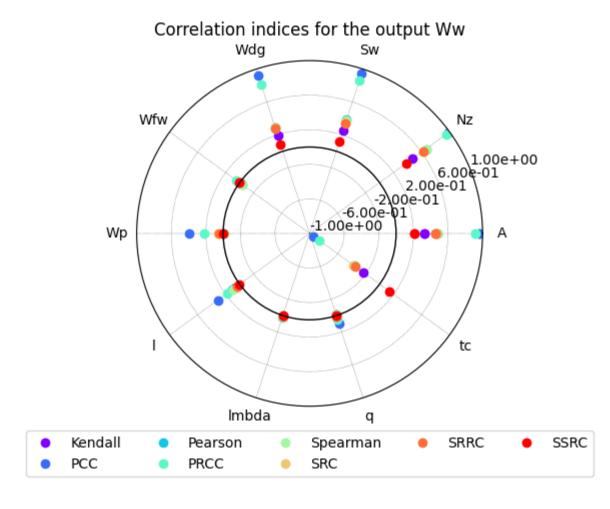
Idea: compare the impact of the uncertain variables on the output based on correlations

#### **Properties:**

- $\mu$  = mean of the FD
- $\mu^*$  = mean of the absolute FD
- $\sigma$  = standard deviation of the FD
- min = minimum value of the output
- max = maximum value of the output

#### **Options:**

- Compute 2nd order indices (True)
- Asymptotic distribution (True)
- Algorithm (Saltelli)
- Confidence level (95%)









# Sensitivity analysis - Sobol' indices



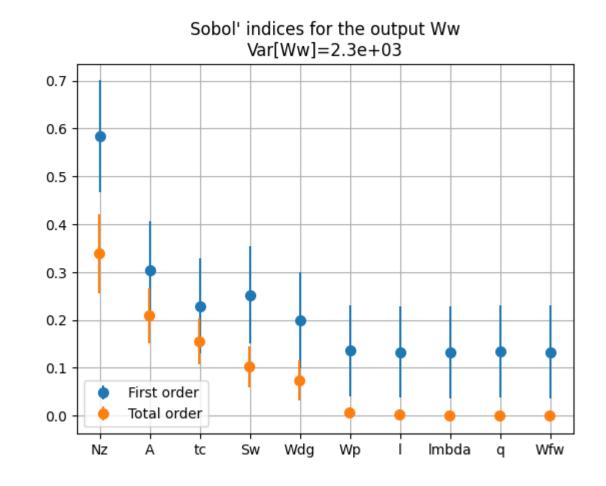
Idea: compare the impact of the uncertain variables on the output based on variance decomposition

#### **Properties:**

- $\mu$  = mean of the FD
- $\mu^*$  = mean of the absolute FD
- $\sigma$  = standard deviation of the FD
- min = minimum value of the output
- max = maximum value of the output

#### **Options:**

- Compute 2nd order indices (True)
- Asymptotic distribution (True)
- Algorithm (Saltelli)
- Confidence level (95%)











# Sensitivity analysis - Sobol' graph



Idea: plot the first-, second- and total-order indices with a graph.



T. Muehlenstaedt, O. Roustant, L. Carraro and S. Kuhnt (2012) Data-driven Kriging models based on FANOVA-decomposition. Statistics and Computing

Nodes:

Name: input variable (total-order in %, first-order in %)

Thickness: total-order index

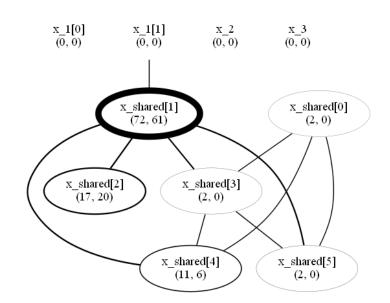
Edges:

Thickness: second-order index

sobol\_analysis = SobolAnalysis(disciplines, uncertain\_space, 1000) sobol\_analysis.compute\_indices()



sobol\_graph = SobolGraph.from\_analysis(sobol\_analysis, output\_name="y\_4") sobol\_graph.visualize(show=True, file\_path="sobol\_graph.pdf")





# Sensitivity analysis - Uncertain coupling graph



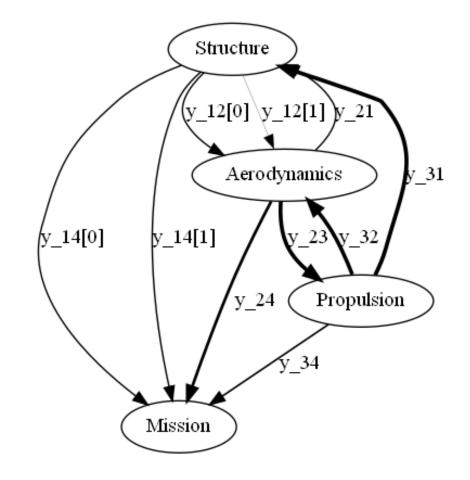
Idea: highlight the most uncertain paths in a multidisciplinary system.

#### **Ingredients:**

- a coupling graph
  - nodes = disciplines
  - edges = coupling variables
- a statistic measuring the dispersion, e.g.
  - coefficient of variation  $\sigma/\mu$ , a.k.a. relative standard deviation
  - quartile coefficient of dispersion

$$(q_{75\%} - q_{25\%})/(q_{25\%} + q_{75\%})$$

edges proportional to the statistics



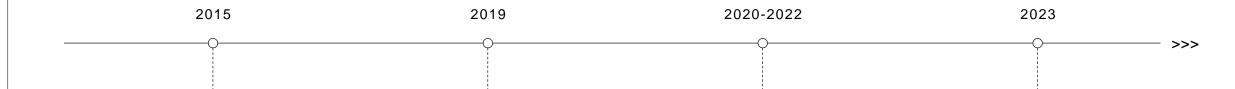




# Conclusion

# **History of GEMSEO's use of OpenTURNS**





#### DOE

LHS,
low-discrepancy
sequences,
stratified DOEs, ...

# **Surrogates**

Polynomial chaos expansion

#### UQ

Distributions, distribution fitting, Sobol' analysis, correlation,

#### . .

## **Surrogates**

Kriging (with LAPACK & HMAT)

#### UQ

Copula, iterative statistics, HSIC, ...



# **Take-home message**



- GEMSEO is made for MDO and can address other multidisciplinary problems.
- It offers MDO features, e.g. optimizers, coupling algorithms, linear solvers, visualization for optimization histories, ...
- These features are fully expandable thanks to factory mechanics (*« Derive from the base class and voilà! »*).



• It has also DOE functionalities for tradeoff studies (« MDO with a DOE instead of an optimizer often gives a first idea. »).



• It proposes a machine learning package to build efficient surrogate models by interfacing specialized libraries.

- For the four past years, we've been adding UQ inside GEMSEO, always starting with abstract classes in pure Python:
  - Probability distributions
  - · Probability distribution fitting



- Sensitivity analysis
- Sometimes we develop functionalities in GEMSEO that would be better placed in a UQ library... if we ever find them in OpenTURNS, we'll surely use them . ©
- The idea is not to create Python wrappers of OpenTURNS functions but to use OpenTURNS in GEMSEO, a Python library for multidisciplinary studies, fully object-oriented and *keen* to be enriched.



# Roadmap





## **Multi-fidelity**

Use of multiple levels of precision for a given discipline to accelerate the computational time



# **Machine learning**

Automate the construction, selection and calibration of surrogate models and extend GEMSEO by plugging specialized ML and IA libraries



## **Active learning**

Improve a model, e.g. surrogate model, by learning new data during a process, e.g. optimization or statistics estimation



## **Sensitivity analysis**

Understand the influence of uncertain inputs on outputs, with a focus on dependency and high dimension for coupling variables



#### **Robust MDO**

Use of MDO formulations and efficient estimation of statistics for MDO under uncertainty



## **Optimizers**

Use of global optimization algorithms for cheap disciplines as well as surrogate-based optimization







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