Application of Gaussian Processes in Uncertainty Quantification and Optimisation

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Warsaw, November 2017

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Uncertainty Quantification

UQ | What the uncertainty is?

It is a lack of knowledge about model parameters and the model itself.

UQ | Sources of the uncertainties

- Manufacturing process (e.g. errors in geometry, material properties, . . .).
- Operating conditions (e.g. geometry deformation due to loads, bird strike, . . .)
- Input data (e.g. air density value, velocity value, . . .).
- Model itself (e.g. simplifications in modeling resulting from simulation cost, . . .).
- Output data (e.g. unconvered results, . . .).
- External changes in a design.

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Is it to safe to ignore uncertainties?

Answer

Like always – it depends.

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UQ | Effects of the uncertainties I

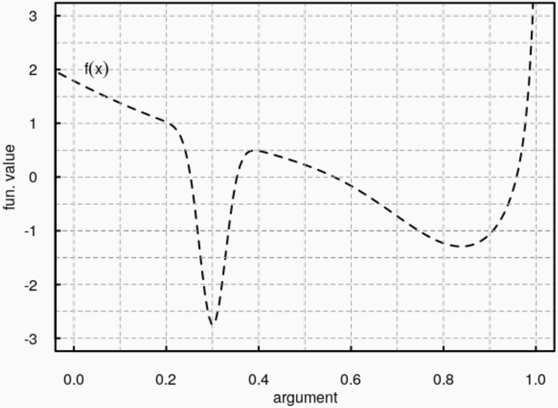


Fig. 1: The effect of the variables uncertainty.

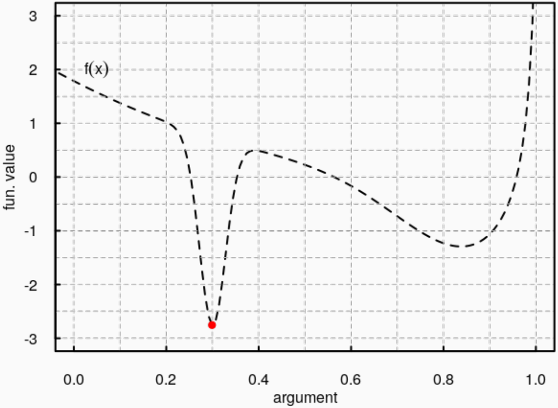
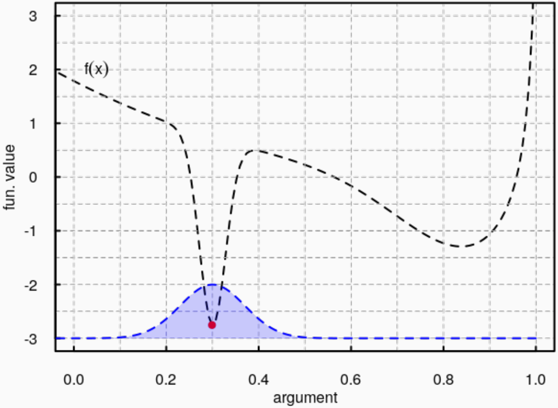


Fig. 2: The effect of the variables uncertainty.

UQ | Effects of the uncertainties III



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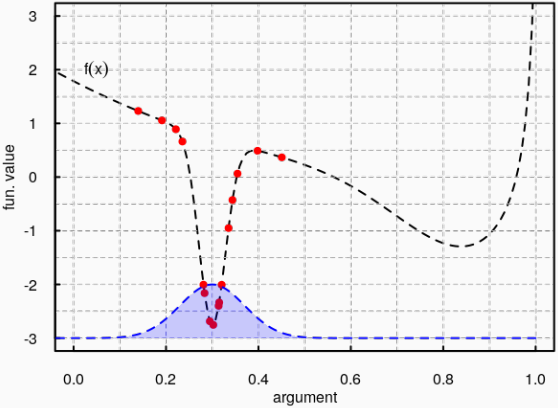

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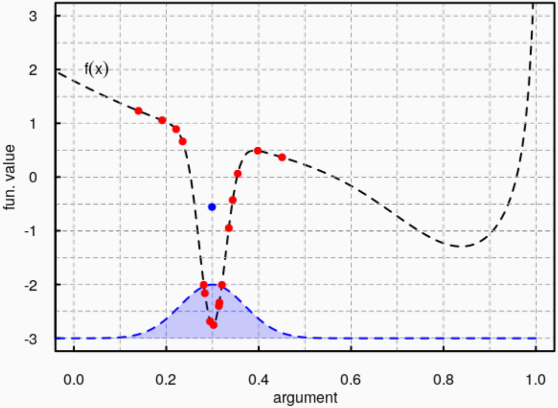

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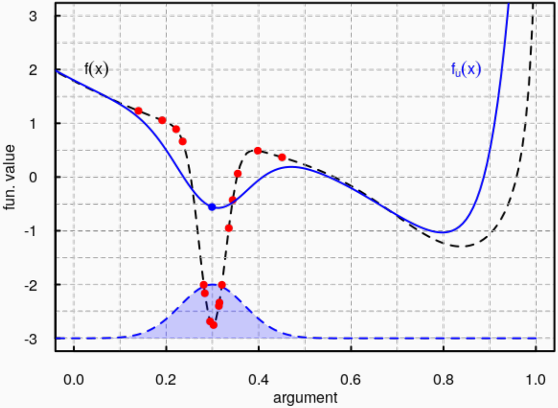

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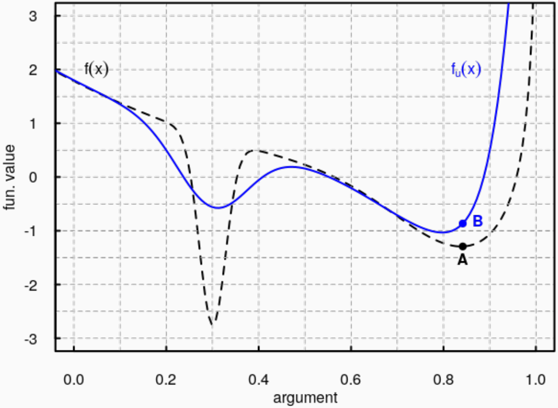

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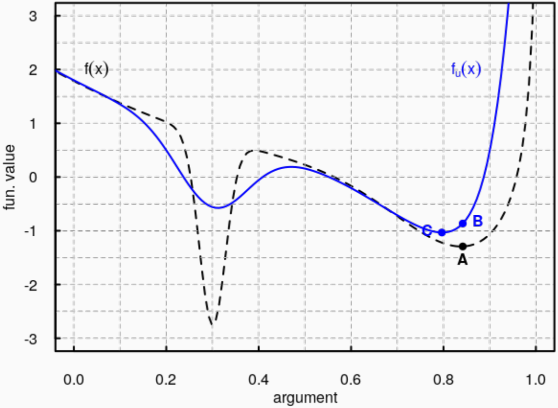

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UQ | Effects of the uncertainties IX

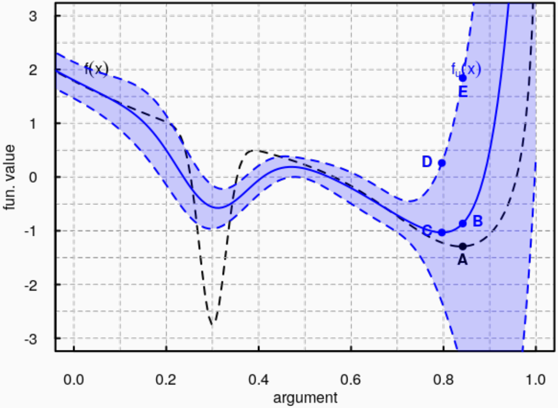

Fig. 9: The effect of the variables uncertainty.

UQ | How we actually quantify the Uncertainties?

1. Obtain an unknown function $f(\mathbf{x})$
2. Calculate a mean function: $f_u(\mathbf{x}) = \mathbb{E}_\Xi\left(f(\mathbf{x}+\Xi)\right)$, where Ξ is a random error and $\mathbb{E}_\Xi$ means expected value.
3. Choose a probability density function $g(\xi)$ describing the random error Ξ.
4. Use the function to calculate

$$f_u(\mathbf{x}) = \int f(\mathbf{x}+\xi)g(\xi)d\xi = (f * g)(\mathbf{x})$$

5. Calculate a variance of the function $f(\mathbf{x})$:

$$\sigma_u^2(\mathbf{x}) = \mathbb{V}\mathrm{ar}_\Xi\left(f(\mathbf{x}+\Xi)\right) =$$

$$= \int f^2(\mathbf{x}+\xi)g(\xi)d\xi - \left(\int f(\mathbf{x}+\xi)g(\xi)d\xi\right)^2 =$$

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Why obtaining of the $f(\mathbf{x})$ function is difficult?

1. Writing a solver capable of calculating values of the function can be time consuming
   $\Longrightarrow$ using external/commercial solvers.
2. It can be very expensive in both time and computer resources needed to calculate it
   $\Longrightarrow$ evaluating of the $f(\mathbf{x})$ function in low number of points.
3. The solver which is used to calculate the function does not have to be reliable in a whole domain (convergence problems)
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1. Assume that the function $f(\mathbf{x})$ is a realization of a random field

$$F(\mathbf{x}) = \mu(\mathbf{x}) + \varepsilon(\mathbf{x}), \text{where}$$

$\mu(\mathbf{x})$ is a deterministic trend function and
$\varepsilon(\mathbf{x})$ is a centered Gaussian Process (GP).

Gaussian Process

- It is a collection (set) of random variables $\{\varepsilon(\mathbf{x}) | \mathbf{x} \in \mathbf{R}^N\}$
- any number of which have a joint Gaussian distribution

In our case we can write that:

$$\varepsilon(\mathbf{x}) \sim \mathbb{GP}(0, c(\mathbf{x}, \mathbf{y}))$$

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2. Chose the covariance kernel of $\varepsilon(\mathbf{x})$:

$$c\left(\mathbf{x}, \mathbf{y}; \sigma^2, \tau^2, \theta\right) = \sigma^2 \prod_{k=1}^{L} g_g(x_k, y_k; \theta_k) + \tau^2 \delta_{\mathbf{x},\mathbf{y}}$$

where:

$$\delta_{\mathbf{x},\mathbf{y}} = \begin{cases} 1, & \mathbf{x} = \mathbf{y} \\ 0, & \mathbf{x} \neq \mathbf{y} \end{cases}$$

$$g_g(x, y; \theta) = \exp\left(-\frac{(x-y)^2}{2\theta^2}\right)$$

UQ | Response Surface Model – Kriging Interpolation III

2. Define estimators of the expected value and variance of the process

$$\hat{F}(\mathbf{x}) = \mathbb{E}_F\left(F(\mathbf{x})\right)$$
$$\hat{\sigma}^2(\mathbf{x}) = \mathbb{V}\mathrm{ar}_F\left(F(\mathbf{x})\right)$$

3. Derive the estimator $\hat{F}$ following:
   - it is a linear combination of known objective function values

$$\hat{F}(\mathbf{x}) = \sum_{i=1}^{N} a^i(\mathbf{x}) F\left(\mathbf{x}^i\right), \text{where}$$

     $F\left(\mathbf{x}^i\right)$ denotes an i-th sample.
   - it is unbiased

$$\mathbb{E}_F\left(\hat{F}(\mathbf{x})\right) = \mathbb{E}_F\left(F(\mathbf{x})\right), \text{and}$$

   - the Mean Squared Error (MSE) is minimal

$$MSE(\mathbf{x}) = \mathbb{E}_F\left(\hat{F}(\mathbf{x}) - F(\mathbf{x})\right)^2 = \min$$

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1. Choose a point in which the uncertainty should be quantified.
2. According to a given error, sample few points.
3. Fit the Kriging Model to obtain the mean response and the variance of the model.

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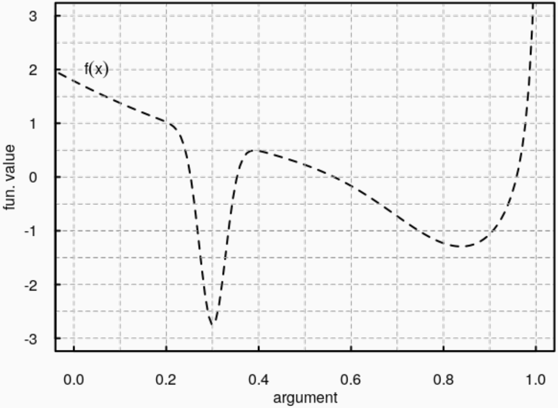


Fig. 10: Uncertainty Quantification with Gaussian Process (GP).

UQ | Procedure III

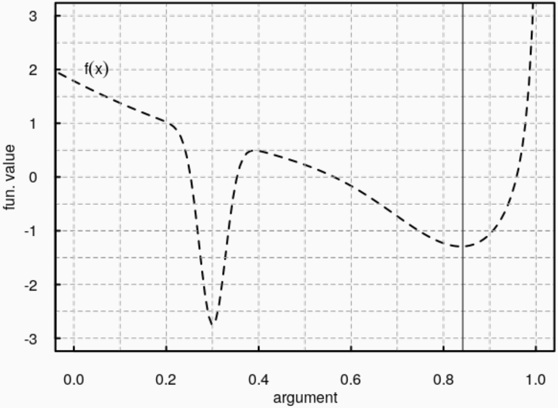


Fig. 11: Uncertainty Quantification with GP.

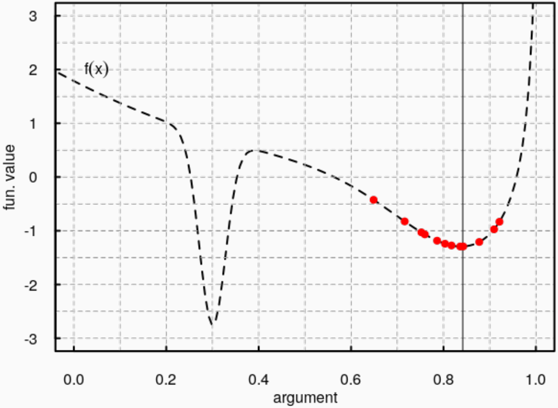


Fig. 12: Uncertainty Quantification with GP.

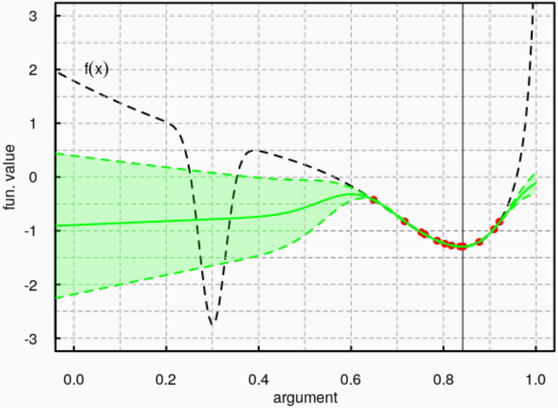


Fig. 13: Uncertainty Quantification with GP.

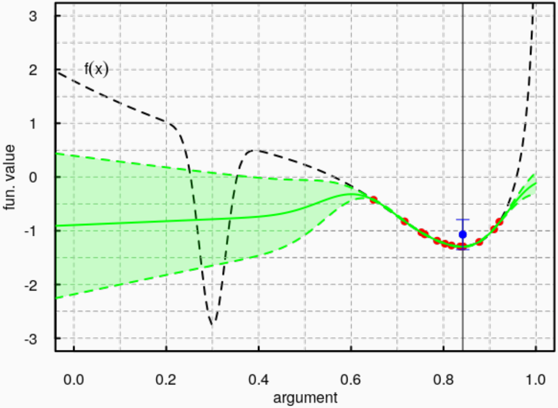


Fig. 14: Uncertainty Quantification with GP.

Robust Optimisation

RO | What the Robust Optimisation is?

It is the optimisation in presence of the variables uncertainties.

1. Take into account the various sources of the uncertainties (in particular: variables errors, parameters errors, solver errors)
2. Optimise not the objective function $f(\mathbf{x})$ but the mean function $f_u(\mathbf{x})$.
3. Simultaneously do the Uncertainty Quantification of the optimal solution.
4. Use as low number of objective function evaluations as possible.

RO | Solution I

Take the advantage of the Kriging method, like in the case of Uncertainty Quantification.

To do so one has to:

1. Perform a Design of Experiment step and evaluate the objective function $f(\mathbf{x})$.
2. Fit the Kriging model to obtain the response $\hat{F}(\mathbf{x})$ and the variance of the response $\hat{\sigma}^2(\mathbf{x})$.
3. Obtain the mean response $\hat{F}_u(\mathbf{x})$ and the variance of the mean response $\hat{\sigma}_u^2(\mathbf{x})$.
4. Find the minimum of the model

$$f_{\min} = \min_{\mathbf{x}_{\min} \in \mathbf{D}} \left(\hat{F}_u(\mathbf{x}_{\min}) + 3 \cdot \hat{\sigma}_u(\mathbf{x}_{\min}) \right)$$

RO | Solution II

Steps 1. – 5. are not sufficient. The UQ of the solution will be poor (the variance of the mean response will be large).

To improve the solution one has to:

6. Use a certain algorithm to add a new point (points) in order to improve the Kriging model.
7. Repeat points 2. – 5. and check if the optimum is good enough (e.g. variance of the optimum is low). If not, go to step 6.

REI is defined as:

$$REI(\mathbf{x}, \mathbf{x}_0) = \mathbb{E}\left(\max_{\mathbf{x},\mathbf{x}_0 \in D}\left(f_{min} - \hat{F}_u(\mathbf{x}), 0\right)\right) =$$

$$= \left(f_{\min} - \hat{F}_u(\mathbf{x})\right)\Phi\left(\frac{f_{\min} - \hat{F}_u(\mathbf{x})}{\hat{\sigma}(\mathbf{x}, \mathbf{x}_0)}\right) + \hat{\sigma}(\mathbf{x}, \mathbf{x}_0)\phi\left(\frac{f_{\min} - \hat{F}_u(\mathbf{x})}{\hat{\sigma}(\mathbf{x}, \mathbf{x}_0)}\right)$$

where:

- ϕ is the probability density function of the standard normal distribution $\mathbb{N}(0, 1)$,
- Φ is the cumulative distribution function of $\mathbb{N}(0, 1)$

$$\Phi(x) = \int_{-\infty}^{x} \phi(t)dt,$$

- $\hat{\sigma}(\mathbf{x}, \mathbf{x}_0)$ is a relative variance between $f(\mathbf{x})$ and $\hat{F}_u(\mathbf{x})$.

Fig. 15: The Relative Variance.

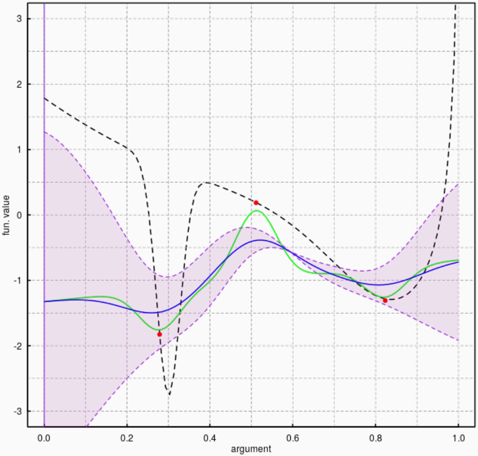
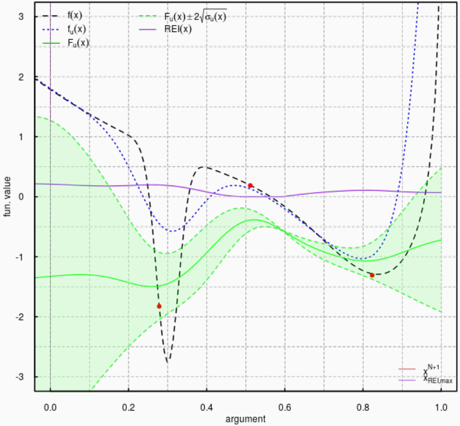


Fig. 16: The process of optimisation.



Test Case

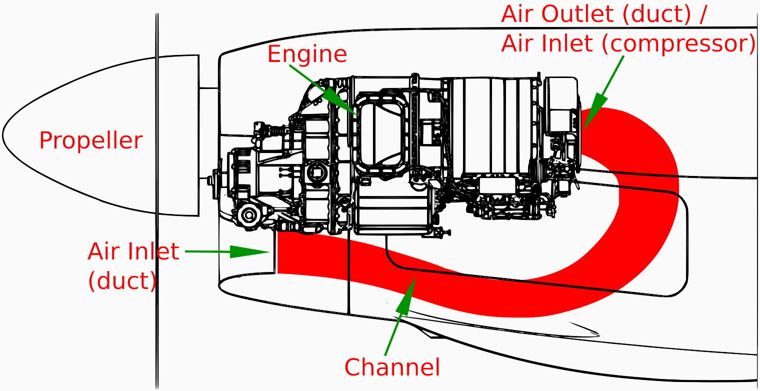


Fig. 17: The engine location and the channel.

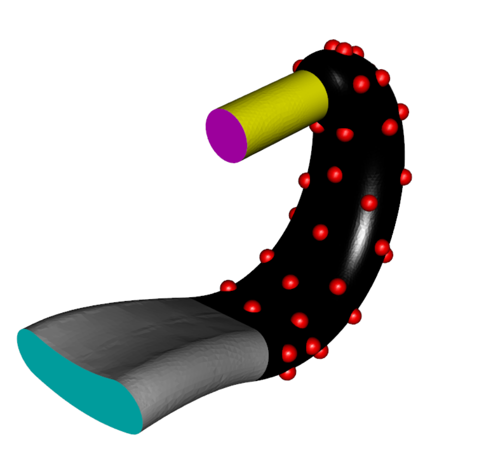


Fig. 18: View of the morphing points locations.

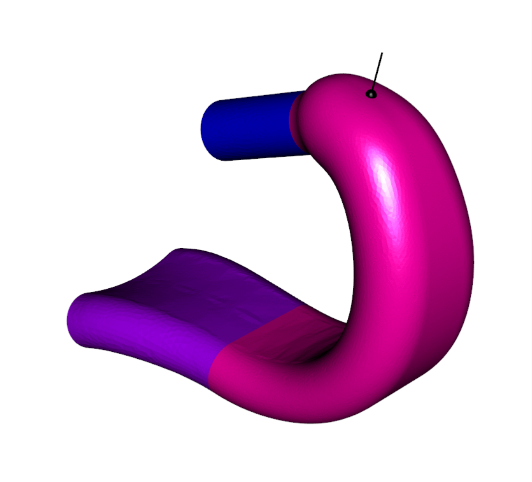


Fig. 19: Movement of chosen morphing point.

TC | Optimisation process I

1. The Design of Experiment: 65 function evaluations, 2 unconverged evaluations.
2. A design region: $[-0.32, 0.32] \times \ldots \times [-0.32, 0.32]$.
3. A sampling space: $[-0.4, 0.4] \times \ldots \times [-0.4, 0.4]$.
4. Parallelization: 5 simultaneous and asynchronized jobs.

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2. A design region: $[-0.32, 0.32] \times \ldots \times [-0.32, 0.32]$.
3. A sampling space: $[-0.4, 0.4] \times \ldots \times [-0.4, 0.4]$.
4. Parallelization: 5 simultaneous and asynchronized jobs.

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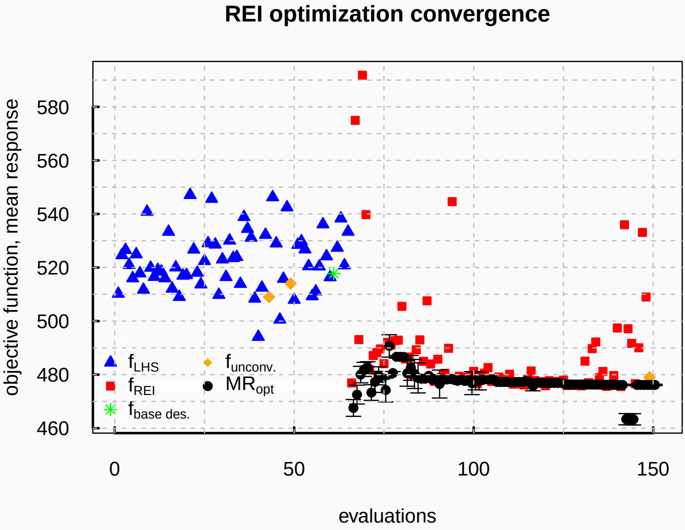
TC | Optimisation process II



TC | Optimisation process III

Pressure loss:

- The base design: 517.8 [Pa]
- The optimum: 474.79 [Pa] (improvement: 8.31 %)
- The robust optimum: 476.16 [Pa] (improvement: 8.04 %)
- The variance of the robust optimum: 0.026 %

TC | Summary

Advantages:

1. black-box functions optimization,
2. robustness to unconverged results and mesh failures,
3. relatively low number of points necessary for optimisation convergence and uncertainty quantification,
4. asynchronous parallel execution,
5. simultaneous optimization and uncertainty quantification.

Disadvantages:

1. relatively low number of design variables (~1–30),
2. low quality of estimation outside the design region.

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Acknowledgements

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UMRIDA

Majority of this research was done as a part of the EU project UMRIDA.