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# Open Source Environment for Multidisciplinary Optimisation

GEMSEO


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# Outline

- **Context and IRT MDA/O approach**
- **Implementation in GEMSEO and results**
- **Conclusion**

# Context and IRT MDA/O approach

# Challenges for applying MDA/O in industry

- Maintainability
  - a wide range of processes, with different types of orchestration depending on the use-cases and numerical resolution strategies
  - complex processes are subject to changes (data and models)
- Scalability
  - numerous analysis models, thousands of design variables, coupling variables and constraints
- Distributed processes
  - MPI processes on many nodes
- Mathematical difficulty
  - design variables of different types (continuous, discrete, categorical), models may be black boxes; can provide derivatives or not.

# Main technical objectives

**Develop optimization strategies (MDO formulations) to efficiently resolve optimization problems**

- A large number of design parameters
- Efficient ways to couple disciplines
- Minimizing the computational cost which is proportional to the number of required simulations and adjoint computations

Development of the BLISS 98 formulation, enhancement of the IRT Bi-level formulations family, application and benchmark

**Evaluate and select the most efficient MDO formulation for a given problem**

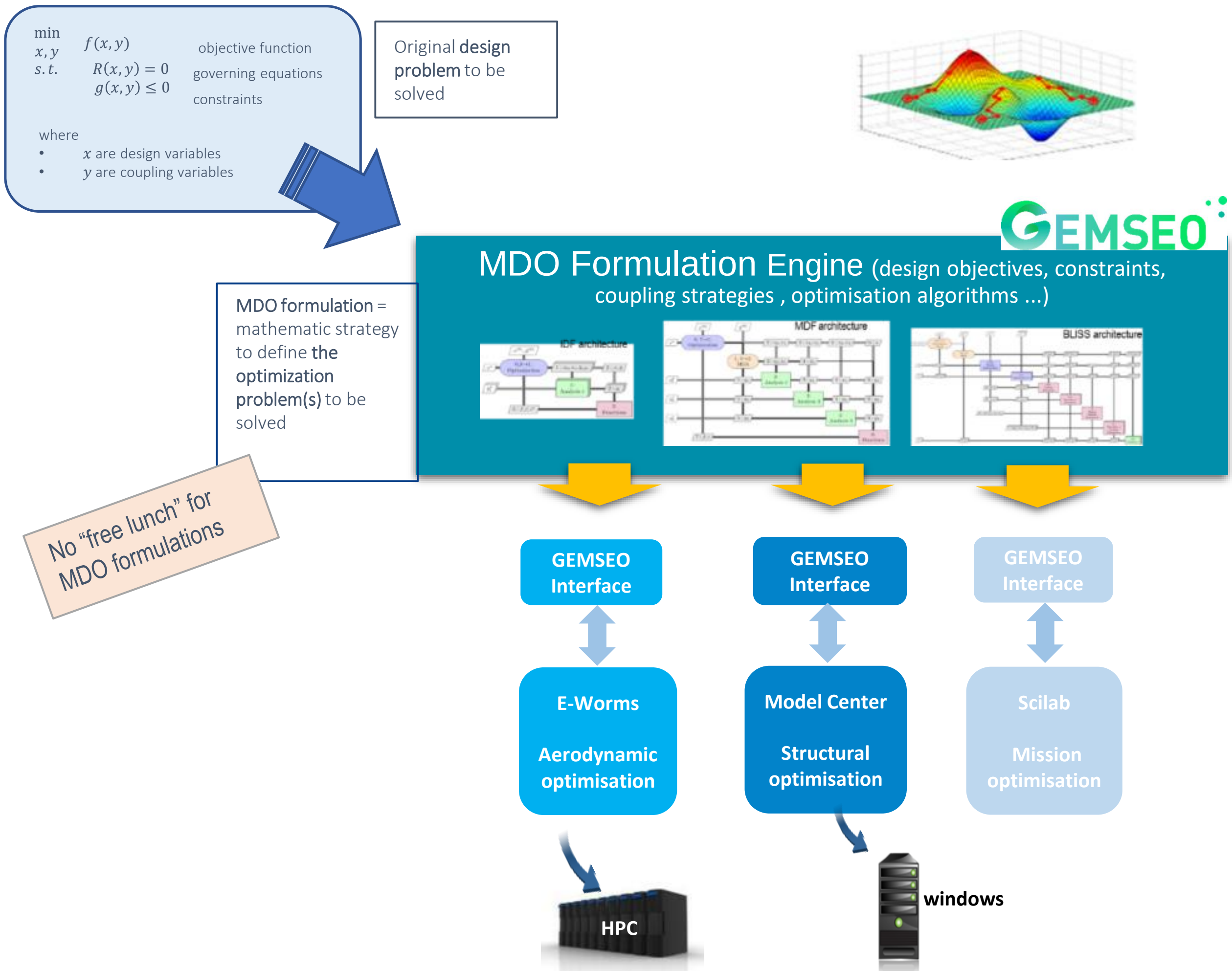
IRT scalable models-based methodology

**Accelerate the MDO processes**

MPI extension of MDA and MDO capabilities in GEMSEO

- Large scale stiff linear systems studied for coupled adjoint

# MDO processes




## MDO formulations for automatic MDO process generation

MDO formulations are « templates » of MDO process organization

MDO formulations are independent of the considered problem.

Hence:

→Programming time saving

→Reduce maintenance issue

Their application to the considered problem is performed through discipline wrapping.

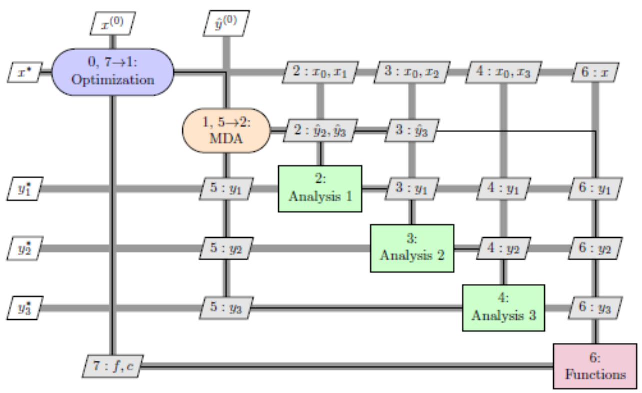
→Facilitates the automatic creation of MDO processes

→Enables to easily reconfigure MDO processes

# MDO formulations

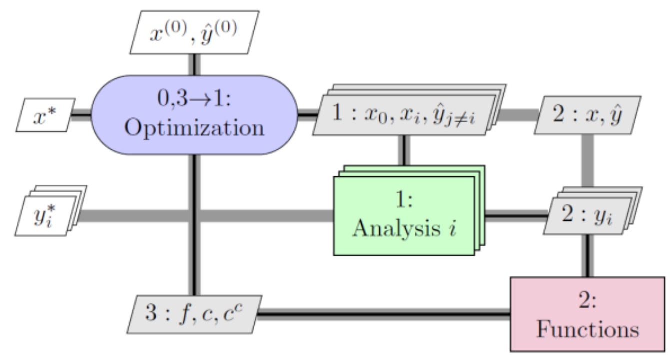
- For a given set of disciplines, design objective and constraints the MDO formulation defines one or multiple **optimization problems** and an **associated process** to compute their criteria.
- There are multiple ways of reformulating the same MDO problem, and theoretically have the **same solution**, although **not with the same convergence**.
- But those alternatives don’t have the same consequences in terms of **process organization**.
- The available formulations in GEMSEO : **MDF, IDF, a family of Bilevel formulations** (distributed disciplinary optimization, distributed MDF)

**MDF**




$$
\begin{aligned}
\text{minimize} \quad & f_0\left(x, y\left(x, y\right)\right) \\
\text{with respect to} \quad & x \\
\text{subject to} \quad & c_0\left(x, y\left(x, y\right)\right) \geq 0 \\
& c_i\left(x_0, x_i, y_i\left(x_0, x_i, y_{j \neq i}\right)\right) \geq 0 \quad \text{for} \quad i = 1, \ldots, N.
\end{aligned}
$$

**IDF**




$$
\begin{aligned}
\text{minimize} \quad & f_0\left(x, y\left(x, \hat{y}\right)\right) \\
\text{with respect to} \quad & x, \hat{y} \\
\text{subject to} \quad & c_0\left(x, y\left(x, \hat{y}\right)\right) \geq 0 \\
& c_i\left(x_0, x_i, y_i\left(x_0, x_i, \hat{y}_{j \neq i}\right)\right) \geq 0 \quad \text{for} \quad i = 1, \ldots, N \\
& c_i^c = \hat{y}_i - y_i\left(x_0, x_i, \hat{y}_{j \neq i}\right) = 0 \quad \text{for} \quad i = 1, \ldots, N.
\end{aligned}
$$

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*[JRRA Martins, A Lambe, Multidisciplinary design optimization: a survey of architectures, AIAA journal 2013]*

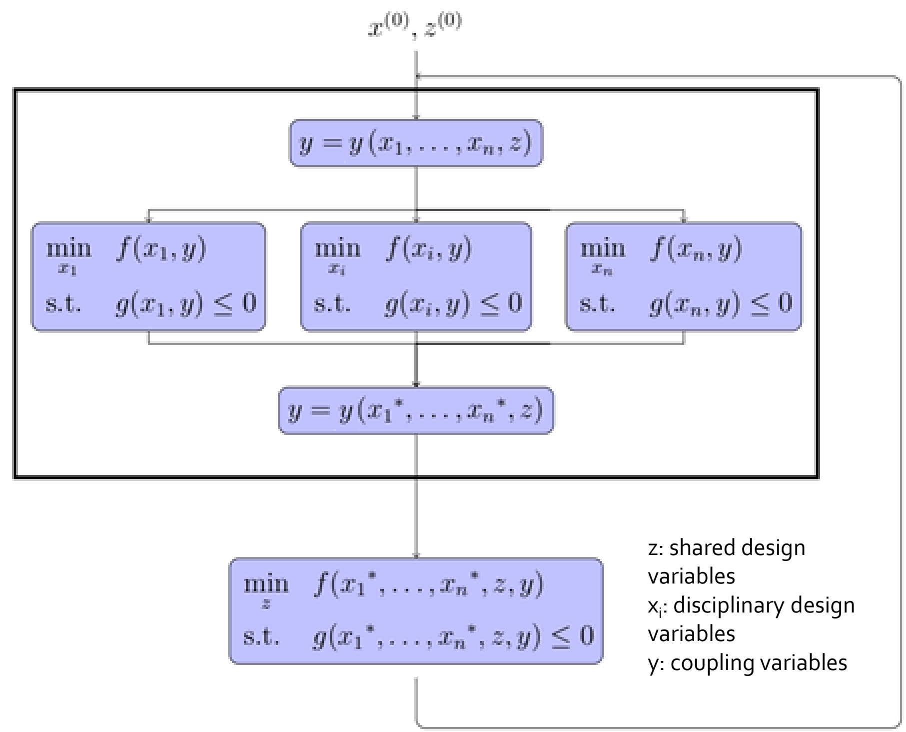
# Bi-level formulations family

**IRT bi-level formulations family is specifically designed to match industrial processes and tools constraints:**

- Re-use of disciplinary optimization processes (preserve some discipline autonomy),
- Alleviate full process derivatives requirement,
- Allow mixed variables (continuous, discrete, categorical),
- Allow different levels of fidelity,
- Ensure that the current solution always has a physical meaning (even before convergence)

**It reconcilies the two a priori contradictory objectives:**

- Being able to create new efficient complex MDO processes challenging usual more conservative solutions
- Taking full benefit from already existing and validated mono-disciplinary optimization processes




$$\min_{z,x} f(z,x) \longrightarrow \min_{z} f(z,x^*(z)) \qquad x^* = \operatorname*{argmin}_{x}(f(z,x))$$

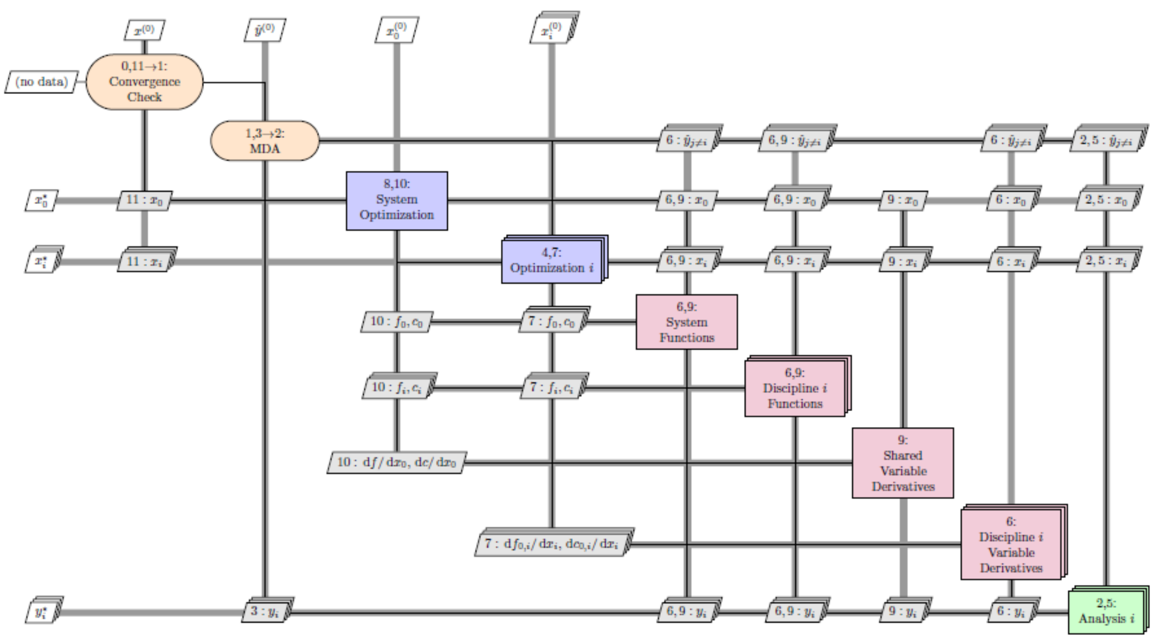
# BLISS 98 – A gradient based bi-level formulation

Computing the **coupled adjoint** is one of the main MADELEINE objectives

→ The opportunity to use it at the **system level** of the bi-level formulation!

The BLISS 98 formulation :

- Relies on **coupled adjoint and post optimal analysis** to compute the **gradient of the system level** in order to accelerate the system level convergence
- Approximates of the system-level and discipline-level objectives by **linear models**, controlled by **trust regions**




**BLISS 98**

The system-level subproblem is

$$
\begin{aligned}
\text{minimize} \quad & (f_0^*)_0 + \left(\frac{\mathrm{d}f_0^*}{\mathrm{d}x_0}\right)\Delta x_0 \\
\text{with respect to} \quad & \Delta x_0 \\
\text{subject to} \quad & (c_0^*)_0 + \left(\frac{\mathrm{d}c_0^*}{\mathrm{d}x_0}\right)\Delta x_0 \geq 0 \\
& (c_i^*)_0 + \left(\frac{\mathrm{d}c_i^*}{\mathrm{d}x_0}\right)\Delta x_0 \geq 0 \quad \text{for} \quad i = 1, \ldots, N \\
& \Delta x_{0L} \leq \Delta x_0 \leq \Delta x_{0U}.
\end{aligned}
$$

The discipline $i$ subproblem is given by

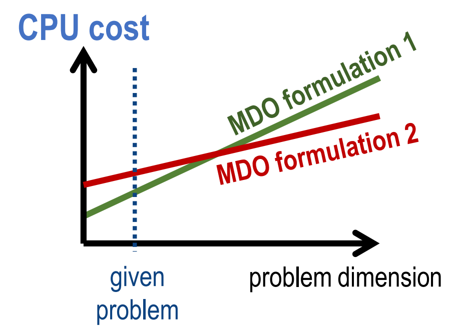
$$
\begin{aligned}
\text{minimize} \quad & (f_0)_0 + \left(\frac{\mathrm{d}f_0}{\mathrm{d}x_i}\right)\Delta x_i \\
\text{with respect to} \quad & \Delta x_i \\
\text{subject to} \quad & (c_0)_0 + \left(\frac{\mathrm{d}c_0}{\mathrm{d}x_i}\right)\Delta x_i \geq 0 \\
& (c_i)_0 + \left(\frac{\mathrm{d}c_i}{\mathrm{d}x_i}\right)\Delta x_i \geq 0 \\
& \Delta x_{iL} \leq \Delta x_i \leq \Delta x_{iU}.
\end{aligned}
$$

# Scalable models-based methodology

For a given MDO problem, we do not know in advance what is **the best MDO formulation.**

And even less **for other problem dimensions.**

→ To benchmark different MDO formulations at low cost, the idea is **to replace each discipline by a « scalable model » and use it for both the original problem and new problem dimensions**




**SCALABLE MODEL**

- MODEL → Associating outputs with inputs
- FAST-RESPONSE → Quick to evaluate
- DATA-DRIVEN → Built from some evaluations of the original discipline
- TARGET → Learning the mathematical features of interest to MDO processes
- SCALABLE → Generalizing these features to higher input and output dimensions

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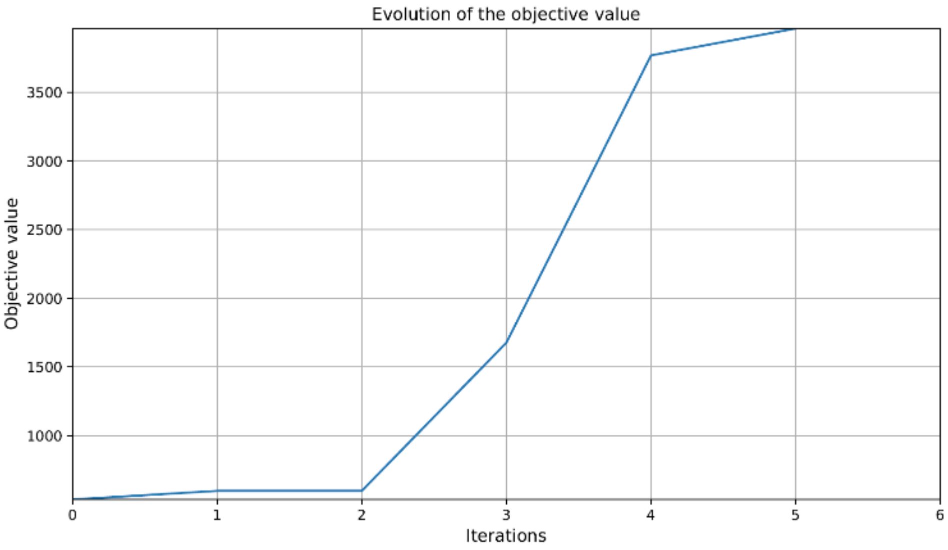
# Implementation in GEMSEO and results

# BLISS 98 – Implementation and validation

The BLISS 98 formulation was implemented in GEMSEO.

- Takes advantage of existing **coupled adjoint and post optimal analysis** capabilities.
- A generic implementation, independent of the MDO problem
- Not straightforward

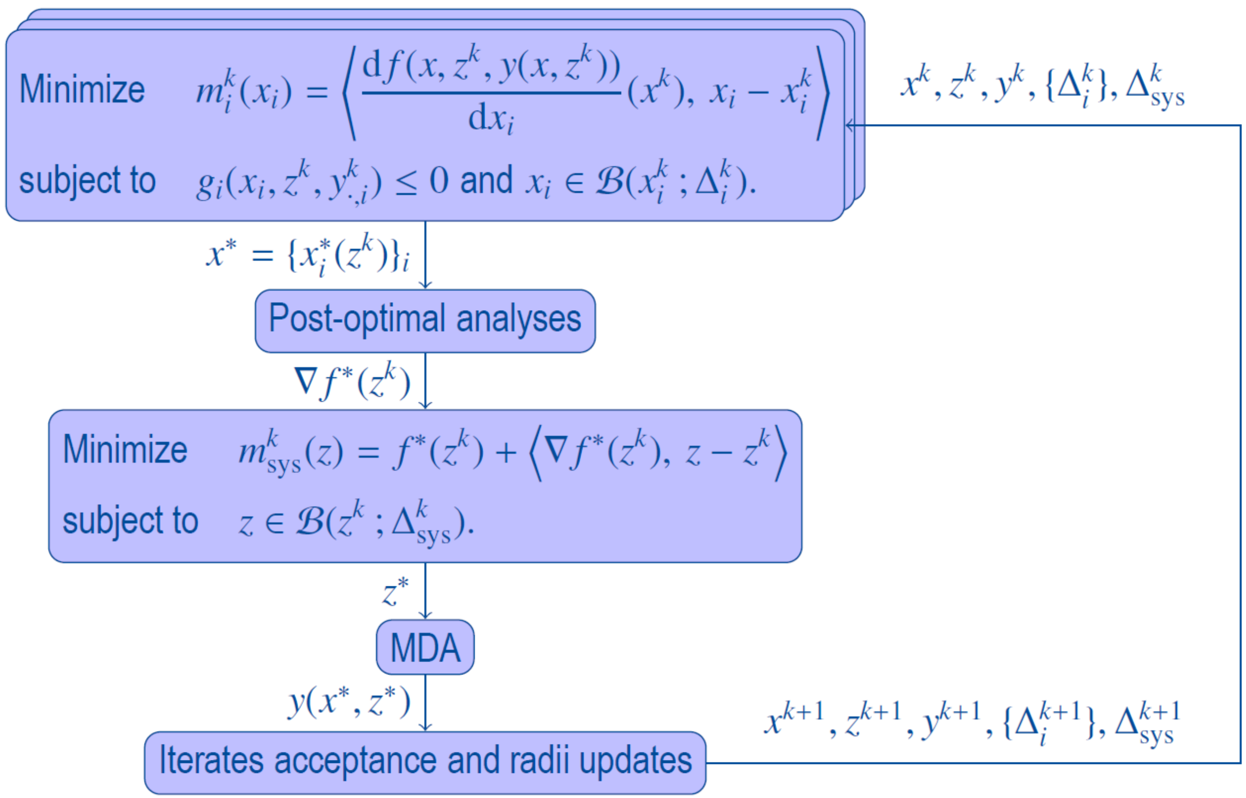
Sobieski's SSBJ benchmark solved in 7 iterations
The original approach, from the 1998 paper



# BLISS 98 – variants

**ONERA** provided expertise to **improve** the original BLISS formulation.

- Adding **a second MDA** right before the post-optimal analysis for interdisciplinary consistency.
- Using **nonlinear** models to better capture nonlinear behaviours (e.g. convex linearizations, quadratic models).
- Replacing discipline-level problems with constrained **non-monotone line searches**



# Enhanced IRT bi-level MDO formulation

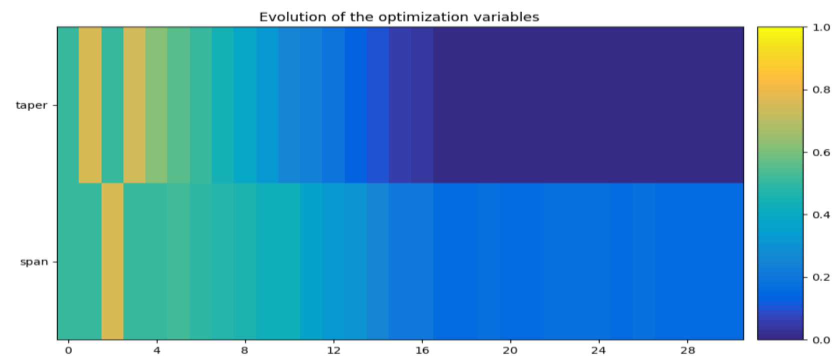
- Onera provided a Nastran wing dynamic – static optimization test case that challenges multi-level MDO formulations
- The standard IRT Bi-level formulation failed to converge

=> A convergence loop was added to iterate over the sub-optimizations, the « Block Coordinated Descent » approach
=> That solved the convergence issues

COBYLA (gradient-free)

| | |
|---|---|
| min | weight(masses, thicknesses) |
| w.r.t. | span and taper |
| s.t. | frequency, strain and strength |

span and taper




Weight, optimal masses and thicknesses

**Block Coordinated Descent (BCD)**

1

| | |
|---|---|
| min | weight |
| w.r.t. | 153 thicknesses |
| s.t. | strain & strength |

SLSQP (gradient-based)

2

| | |
|---|---|
| min | weight |
| w.r.t. | 39 concentrated masses |
| s.t. | frequency |

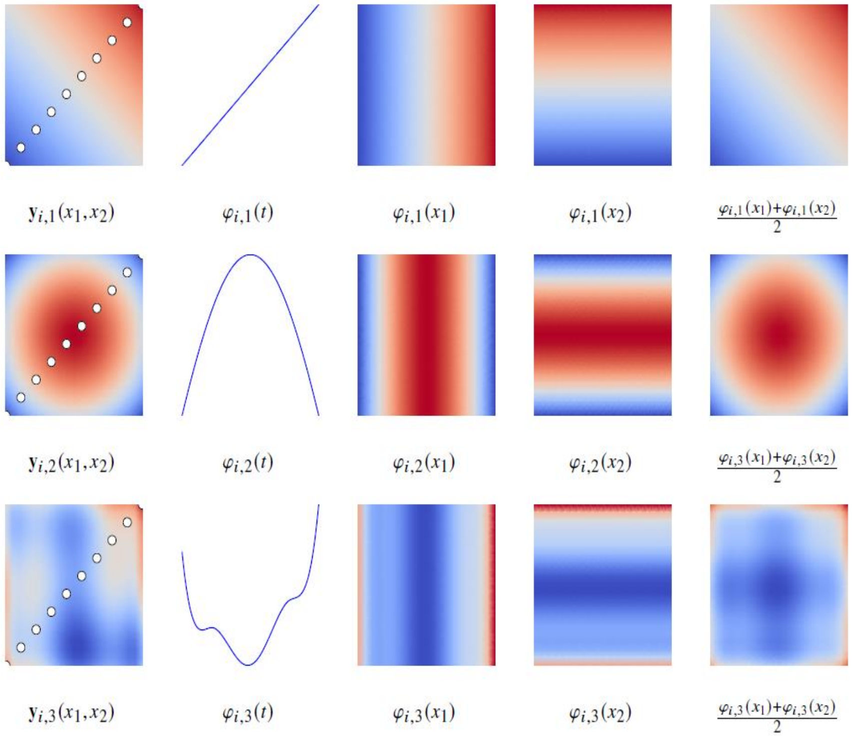
SLSQP (gradient-based)

# Scalable model-based methodology

Objective: to assist the choice of MDO formulation with a quantitative approach

Difficulties:

- Benchmark on real problems is too expansive
- Arbitrary analytic problems have not the sames mathematical properties as real problems
- Classical surrogate models are inappropriate here




Proposed approach:

- A data driven approach using minimal data
- GEMSEO generates automatically the DOE
- Model the computational cost of the real problems
- Simulate many processes and perform statistics

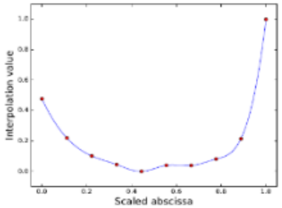
*De Lozzo, Matthias, et al. "A data-driven scalable MDO problem to compare MDO formulations." AIAA AVIATION 2021 FORUM. 2021.*

*Abu-Zurayk, Mohammad, et al. "Comparing Two Multidisciplinary Optimization Formulations of Trimmed Aircraft Subject to Industry-relevant Loads and Constraints." AIAA AVIATION 2021 FORUM. 2021.*

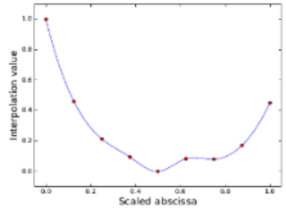
# Results on wing MDO use cases

## Basis functions

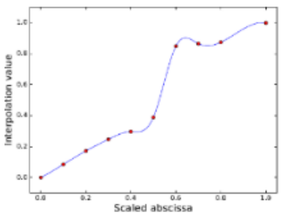
XRF1:
DLR data



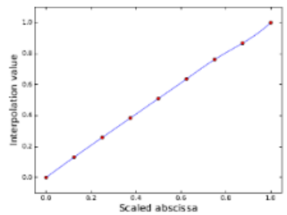
(a) Seq



(b) AAO

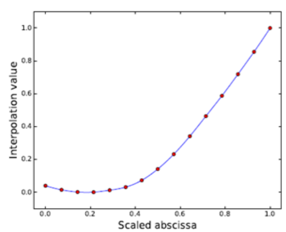


(a) Seq

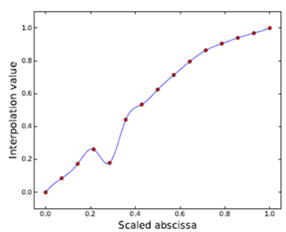


(b) AAO

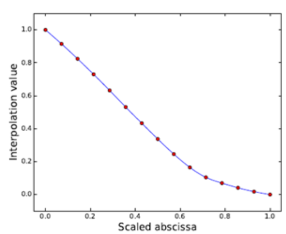
GBJ:
Dassault
& ESI
data



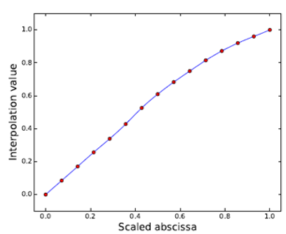
**(a) CD**



**(b) CL**

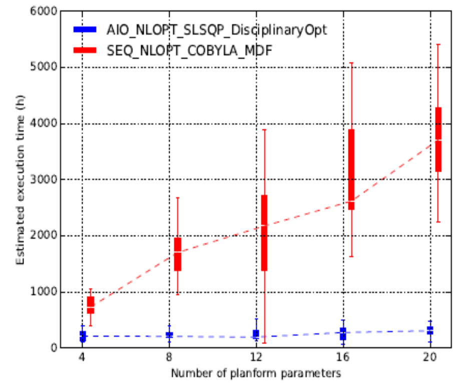


**(d) FS1**

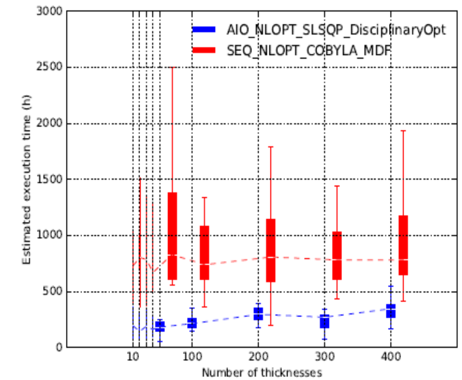


**(e) FS2**

## Estimated CPU cost

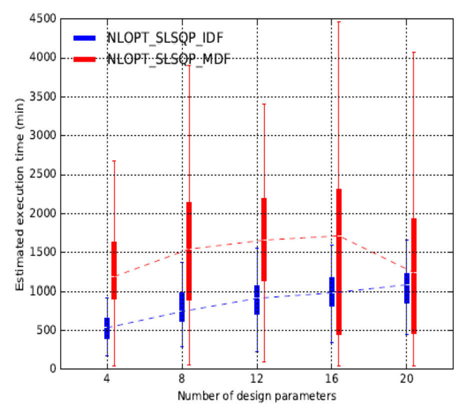


(a) Scaling material parameters

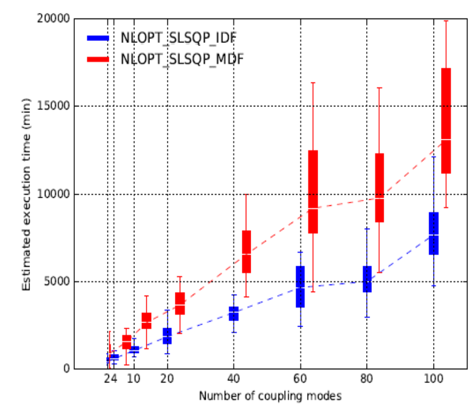


(b) Scaling coupling parameters

AIO formulation is faster



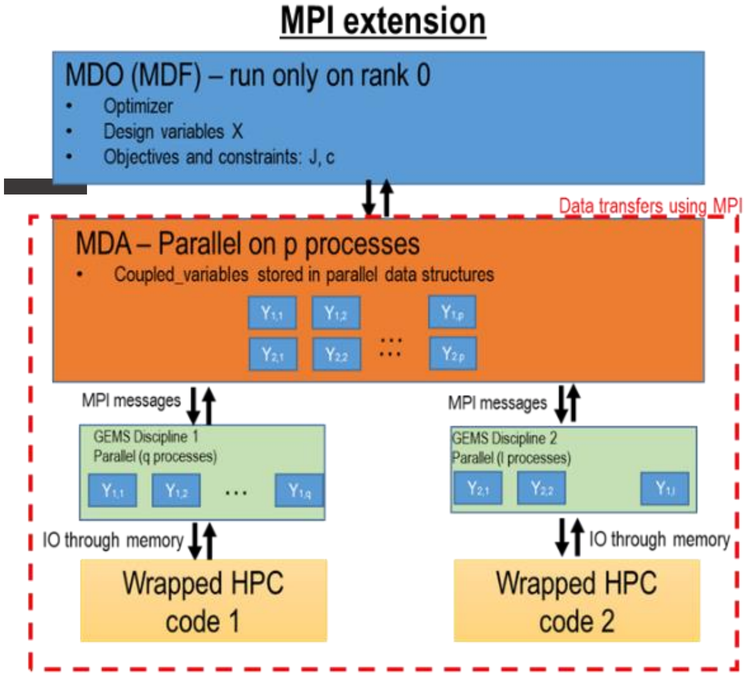
**(a) Scaling material parameters**

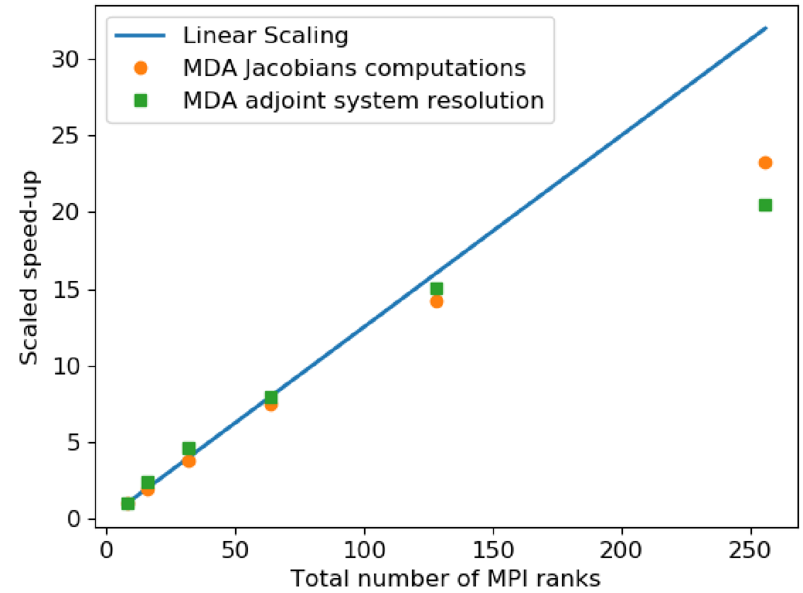


**(b) Scaling coupling parameters**

IDF formulation is faster

# MPI extension of MDO processes




Extension of GEMSEO parallel capabilities to distribute the computation on many HPC nodes.

Driving concepts:

- Each discipline or process has its own MPI communicator
- Data transfers and synchronizations are automated
- Does not break the reconfigurable process features of GEMS.

Key results:

- A focus was made on efficient coupled adjoint solvers using PetsC
- Results on 250 cores with 5 millions coupling variables, with coupled adjoint, are promising

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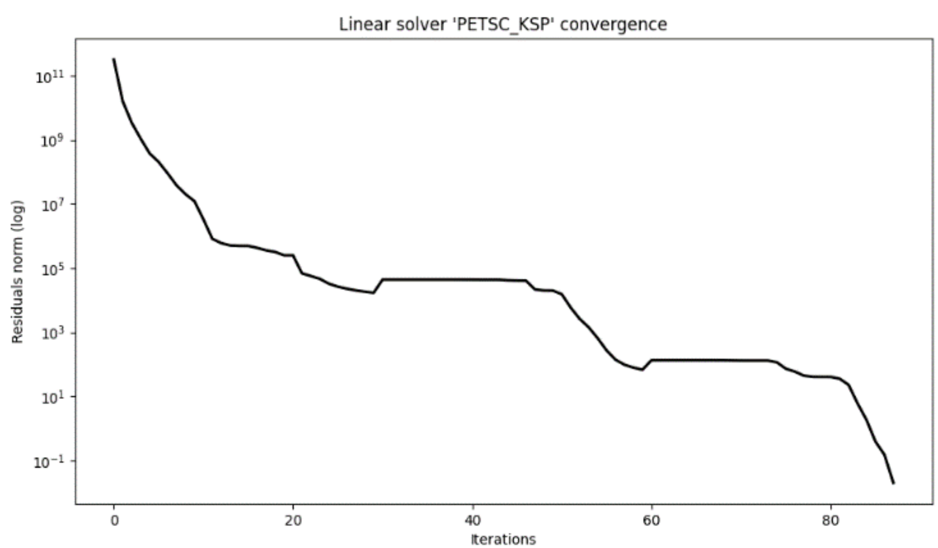
# New GEMSEO-PetsC linear solvers plugin

- Usages:
  - Coupled adjoint linear system
  - Newton MDA steps calculation

- Provides large speedup and robustness improvement compared to current Krylov methods in GEMSEO, thanks to the many available solvers and preconditioners.

- Validation on a real coupled adjoint use case provided by Airbus, high condition number, which was dealing issues

  **=> Speedup factor >20**



# Conclusion

# Conclusion

## Collaborative work in MADELEINE offered several opportunities:

- ❑ An increased experience in terms of applying and testing MDO formulations in real applications
- ❑ A better understanding of MDO formulations and their impact on the performance of the processes and on the optimal designs
- ❑ An increase of shared experience and expertise within the MADELEINE consortium
- ❑ Enrichment of GEMSEO MDO formulations
  - BLISS 98 with interesting refinements coming from ONERA’s expertise
  - Enhanced Bi-level formulations engine enabling to accelerate the convergence
- ❑ First real applications of the scalable methodology facilitating comparing the efficiency of MDO formulations, realized in collaboration with DLR, ESI and Dassault
- ❑ Extension of GEMSEO parallel capabilities and development of GEMSEO-PetsC linear solvers plugin, in collaboration with Optimad
- ❑ An increased experience of using GEMSEO thanks to Airbus, DLR and ONERA with very interesting feedback contributing to improve the software

**MADELEINE allowed us to take an important step in terms of MDO experience and enrichment of GEMSEO with capabilities crucial for industry!**

# GEMSEO, open source since May 2021

## FEATURES

### Study Prototyping

An intuitive tool to discover MDO without writing any code, and define the right MDO problem and process. From an Excel workbook, specify your disciplines, design space, objective and constraints, select a MDO formulation and plot both coupling structure (N2 chart) and MDO process (XDSM), even before wrapping any software.

Read more | Examples

### Optimization

Define, solve and post-process an optimization problem from an optimization algorithm.

**Algorithms:** BFGS, BOBYQA, COBYLA, L-BFGS-B, MMA, NEWUOA, ODD, SLSQP, TNC

*based on nlopt, scipy and snopt.*

Read more | Examples | Options

### DOE & Trade-off

Define, solve and post-process a trade-off problem from a DOE (design of experiments) algorithm.

**Design of experiments:** axial, bilevel full-factorial, Box-Behnken, central-composite, composite, custom, diagonal, Faure, full factorial, Halton, Haselgrove, LHS, Monte-Carlo, Plackett-Burman, reverse Halton, Sobol

*based on OpenTURNS and pyDOE*

Read more | Examples | Options

### MDO formulations

Define the way as the disciplinary coupling is formulated and managed by the optimization or DOE algorithm.

**Formulations:** bilevel, IDF, MDF, standard optimization

Read more | Examples | Options

### MDA

Find the coupled state of a multidisciplinary system using a Multi-Disciplinary Analysis.

**Algorithms:** Gauss-Seidel, Jacobi, MDA chain, Newton-Raphson, Quasi-Newton, Gauss-Seidel/Newton

Read more | Examples | Options

### Visualization

Generate graphical post-processings of optimization histories.

**Visualizations::** basic history, constraint history, correlations, gradient sensitivity, k-means, objective and constraint history, optimization history view, parallel coordinates, quadratic approximation, radar chart, robustness, scatter matrix, self organizing map, variable influence.

Read more | Examples | Options

### Surrogate models

Replace a discipline by a surrogate one relying on a machine learning regression model.

**Surrogate models:** Gaussian process regression (kriging), linear model, radial basis regression, polynomial chaos expansion and surrogate quality measures.

*based on scikit-learn and OpenTURNS*

Read more | Examples | Options

### Scalable models

Use scalable data-driven models to compare MDO formulations and algorithms for different problem dimensions.

**Features:** scalability study, scalable problem, scalable discipline, diagonal-based, ...

Read more | Examples

### Machine learning

Apply clustering, classification and regression methods from the machine learning community.

**Features:** clustering, classification, regression, quality measures, calibration, data transformation.

*based on scikit-learn and OpenTURNS*

Read more | Examples | Options

</> beta version

### Uncertainty

Define, propagate, analyze and manage uncertainties.

**Roadmap under development**

- Enhanced MDO techniques
- Multi-fidelity MDO
- Mixed categorical – continuous variables
- Uncertainty quantification & management
- Robust MDO
- Platform services, MDO in distributed heterogeneous environments

**You are welcome to contribute!**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N° 769025.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