Multi-fidelity Optimization under Uncertainty for the Design of Complex Systems

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Grants : ONERA – CERFACS

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Introduction – Optimization under uncertainty

- Optimization of complex systems under uncertainties:
  → Reliability-Based Design Optimization (RBDO) [1,2]

Figure – Uncertainty on the flight conditions of a sounding rocket

RANS: Reynolds Averaged Navier-Stokes

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- **Uncertainty sources**
  - Aleatory : system environment (*e.g.*, wind gusts, atmospheric density)
  - Epistemic : modelling, level of fidelity with respect to the physical phenomenon (*e.g.*, for aerodynamic simulation with "high-fidelity" RANS type code and "low-fidelity" Euler type code)

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- High-fidelity (HF) codes often very expensive to evaluate: finite element codes, CFD code (*e.g.*, RANS)

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RBDO Problem Formulation

Problem formulation

$$\min_{\boldsymbol{d},\boldsymbol{p}} f(\boldsymbol{d},\boldsymbol{p}) \quad s.t. \begin{cases} \boldsymbol{h}(\boldsymbol{d},\boldsymbol{p}) \leq 0 \\ \mathbb{P}[\boldsymbol{g}(\boldsymbol{d},\boldsymbol{X}(\boldsymbol{p}),\boldsymbol{Z}) \leq 0] \leq P_f^T \end{cases}$$

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Deterministic constraint vector

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Acceptable probability of failure: P_f^T

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Acceptable probability of failure: P_f^T

Classical RBDO techniques

Two-level approach

Optimization

Reliability Analysis

- **Reliability analysis by MCS** [3]
- Methods using a linear approximation for the reliability analysis:
  - **Reliability Index Approach (RIA)** [4]
  - **Performance Measure Approach (PMA)** [5]

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Single-level approach

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Constraints integrated in objective function

- **Single-Loop Approach (SLA)** [6]

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Decoupled approach

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Reliability Analysis

➢ **Sequential Optimization and Reliability Assessment (SORA)** [7]

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Surrogate-based approach

Functions $\{f, \boldsymbol{g}, \boldsymbol{h}\}$ replaced by a surrogate model in the RBDO problem

- Gaussian Process, polynomial chaos expansions, support vector machines [2]

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Objective of the present work is to couple:

- Decoupled approach
- Surrogate-based approach
- Multi-fidelity

Useful reliability analysis techniques

Objective: estimate if $\mathbb{P}[g(\boldsymbol{X},\boldsymbol{Z}) \leq 0] \leq P_f^T$

Use of Iso-probabilistic transformation: $\boldsymbol{u} = \mathcal{T}([\boldsymbol{X},\boldsymbol{Z}]^T)$

- **First Order Reliability Method (FORM)** [8]
  - Optimization problem to solve to find the MPFP (Most Probable failure Point):

$$\boldsymbol{u}^* = \underset{\mathbf{u}}{\operatorname{argmin}}\|\boldsymbol{u}\| \quad s.t. \;\; g(\boldsymbol{u}) = 0$$

And: $\widehat{P_f} = \Phi(-\|\boldsymbol{u}^*\|)$

- **Inverse FORM (inverse problem)**
  - Optimization problem to solve to find the MPTP (Minimum Performance Target Point):

$$\min_{\mathbf{u}} g(\boldsymbol{u}) \quad s.t. \;\; \left|\left|\boldsymbol{u}\right|\right| = \beta^T$$

With $\beta^T = -\Phi^{-1}(P_f^T)$, and Φ^{-1} the inverse CDF of the Normal law

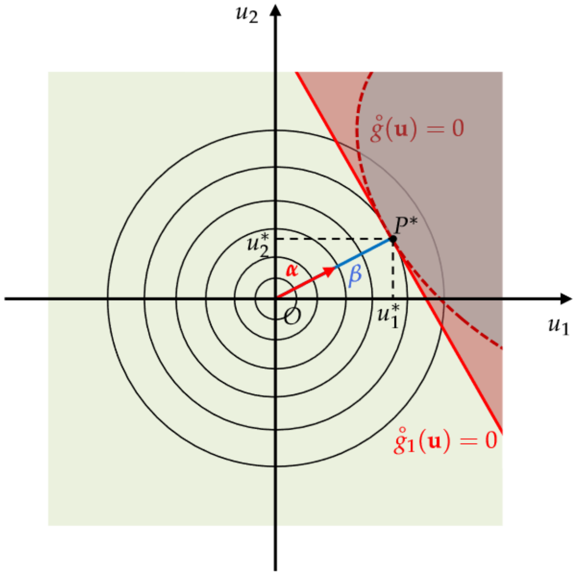

Figure – Illustration of FORM [9]

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Sequential Optimization and Reliability Assessment (SORA)

In blue: fixed during the process

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Deterministic Optimization (DO)

$$\min_{\mathbf{d},\mathbf{p}} f(\boldsymbol{d},\boldsymbol{p}) \quad s.t. \begin{cases} g\left(\boldsymbol{d},\boldsymbol{p} - \boldsymbol{s}^{(k)}, \boldsymbol{Z}_{MPTP}^{(k)}\right) \geq 0 \\ h(\boldsymbol{d},\boldsymbol{p}) \leq 0 \end{cases}$$

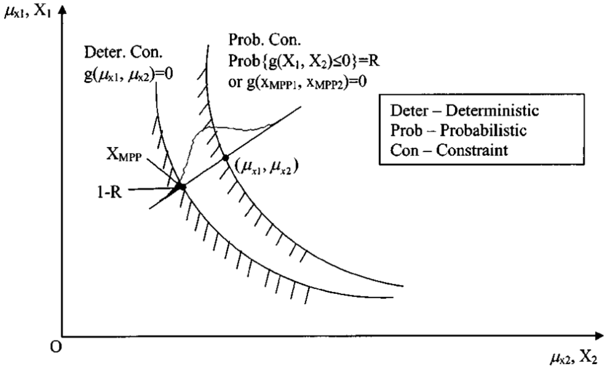

Figure – Constraint function translated for the deterministic optimization [7]

Sequential Optimization and Reliability Assessment (SORA)

In blue: fixed during the process

Initialization $(k = 0)$
$\boldsymbol{s}^{(k)} = 0$ and $\boldsymbol{Z}_{\mathrm{MPTP}} = \boldsymbol{\mu}_Z$

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$\boldsymbol{d}^{(k)}, \boldsymbol{p}^{(k)}$

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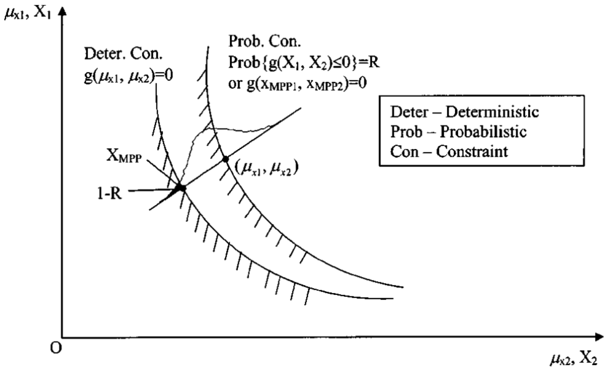

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Reliability Assessment (RA): Inverse FORM

$$\min_{\boldsymbol{X},\boldsymbol{Z}} g\left(\boldsymbol{d}^{(k)}, \boldsymbol{X}, \boldsymbol{Z}\right) \quad s.t. \quad \left\|\mathcal{T}_{\boldsymbol{p}^{(k)}}(\boldsymbol{X},\boldsymbol{Z})\right\| = -\phi^{-1}\left(P_f^T\right)$$

$\boldsymbol{X}_{\mathrm{MPTP}}^{(k)}, \boldsymbol{Z}_{MPTP}^{(k)}$

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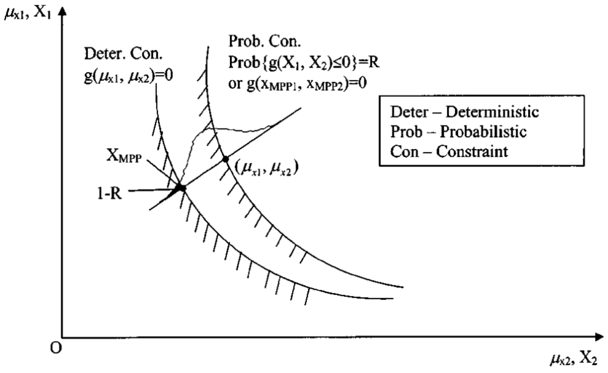

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$\boldsymbol{X}_{\mathrm{MPTP}}^{(k)}, \boldsymbol{Z}_{MPTP}^{(k)}$

Convergence ?

No

$\boldsymbol{s}^{(k+1)} = \boldsymbol{p}^{(k)} - \boldsymbol{X}_{\mathrm{MPTP}}^{(k)}$

$k = k+1$

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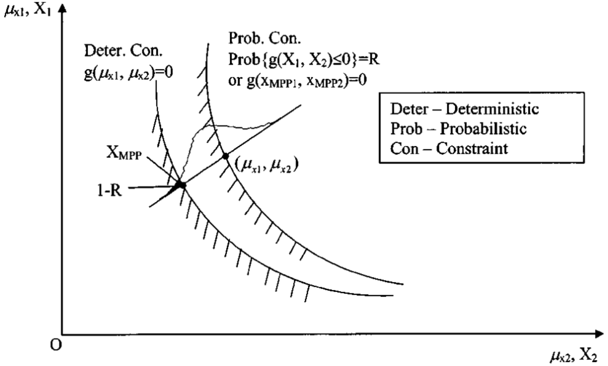

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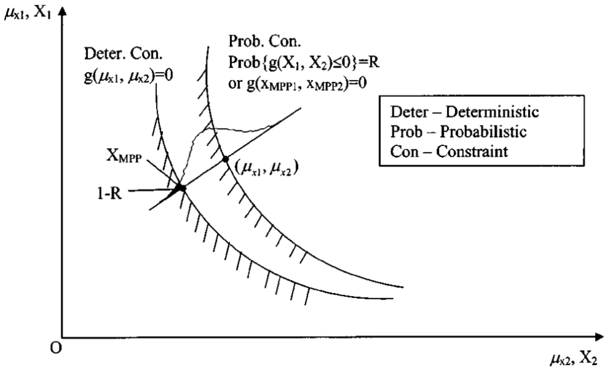
No → $\boldsymbol{s}^{(k+1)} = \boldsymbol{p}^{(k)} - \boldsymbol{X}_{\mathrm{MPTP}}^{(k)}$ → $k = k + 1$

Yes → Optimal Design



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Multi-fidelity Bayesian SORA (MFB-SORA)

1st contribution: Bayesian Optimization

- Construction of surrogate models of objective and constraint functions using Gaussian Process (GP) [10]
- Optimize the sub-problems by Bayesian approach [11] (*i.e.*, using an enrichment criterion: lower confidence bound (LCB), expected violation (EV), *etc.*)

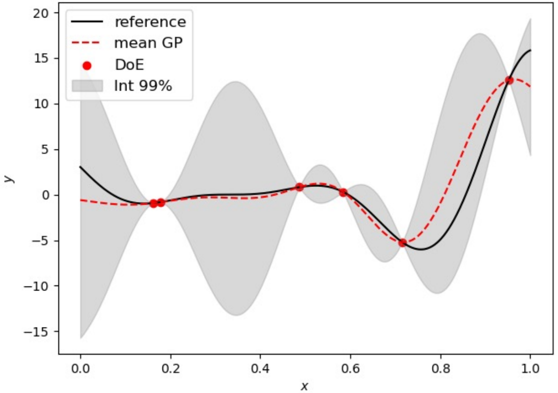
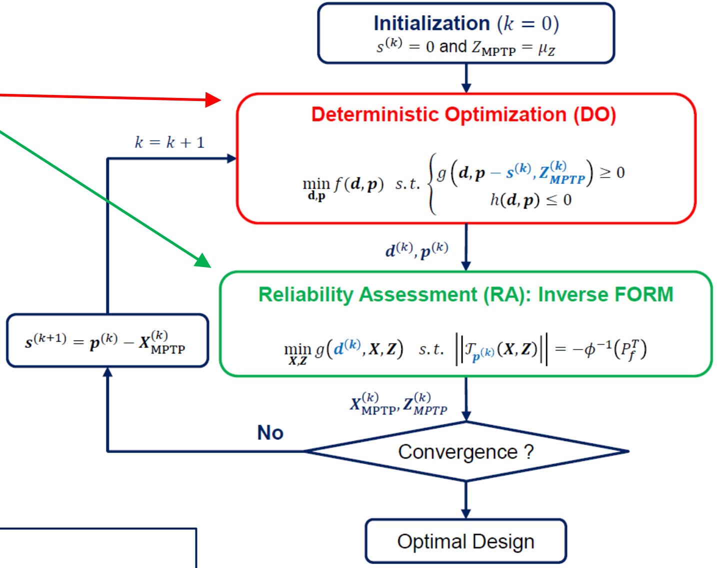


Figure – Mean function μ and associated variance σ^2 of the GP prediction.

Enrichment phase for DO:

$$\boldsymbol{d}^{new}, \boldsymbol{p}^{new} = \arg\min_{\mathbf{d},\mathbf{p}} LCB(\mathbf{d},\mathbf{p}) \quad s.t. \;\; EV(\mathbf{d},\mathbf{p}) \leq t$$

⟶ Criterion adapted for RA



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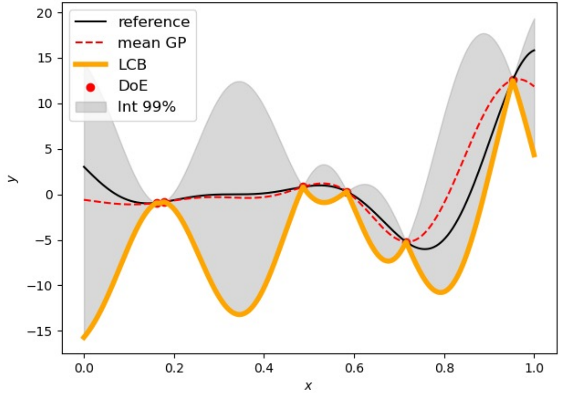

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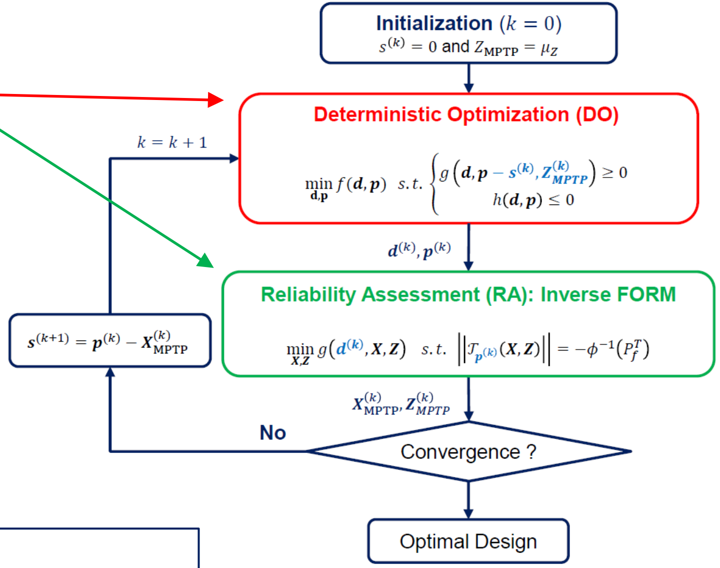


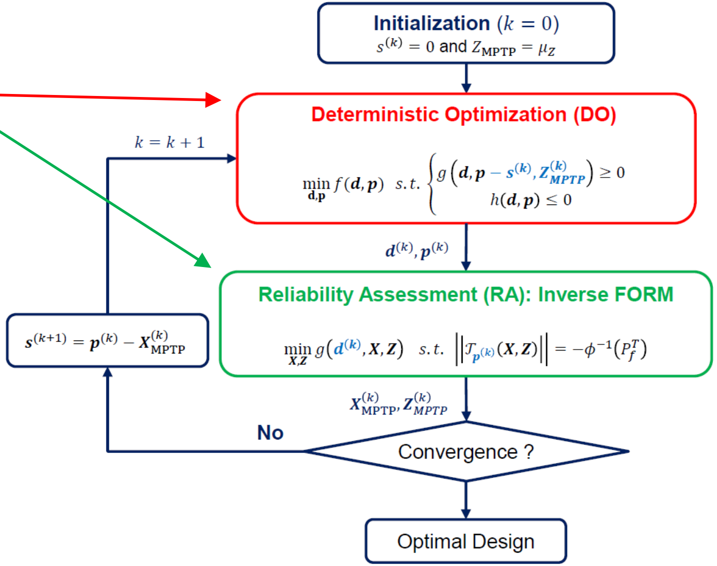
Multi-fidelity Bayesian SORA (MFB-SORA)

2nd contribution: Augmented space

- Construction of the surrogate model of the constraint function in the augmented (joint) space (design and random variables)

$$g(\boldsymbol{d}, \boldsymbol{X}(\boldsymbol{p}), \boldsymbol{Z})$$

- Reuse of information in the design of experiment (DoE) obtained in previous iterations of SORA (*e.g.*, costly model evaluations)



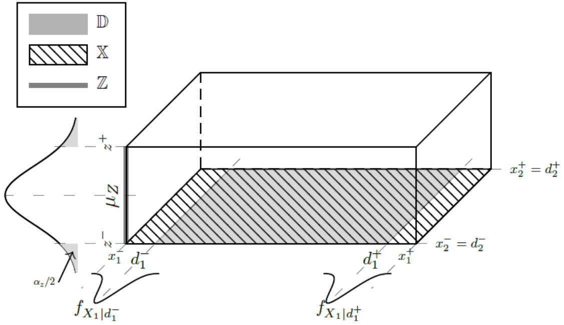
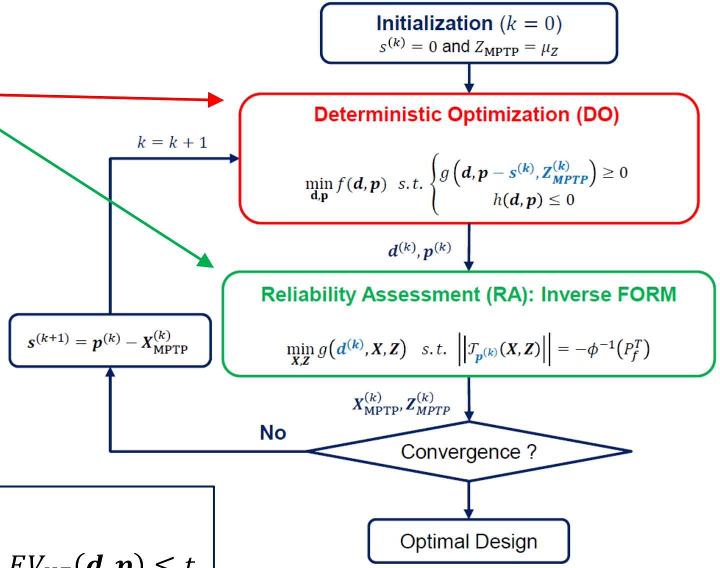


Figure – Illustration of the augmented space for a problem with two design variables $X_1(d_1)$ and d_2, and a random variable Z. [2]

Multi-fidelity Bayesian SORA (MFB-SORA)

3rd contribution: Multi-fidelity

- Aggregation of solvers of different level of fidelity
- Construction of a multi-fidelity GP using co-kriging [12]
- Adapted enrichment criterion: selection of a new point $\{\boldsymbol{d}^{new}, \boldsymbol{p}^{new}\}$ and of the information source l^{new}



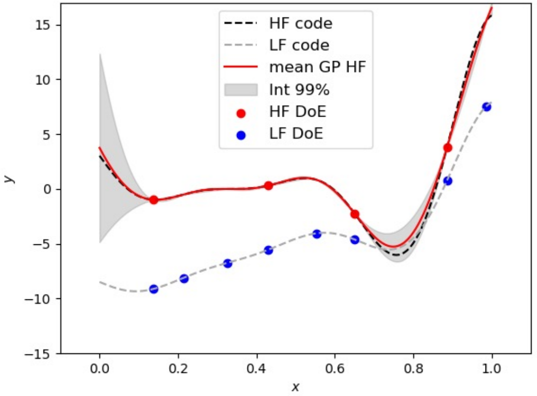


Figure – Illustration of the outputs of a high-fidelity (HF) and low-fidelity (LF) code.

Enrichment phase for DO:

$$\begin{cases} \boldsymbol{d}^{new}, \boldsymbol{p}^{new} = \arg\min_{\boldsymbol{d},\boldsymbol{p}} LCB_{HF}(\boldsymbol{d},\boldsymbol{p}) \quad s.t. \ \ EV_{HF}(\boldsymbol{d},\boldsymbol{p}) \leq t \\ l^{new} = \arg \max_{l \in \{LF,HF\}} \dfrac{\sigma^2_{red}(l, \{\boldsymbol{d}^{new}, \boldsymbol{p}^{new}\})}{cost(l)^2} \qquad [13] \end{cases}$$

⟶ Criterion adapted for RA

Experiments on a physical test case

Sounding rocket test case

➢ **Optimization problem**

$$\min GLOW(d_0, d_1, p_0, p_1)$$
$$s.t. \quad \mathbb{P}[Alt(d_0, d_1, \boldsymbol{X}(p_0, p_1), Z_0) \leq 300\ km] \leq 10^{-3}$$

GLOW: Gross Lift-Off Weight
Alt: altitude of the sounding rocket at its trajectory apogee

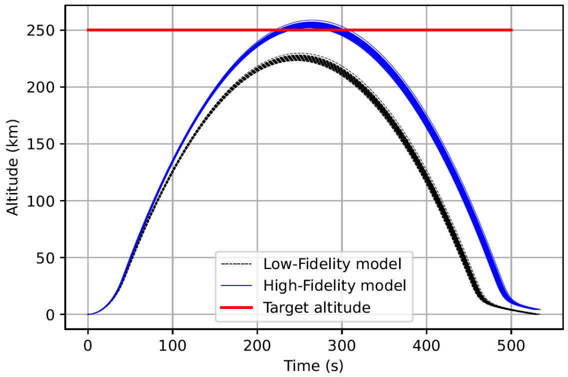


Figure – Dispersion of trajectories of the sounding rocket due to uncertainties, computed with the HF and LF codes

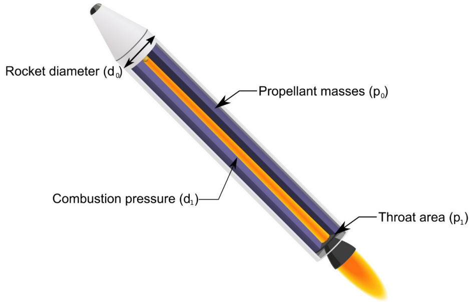


Figure – Illustration of a solid propellant single stage sounding rocket with the different design parameters ($\boldsymbol{d}$ and $\boldsymbol{p}$)

Experiments on a physical test case

Sounding rocket test case

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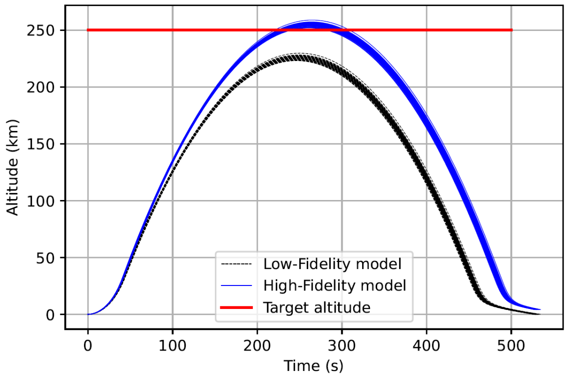
➢ Design and uncertain parameters

- d_0 the stage diameter
- d_1 the combustion chamber pressure (solid propulsion)
- p_0 the propellant mass
- p_1 the throat area
- Z_0 the uncertainty on the ascent drag coefficient

p_0, p_1: $\boldsymbol{X}$ the uncertainty due to manufacturing



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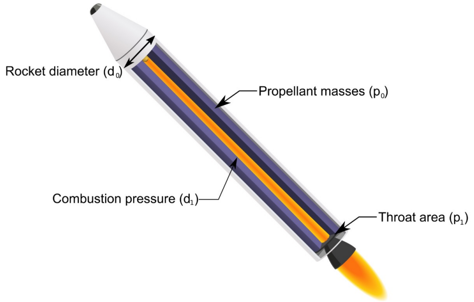

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➢ Solvers

- HF code: multidisciplinary code (trajectory, aerodynamics, structure, propulsion)
- LF code: HF code with simplifications on aerodynamics and structure disciplines

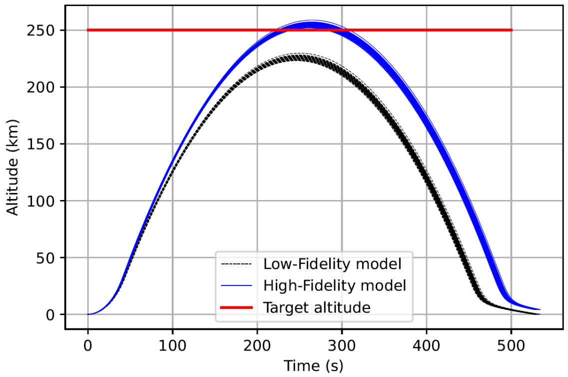

Figure – Dispersion of trajectories of the sounding rocket due to uncertainties, computed with the HF and LF codes

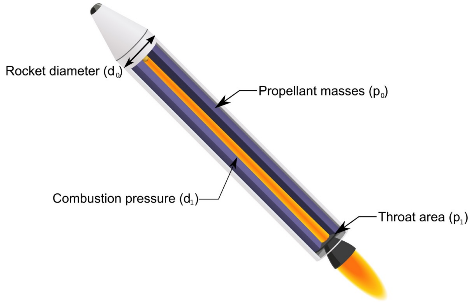

Figure – Illustration of a solid propellant single stage sounding rocket with the different design parameters ($\boldsymbol{d}$ and $\boldsymbol{p}$)

Experiments on a physical test case

Sounding rocket test case

➢ Optimization problem

$$\min GLOW(d_0, d_1, p_0, p_1)$$
$$s.t.\quad \mathbb{P}[Alt(d_0, d_1, \boldsymbol{X}(p_0, p_1), Z_0) \leq 300\ km] \leq 10^{-3}$$

GLOW: Gross Lift-Off Weight
Alt: altitude of the sounding rocket at its trajectory apogee

➢ Design and uncertain parameters

- d_0 the stage diameter
- d_1 the combustion chamber pressure (solid propulsion)
- p_0 the propellant mass
- p_1 the throat area

$\Big\}$ $\boldsymbol{X}$ the uncertainty due to manufacturing

- Z_0 the uncertainty on the ascent drag coefficient

➢ Solvers

- HF code: multidisciplinary code (trajectory, aerodynamics, structure, propulsion)
- LF code: HF code with simplifications on aerodynamics and structure disciplines

Computational settings

➢ Computational costs: $c_{LF} = 0.1$ and $c_{HF} = 1$

➢ Initial Design of Experiments (DoE)
- $3 * \dim$ points in each fidelity level ($\dim$ the dimension of each function)

➢ 10 repetitions of the method with differents DoEs

➢ Stopping criterion for the Bayesian optimizations
- $\left\| \{\boldsymbol{d}^{new}, \boldsymbol{p}^{new}\}_{(i)} - \{\boldsymbol{d}^{new}, \boldsymbol{p}^{new}\}_{(i-1)} \right\| \leq \delta$

Experiments on a physical test case

Results

Double-loop approach

- **Optimizer:** ~ 100 iterations
- **Reliability analysis by MCS:** $\sim 10^5$ points to estimate P_f of the order of 10^{-3}

Remarks

Experiments on a physical test case

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Experiments on a physical test case

Results

Table – Solution of the optimization problem

	$x^{\text{opt}} = [d_0, d_1, p_0, p_1]^{opt}$	$f_{HF}(x^{opt})$	$P_f(x^{opt})$	Coût total HF
Standard SORA	$[\,51{,}1;\ 9{,}75;\ 438;\ 1{,}48\,]$	$683{,}5$	10^{-3}	4054

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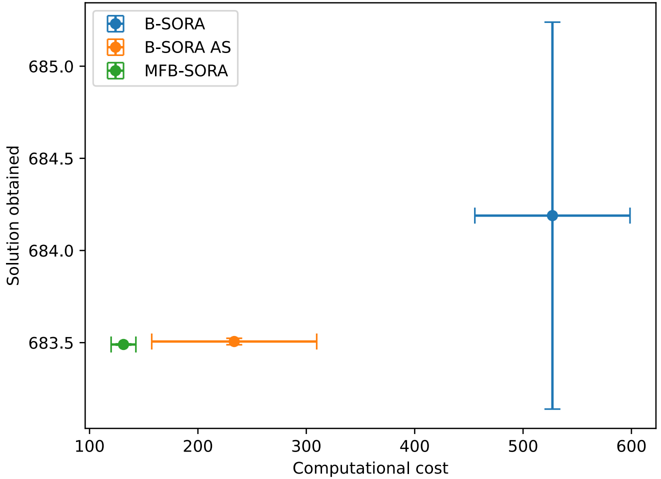

Figure – Solutions obtained for the 10 repetitions, as a function of the associated computational cost

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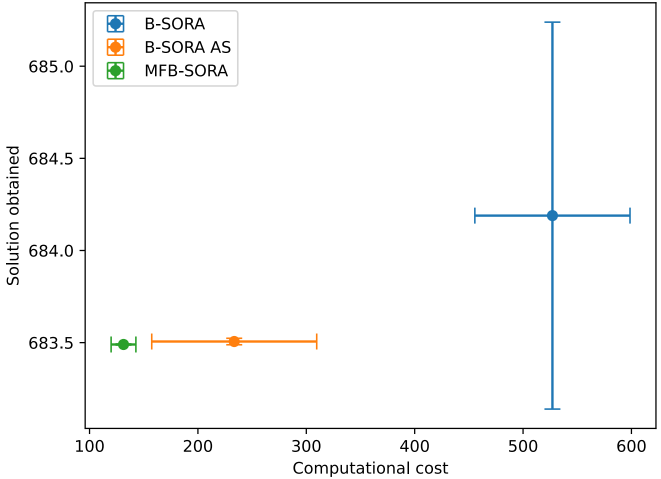

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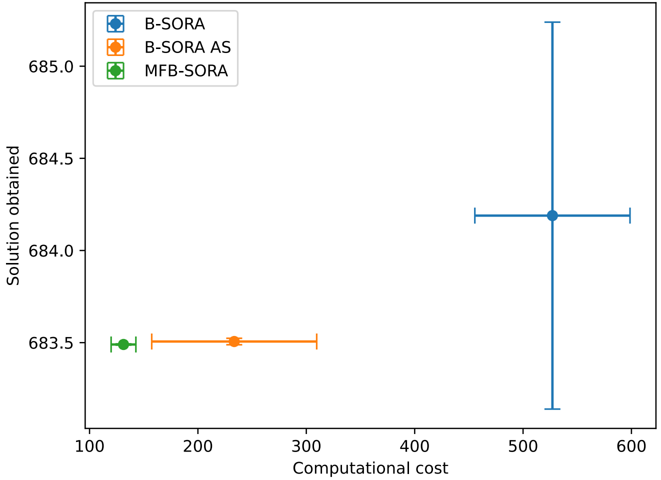

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Remarks

- The proposed MFB-SORA approach provide the feasible solution of the RBDO problem
- Each improvment of SORA reduces the computational cost, from 7,7 to 31 times

Contents

Conclusions and perspectives

Conclusions

- SORA method have been investigated, which is a decoupled RBDO technique
- 3 different contributions have been implemented:
  - The integration of Bayesian optimization in the SORA framework
  - The construction of the surrogate models in an augmented space to reuse information through the SORA iterations
  - The use of multi-fidelity surrogate model to combine different fidelity models

- MFB-SORA improves the efficiency of the method by reducing the computational cost, while ensuring the accuracy on the optimum of the optimization problem

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Perspectives

- Compare different infill criteria for the multi-fidelity Bayesian optimization
- Test other multi-fidelity GP models (*e.g.,* Non-linear Auto-Regressive Gaussian Process (NARGP) [14] or Linear Model of Coregionalization (LMC) [15])

Thank you for your attention!

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Appendix

Bayesian Optimization

- Construct a GP based on a DoE
- Enrich the DoE to improve the prediction of the surrogate model

Problem formulation

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad s.t. \quad g(\boldsymbol{x}) \geq 0$$

- Enrichment of the DoE:

$$\boldsymbol{x}^{new} = \underset{\boldsymbol{x}}{\operatorname{argmin}}\, LCB(\boldsymbol{x}) \quad s.t. \quad EV(\boldsymbol{x}) \leq T$$

- $LCB(\boldsymbol{x}) = \mu_f(\boldsymbol{x}) - \alpha * \sigma_f(\boldsymbol{x})$
- $EV(\boldsymbol{x}) = -\mu_g(\boldsymbol{x}) * \Phi\left(\frac{-\mu_g(\boldsymbol{x})}{\sigma_g(\boldsymbol{x})}\right) + \sigma_g(\boldsymbol{x}) * \phi\left(\frac{-\mu_g(\boldsymbol{x})}{\sigma_g(\boldsymbol{x})}\right)$
- $\{\mu_f, \sigma_f^2\}$ the posterior mean and variance of the surrogate model of f
- $\{\mu_g, \sigma_g^2\}$ the posterior mean and variance of the surrogate model of g

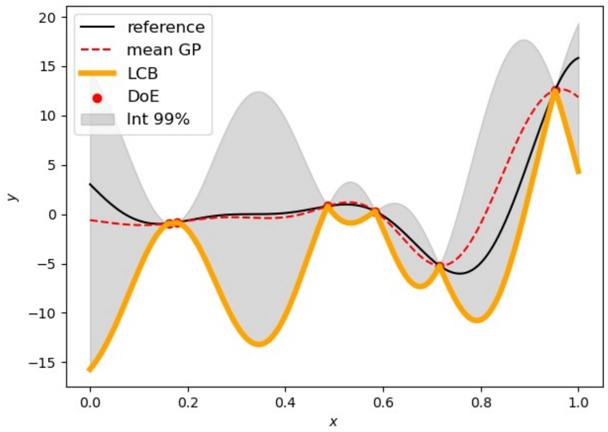


Figure – Illustration of the LCB enrichment criterion

Auto-Regressive model AR1 (co-kriging)

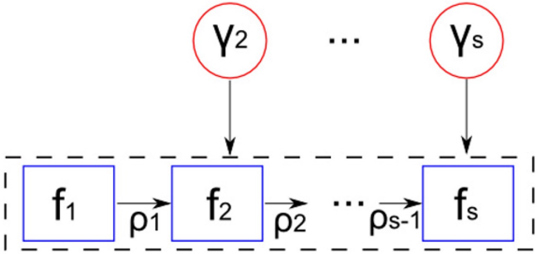
- Construction of a multi-fidelity GP, based on a hypothesis of linear dependency bewteen two successive levels of fidelity

GP HF GP LF GP corrector

- $f_t(x) = \rho_{t-1} \times f_{t-1}(x) + \gamma_t(x)$

Scalar coefficient

- Recursive construction possible if the DoEs are nested



Appendix

Multi-fidelity Bayesian Optimization

Problem formulation

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad s.t. \quad g(\boldsymbol{x}) \geq 0$$

- Construct a multi-fidelity GP based on a multi-fidelity DoE (a DoE per fidelity)
- Enrich the DoE to improve the prediction (by selecting a new point and a fidelity level to compute it)

- Enrichment of the DoE:

$$\begin{cases} x^{new} = \underset{x}{\operatorname{argmin}}\, LCB_{HF}(\boldsymbol{x}) \quad s.t. \quad EV_{HF}(\boldsymbol{x}) \leq \mathrm{t} \\ l^{new} = \arg \max_{l \in \{LF,HF\}} \dfrac{\sigma_{red}^2(l, \boldsymbol{x}^{new})}{cost(l)^2} \end{cases}$$

- With $cost(l)^2 = \sum_{i=1}^{l} c_i$, and with i the cost of each level of fidelity

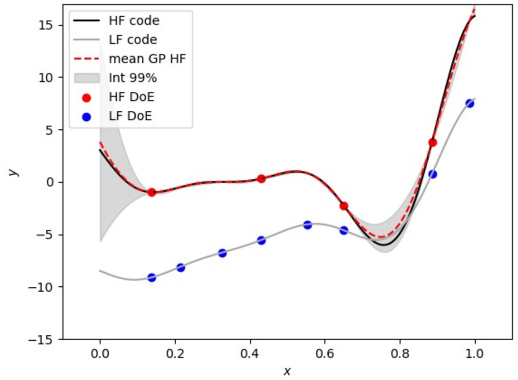


Figure – Illustration of the outputs of a high-fidelity (HF) and low-fidelity (LF) code.