# Dealing with a non-Gaussian objective function in aeroelastic Bayesian optimization with disciplinary Gaussian Processes

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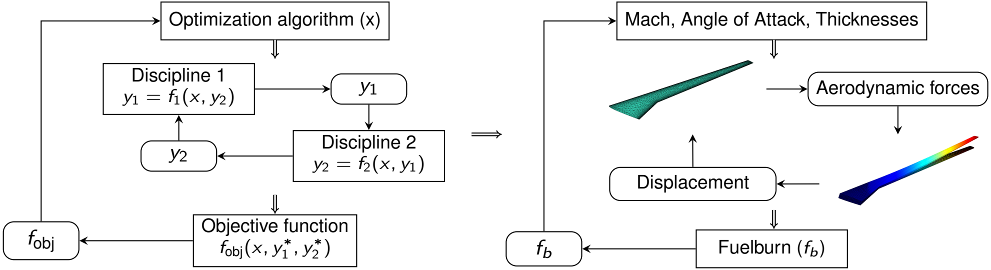
# Outline

# Context

## Multidisciplinary Analysis and Optimization

MDO problem: 2-discipline optimization problem (MDF approach)




Multidisciplinary analysis (MDA): non-linear system of equations

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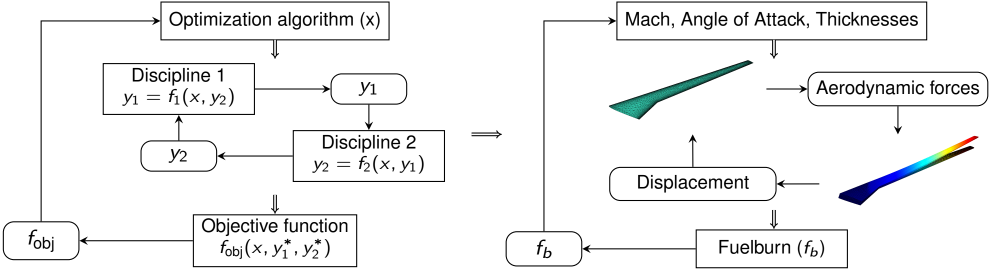


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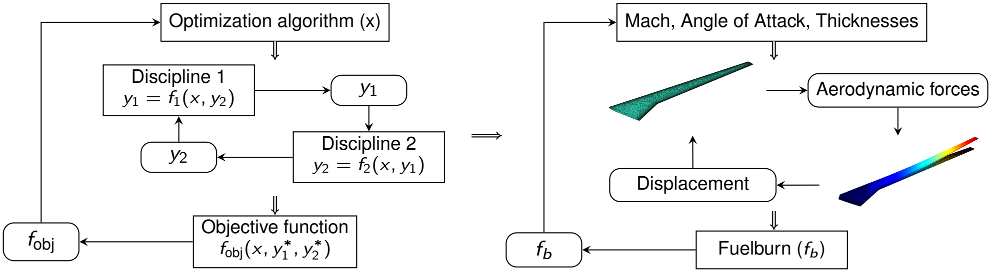


Multidisciplinary analysis (MDA): non-linear system of equations

$\Longrightarrow$ Costly disciplinary solvers: one call to a disciplinary solver takes a long time to compute.

$\Longrightarrow$ Partitioned approach: disciplinary solvers are called iteratively until convergence.

$\Longrightarrow$ Heavy computational cost: the MDA must be solved several times during the optimization.

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## Bayesian framework for MDO

Bayesian framework:

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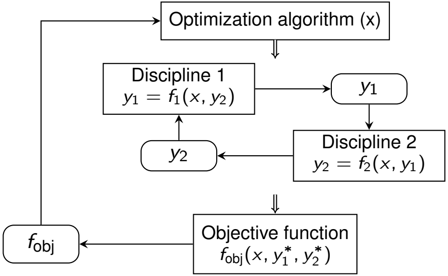

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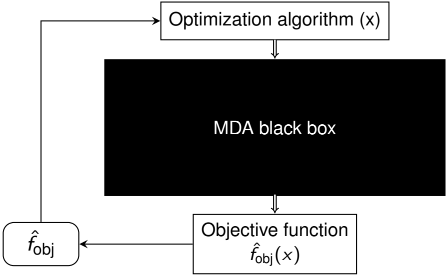
Efficient Global Optimization (EGO) [1]:

- The **objective function** is replaced by a Gaussian Process (GP).
- ✓ Surrogate is exact at training points.
- ✗ Each enrichment of the surrogate model requires the resolution of the MDA.




[1] Donald Jones, Matthias Schonlau, and William Welch. Efficient global optimization of expensive black-box functions. *Journal of Global Optimization*, 13:455–492, 1998.

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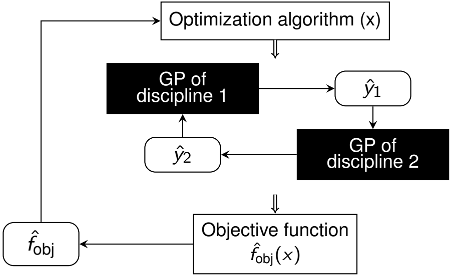
2. Adaptive enrichment of the GPs until the global optimum is found.

Efficient Global Multidisciplinary Design Optimization (EGMDO) [2]:

- The **disciplinary solvers** are replaced by independent Gaussian Processes.

✓ Resolution of the MDA requires only surrogate evaluations.

✓ The disciplines are uncoupled.





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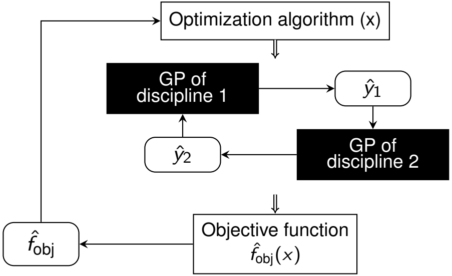
2. Adaptive enrichment of the GPs until the global optimum is found.

Efficient Global Multidisciplinary Design Optimization (EGMDO) [2]:

- ✗ The resulting objective function approximation is not exact at the training points.
- ✗ Due to the non-linearity of the MDA, it is a non-Gaussian random field.





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# Objectives

## Dealing with non-Gaussian objective and constraint functions

- The EGMDO framework proposes a solution to represent the random field modeling the random objective function.
- It equally provides a strategy to reduce the uncertainty of the obtained objective function model, here used to perform global optimization.
- Extension of the EGMDO framework to handle constraint functions which depend on the solution of the MDA. Like the objective function, they are a non-Gaussian random field.

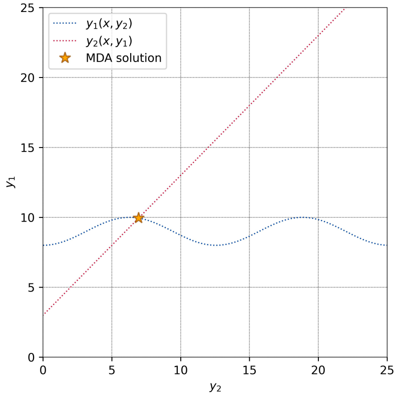
# Outline

# Efficient Global Multidisciplinary Design Optimization

## Using disciplinary surrogates

For a single design space point $x$, the MDA is described by the non-linear system of equations:

$$\begin{cases} y_1 = f_1(x, y_2) \\ y_2 = f_2(x, y_1) \end{cases}$$

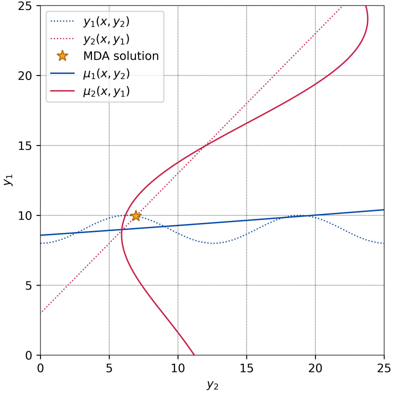


# Efficient Global Multidisciplinary Design Optimization

## Using disciplinary surrogates

We want to estimate the solution of the MDA $(y^*(x))$ by replacing each disciplinary solver by a GP:

$$\begin{cases} \hat{y}_1 = \mu_1(x, \hat{y}_2) + \epsilon_1(x, \hat{y}_2) \\ \hat{y}_2 = \mu_2(x, \hat{y}_1) + \epsilon_2(x, \hat{y}_1) \end{cases}$$



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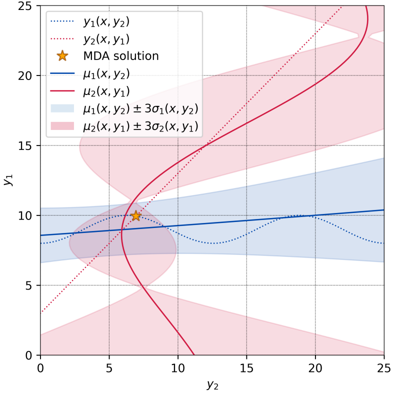

# Efficient Global Multidisciplinary Design Optimization

## Using disciplinary surrogates

Let $\Xi = \{\xi_1, \dots, \xi_{n_d}\}$ be a vector of standard Gaussian random variables, we can model the uncertainty of the random MDA as:

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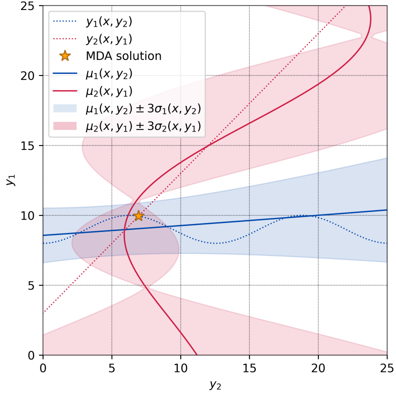

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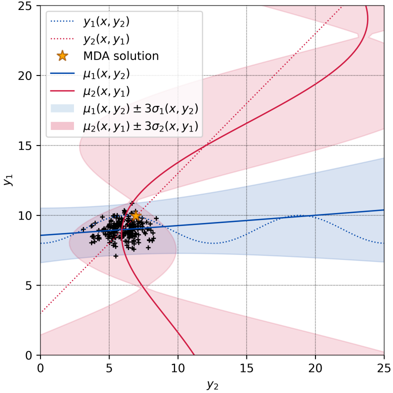
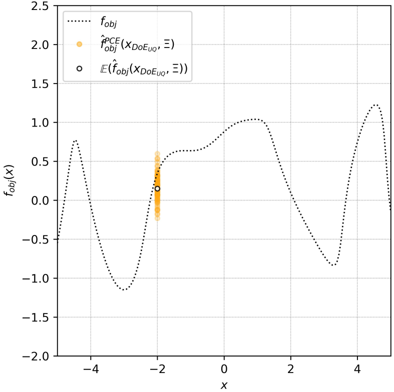


# Efficient Global Multidisciplinary Design Optimization

## Objective function approximation

Due to the random MDA, the objective function is a random variable, of unknown distribution, at any point $x \in X$.



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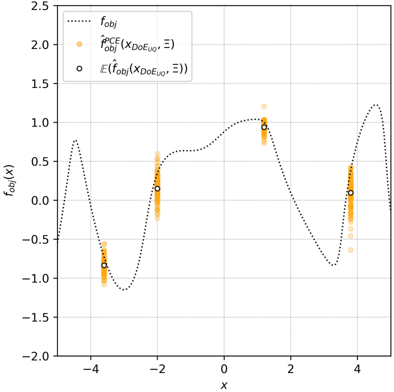

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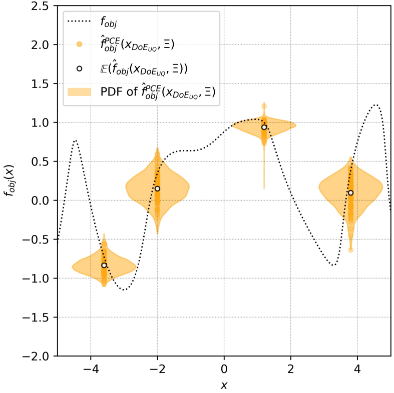
In EGMDO it is proposed to approximate this random variable via Polynomial Chaos Expansion (PCE) [3]:

$$\hat{f}_{\text{obj}}^{\text{PCE}}(x_i, \Xi) = \sum_{j=1}^{P} a_j(x_i)\text{H}_j(\Xi), \quad \forall x_i \in \text{DoE}_{\text{UQ}}$$

[3] R. Ghanem and P. Spanos, Stochastic Finite Elements: A Spectral Approach, Civil, Mechanical and Other Engineering Series. Dover Publications (2003).



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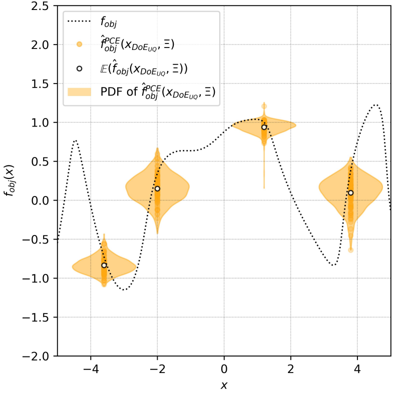
## Objective function approximation

$\text{DoE}_{\text{UQ}}$ is a design of experiments that we can use to obtain a continuous approximation of the random field $\hat{f}_{\text{obj}}^{\text{PCE}}(x, \Xi)$.



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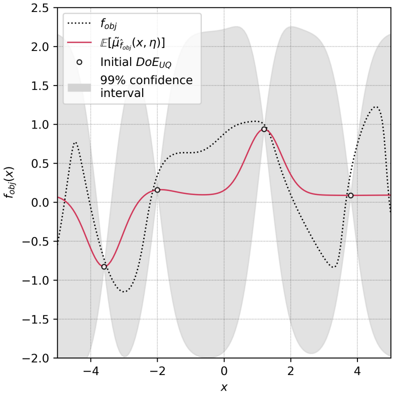
In EGMDO the continuous model [4] is obtained by a combined Karhunen-Loève (KL) decomposition and GP interpolation:

$$\tilde{f}_{\text{obj}}(x, \Xi, \eta) = \tilde{\mu}_{\hat{f}_{\text{obj}}}(x, \eta) + \sum_{k=1}^{m} \left( \sum_{l=2}^{P} a_l^{\text{T}} \varphi_k \text{H}_l(\Xi) \right) \tilde{\varphi}_k(x, \eta)$$

In the figure, only the GP associated with $\tilde{\mu}_{\hat{f}_{\text{obj}}}(x, \eta)$ is represented.





[4] S. Dubreuil, N. Bartoli, C. Gogu, T. Lefebvre and J. Mas Colomer, Extreme value oriented random field discretization based on an hybrid polynomial chaos expansion - Kriging approach, Computer Methods in Applied Mechanics and Engineering, 332, pp. 540–571 (2018).

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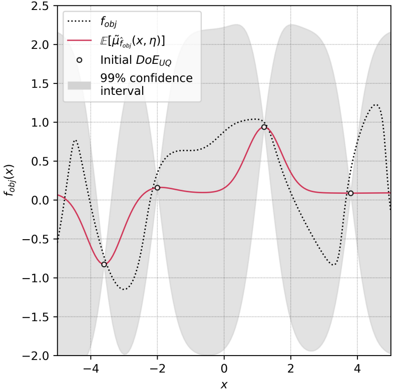
## Uncertainty reduction steps

The purpose of the Bayesian framework is to reduce the uncertainty of the model where the global optimum is likely to be.



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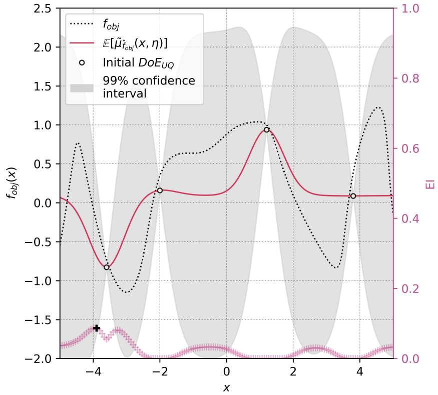

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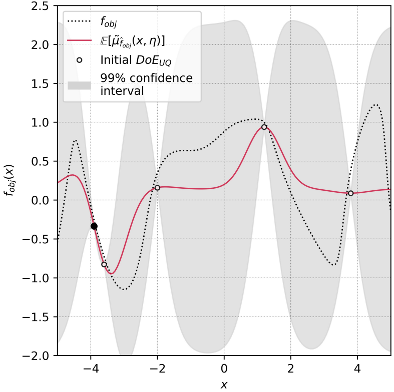

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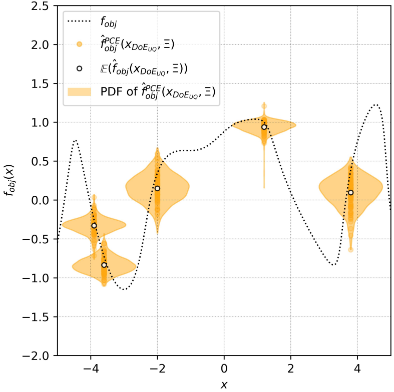
   Reduces the uncertainty with respect to the random variable $\Xi$.



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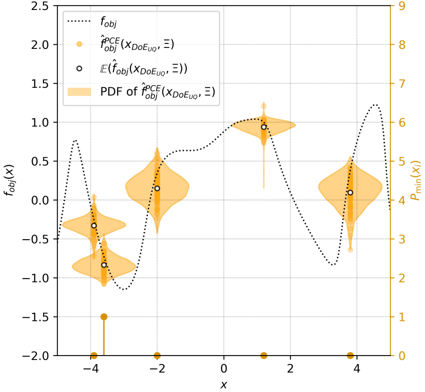

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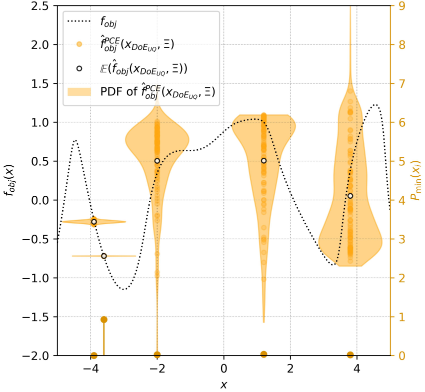

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## Uncertainty reduction steps

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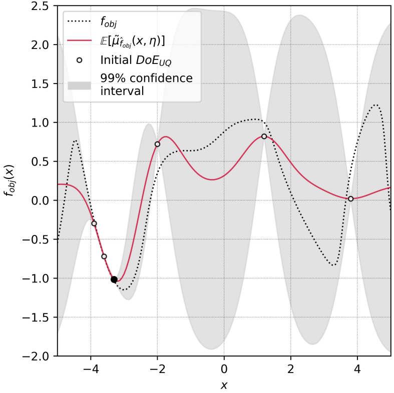

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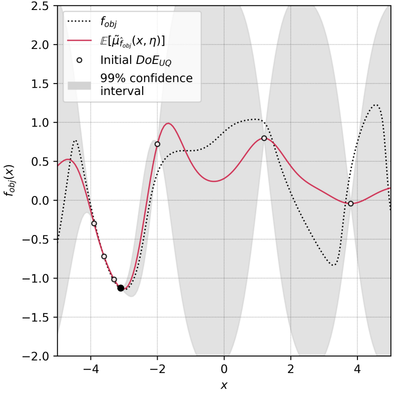

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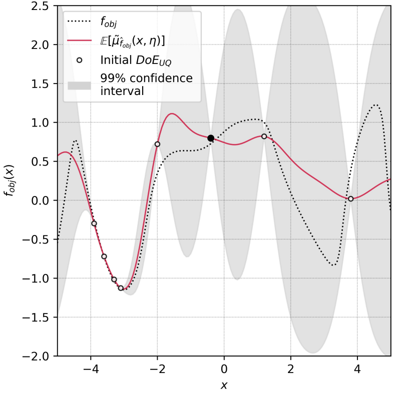

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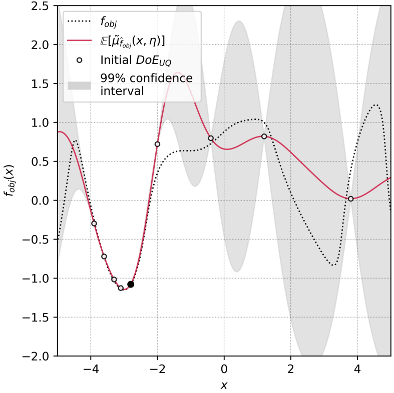
By iteratively sampling the design space and enriching the disciplinary solvers the EGMDO algorithm is capable of finding the unconstrained global optimum using few disciplinary solver calls.

How do we introduce constraints in the EGMDO framework while still retaining the Bayesian framework?

Remarks:

We will focus on constraint functions which depend on any subset of the converged coupling variables.



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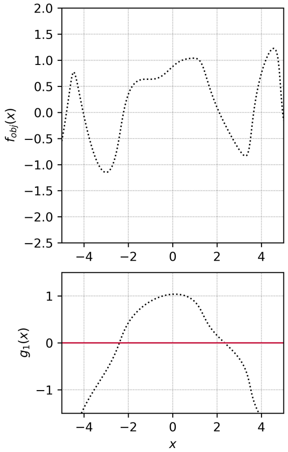
# C-EGMDO

## Extension of the EGMDO framework to constrained problems

We introduce the inequality constraint $g_1(y_1) \geq 0$.



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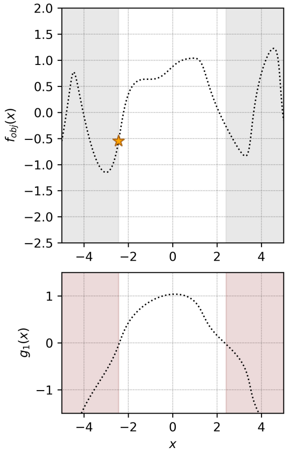

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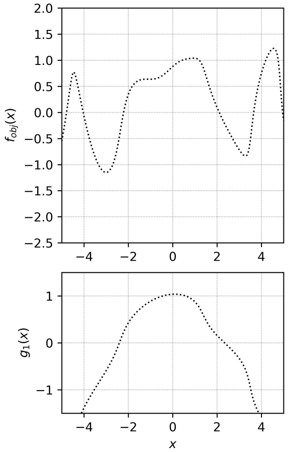

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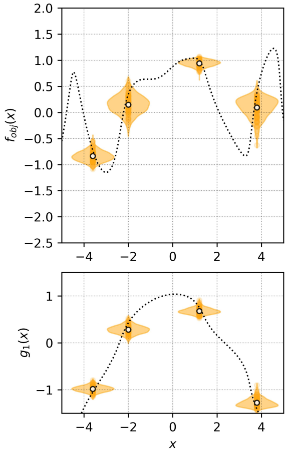

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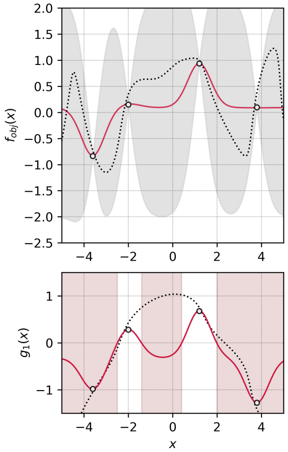
  An **approximate unfeasible region** is obtained based on the continuous model of the constraint function.



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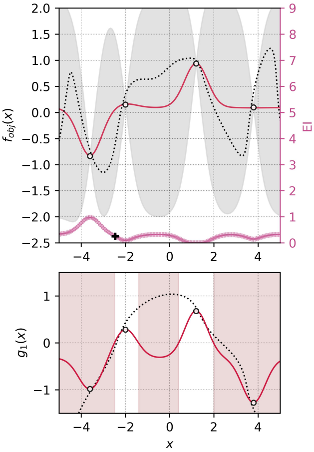
   New points should be in the current feasible region.



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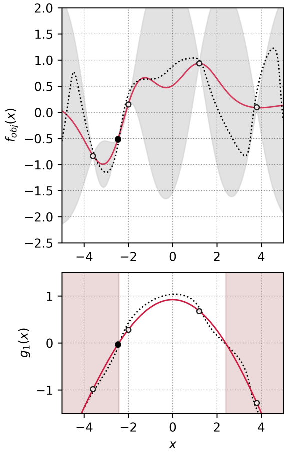

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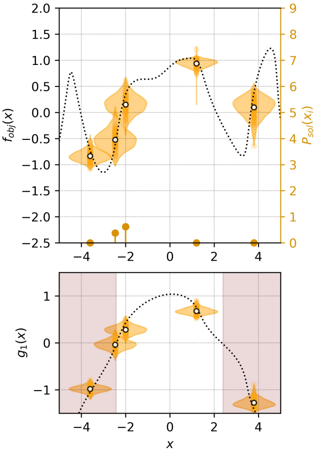


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1. Sampling of the design space subject to constraints.
   New points should be in the current feasible region.
2. Enrichment of the disciplinary solvers in points with **high probability of solving the constrained problem.**
   Uncertainty of the constraint function is accounted for.

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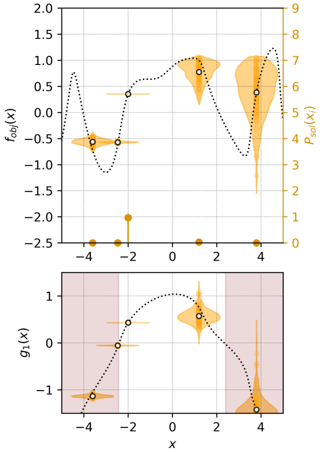
  An **approximate unfeasible region** is obtained based on the continuous model of the constraint function.

Adapted uncertainty reduction strategy:

1. Sampling of the design space subject to constraints.
   New points should be in the current feasible region.
2. Enrichment of the disciplinary solvers in points with **high probability of solving the constrained problem.**
   Uncertainty of the constraint function is accounted for.



# Outline

1. Context
2. Objectives
3. EGMDO
4. C-EGMDO
5. **Applications**
6. Conclusion

# Applications: analytical test case

## Comparison with other optimization frameworks

Application to the analytical Sellar benchmark test case [5]:

$$\begin{aligned} \arg\min_{z \in \mathcal{Z}} \quad & f_{\text{obj}}(\boldsymbol{z}, y^*_{c_{\text{obj}}}) = z_3^3 + z_2 + y_1^* + \exp(-y_2^*) \\ \text{s.t.} \quad & 3.16 - y_1^* \leq 0 \\ & y_2^* - 24 \leq 0 \end{aligned}$$

| | Gradient-based | | Gradient-free | | Bayesian | |
|---|---|---|---|---|---|---|
| | MDF-SLSQP | IDF-SLSQP | MDF-COBYLA | IDF-COBYLA | SEGO-WB2 | C-EGMDO-WB2 |
| Success† | 43/100 | 59/100 | 55/100 | 90/100 | 95/100 | 96/100 |
| $\mathbb{E}$(N1) | 68.1 | 51.6 | 167.1 | 105.5 | 28.3 | 13 |
| $\mathbb{E}$(N2) | 68.1 | 51.6 | 167.1 | 105.5 | 28.3 | 9.8 |

†A run was considered successful if the solution found presented a relative error of no more than 1%.

[5] R. S. Sellar, S. M. Batill and J. E. Renaud, Response surface based, concurrent subspace optimization for multidisciplinary system design (1996).

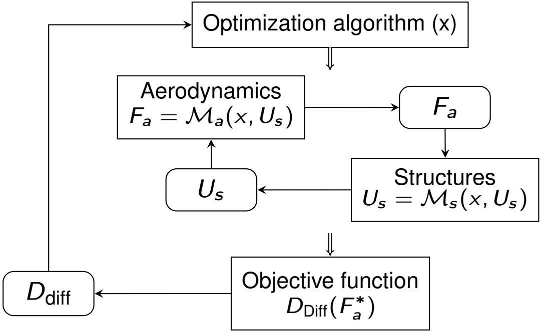
# Applications: engineering test case

## Bayesian framework for MDO

We define the following MDO problem which couples an aerodynamic and structural solver:

$$\begin{aligned} \arg\min_{x \in X} \quad & D_{\text{diff}} = \frac{\|D - D_{\text{ref}}\|_2}{D_{\text{ref}}} \\ \text{s.t.} \quad & L = W \\ & \delta z \leq \delta z_{\text{max}} \end{aligned}$$

where $D$ is the drag, $L$ is the lift, $W$ is the weight and $\delta z$ is the vertical wing tip displacement.



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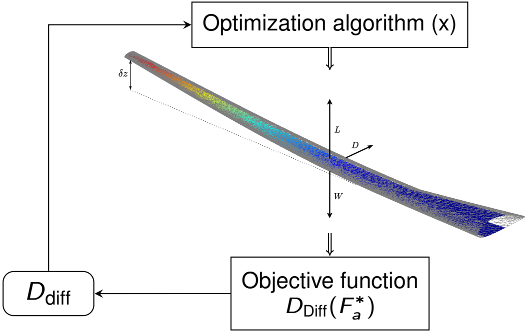

# Applications: engineering test case

## Aerostructural optimization: problem definition

- As design variables we take wing's the angle of attack ($\alpha$) and the twist at tip ($\theta_t$).
- The reference solutions are established using a gradient-based algorithm.

| | | Bounds | | Optima | |
|---|---|---|---|---|---|
| | | Lower | Upper | Global | Local |
| **minimize** | $D_{\text{diff}}$ | $--$ | $--$ | $\approx 1 \times 10^{-6}$ | $\approx 8 \times 10^{-2}$ |
| **w.r.t.** | $\alpha$ | 0 | 1 | 0.2287 | 0.5885 |
| | $\theta_t$ | 0 | 1 | 0.1462 | 0.8821 |
| **subject to** | $L = W$ | 0 | 0 | 0 | 0 |
| | $\delta z - \delta z_{\text{max}}$ | $--$ | 0 | $-0.1589$ | 0 |

# Applications: engineering test case

## Aerostructural optimization: results

✓ C-EGMDO finds the global optimum for 7/10 runs when $n_{\max} = 15$.

# Applications: engineering test case

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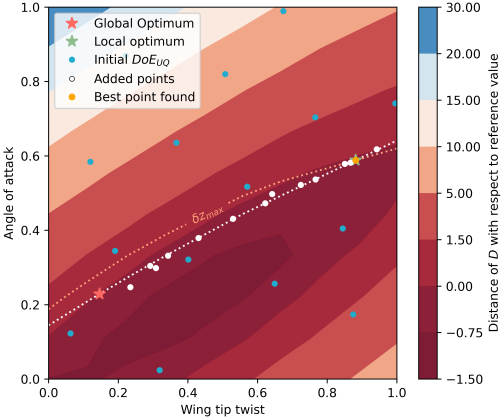
✓ C-EGMDO finds the global optimum for 7/10 runs when $n_{\max} = 15$. What causes failed runs?



# Applications: engineering test case

## Aerostructural optimization: results

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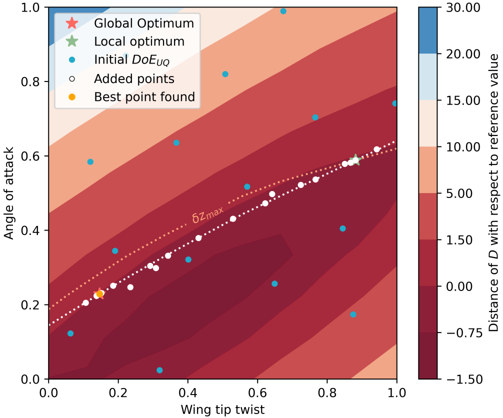

# Applications: engineering test case

## Aerostructural optimization: results

- ✓ With a sufficiently large number of iterations, all runs are able to find the global optimum;
- ✓ The number of disciplinary solver calls does not increase significantly after 15 iterations;
- ✓ For $n_{\max} = 25$, C-EGMDO is still much cheaper than the gradient based MDF-SLSQP framework.

| | C-EGMDO | | | | | MDF-SLSQP |
|---|---|---|---|---|---|---|
| $n_{\max}$ | 5 | 10 | 15 | 20 | 25 | $--$ |
| Success[†] | 2/10 | 6/10 | 7/10 | 9/10 | 10/10 | 2/10 |
| $\mathbb{E}(n_a)$ | 17.5 | 22.83 | 25.71 | 26.33 | 26.4 | 133.5 |
| $\mathbb{E}(n_s)$ | 13.0 | 14.17 | 14.29 | 14.78 | 15.0 | 133.5 |

[†]A run was considered successful if the solution found presented a relative error of no more than 5%.

# Outline

# Conclusion and future perspectives

## The curse of dimensionality

The presented developments provided us with a Bayesian optimization framework that:

- ✓ Uses disciplinary surrogates to reduce the computational cost of the MDO problem;
- ✓ Is capable of handling equality and inequality constraints;
- ✓ Has been validated on an analytical benchmark problem as well as on an engineering application problem;
- ✗ Is limited to a low number of design variables and low-dimensional coupling variable space.

Possible leads for future work thus include dimension reduction techniques, such as:

1. Kriging with Partial Least Squares [6] to handle a greater number of design variables;
2. Proper Orthogonal Decomposition to handle high-dimensional coupling variables in an MDA context (as is done in [7]).

[6] M. Bouhlel, N. Bartoli, J. Morlier and A. Otsmane, Improving kriging surrogates of high-dimensional design models by Partial Least Squares dimension reduction, Structural and Multidisciplinary Optimization, 53 (5), pp. 935–952 (2016)
[7] G. Berthelin, S. Dubreuil, M. Salaün, N. Bartoli and C. Gogu, Disciplinary proper orthogonal decomposition and interpolation for the resolution of parameterized multidisciplinary analysis, International Journal for Numerical Methods in Engineering, 123 (15), pp. 3594–3626 (2022).

**Thank you for your attention!**

**Any questions?**

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