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OPTIMIZATION OF A PHOTOACOUSTIC GAS SENSOR USING MULTIFIDELITY RBF METAMODELING

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Absorption spectroscopy principle is the basis of optical sensors.



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• Gas sensor design: the miniaturized photoacoustic cell



Synchronous detection system



Leti MAIN OPTIMIZATION PROBLEM

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• Two different simulation model are available:





PRELIMINARY RESULTS

		High fidelity	Low fidelity	
Resonance frequency	RBF	1,07±0,52	0,07±0,01	
	Kriging	2,94±0,32	0,12±0,03	
Signal	RBF	3,26±1,10	0,04±0,01	
	Kriging	3,23±1,08	0,08±0,03	



- Radial Basis Function
- RBF-based multifidelity metamodel
- Benchmark with co-kriging
- **RBF optimization algorithm extended to multifidelity**

Leti RADIAL BASIS FUNCTION (RBF)

• Objective function is decomposed on a basis of function :

$$\hat{Y}(\mathbf{x}) = \sum_{i=1}^{n} \beta_{i} \varphi(\|\mathbf{x} - \mathbf{x}_{i}\|) + Q(\mathbf{x})$$

RBF
$$\varphi (\|\mathbf{x} - \mathbf{x}'\|)$$
 $Q(\mathbf{x})$ Cubic $(\|\mathbf{x} - \mathbf{x}'\|)^3$ $\alpha_1 p_1(\mathbf{x}) + \alpha_2 p_2(\mathbf{x})$ Gaussian $\exp\left(-\sum_{i=1}^d \gamma_i \|\mathbf{x}_i - \mathbf{x}'_i\|^2\right), \ \gamma_i > 0$ $\{\emptyset\}$

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Interpolating condition

•
$$(-1)^{l_0+1} \boldsymbol{\beta}^T \boldsymbol{\Phi} \boldsymbol{\beta} > 0 \quad \forall \boldsymbol{\beta} \in \mathcal{V}_{l_0} \setminus \{0\}$$

$$\sum_{i=1}^{n}\beta_{i}Q(\mathbf{x}_{i})=0 \quad \forall Q\in \Pi_{l_{0}}$$

$$\boldsymbol{\Phi}_{ij} \coloneqq \boldsymbol{\varphi} [| \mathbf{x}_i - \mathbf{x}_j | |) \quad i, j = 1, \dots, n$$

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$$\frac{\text{RBF}}{\text{Cubic}} \frac{\varphi \left(\|\mathbf{x} - \mathbf{x}'\| \right)}{\left(\|\mathbf{x} - \mathbf{x}'\| \right)^3} \qquad Q(\mathbf{x}) \\
\frac{\varphi \left(\|\mathbf{x} - \mathbf{x}'\| \right)^3}{\text{Gaussian}} \exp \left(-\sum_{i=1}^d \gamma_i \|\mathbf{x}_i - \mathbf{x}'_i\|^2 \right), \quad \gamma_i > 0 \qquad \{\emptyset\}$$

$$\begin{pmatrix} \mathbf{\Phi} & \mathbf{F} \\ \mathbf{F}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{\beta} \\ \mathbf{\alpha} \end{pmatrix} = \begin{pmatrix} \mathbf{z} \\ \mathbf{0} \end{pmatrix}$$

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$$\mathbf{\Phi}_{ij} \coloneqq \varphi [\mathbf{X}_i - \mathbf{X}_j] |) \quad i, j = 1, \dots, n$$

$$\mathbf{F} = \left(p_1(\mathcal{X}), \dots, p_{l_0+1}(\mathcal{X}) \right)$$

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$$LOO = \sum_{i=1}^{n} \left(\frac{\beta_i}{\mathbf{\Phi}_{ii}^{-1}}\right)^2$$

Interpolating condition

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M. J. D. Powell. Radial basis functions for multivariable interpolation: a review. In J. C. Mason and M. G. Cox, editors, *Algorithms for Approximation*, pages 143-167 Clarendon Press, New York, NY, USA, 1987.

RBF-BASED MULTIFIDELITY METAMODEL

- Different fidelity level between models involves different computational time:
 - 2D and 3D modeling.
 - Multiple physical approaches.
 - Different solver.

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• The multifidelity model is built using:



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BENCHMARK : ANALYTICAL EXAMPLE

$$y_{e} = \frac{2\pi T_{u} (H_{u} - H_{l})}{\log(r/r_{w}) \left[1 + \frac{2LT_{u}}{\log(r/r_{w})r_{w}^{2}K_{w}} + T_{u}/T_{l}\right]} \qquad y_{c} = \frac{5\pi T_{u} (H_{u} - H_{l})}{\log(r/r_{w}) \left[1.5 + \frac{2LT_{u}}{\log(r/r_{w})r_{w}^{2}K_{w}} + T_{u}/T_{l}\right]}$$

Mean value of the prediction error over 20 random initial designs





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BENCHMARK : PHOTOACOUSTIC SIGNAL

Mean value of the prediction error over 5 random initial designs



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BENCHMARK : RESONANCE CELL FREQUENCY

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• Difference in computational time and accuracy:

Output	Model	5 points	10 points	15 points	20 points
Resonance frequency	RBF	$8.0{\pm}1.1$	3.2 ± 1.6	1.4 ± 0.1	1.1 ± 0.5
	$\operatorname{co-RBF}$	$0.44 {\pm} 0.11$	$0.43 {\pm} 0.11$	$0.51 {\pm} 0.12$	$0.33 {\pm} 0.08$
	co-kriging	$0.33 {\pm} 0.05$	$0.42 {\pm} 0.08$	$0.34{\pm}0.1$	$0.37 {\pm} 0.1$
Signal	RBF	6.0 ± 2.4	5.0 ± 3	$3.9{\pm}1.9$	3.2 ± 1.2
	$\operatorname{co-RBF}$	4.48 ± 1.6	$3.75 {\pm} 1.72$	$3.20{\pm}1.65$	$2.83 {\pm} 1.37$
	co-kriging	$2.16{\pm}1.07$	$4.70 {\pm} 5.14$	$2.13 {\pm} 0.66$	$2.32{\pm}1.03$



- A criterion to refine RBF toward the minimum of the function is defined by Gutmann.
 - $\langle s, s \rangle = (-1)^{l_0+1} \boldsymbol{\beta}^T \boldsymbol{\Phi} \boldsymbol{\beta}$ $h(t) = \langle s_t, s_t \rangle \langle s, s \rangle$



$$\langle s,s\rangle = (-1)^{l_0+1} \boldsymbol{\beta}^T \boldsymbol{\Phi} \boldsymbol{\beta}$$

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 In the co-RBF framework, only the difference model is refined using the detailed simulation.

H.-M. Gutmann. "A radial basis function method for global optimization". Journal of Global Optimization, 2001.



OPTIMIZATION OF THE PHOTOACOUSTIC GAS SENSOR

• Signal optimization:

Initial DOE	Minimum value		Minimum location		
	Co-kriging	Co-RBF	Co-kriging	Co-RBF	
1	-1.88	-1.91	$[0.02, 4.18e^{-4}, 0.0179]$	$[0.02, 5.00e^{-4}, 0.0177]$	
2	-1.87	-1.90	$[0.02, 5.00e^{-4}, 0.0159]$	$[0.02, 4.97e^{-4}, 0.0173]$	
3	-1.91	-1.90	$[0.02, 4.86e^{-4}, 0.0188]$	$[0.02, 4.73e^{-4}, 0.0200]$	
4	-1.90	-1.88	$[0.02, 4.54e^{-4}, 0.0200]$	$[0.02, 5.00e^{-4}, 0.0200]$	
5	-1.87	-1.91	$[0.02, 4.58e^{-4}, 0.0200]$	$[0.02, 4.46e^{-4}, 0.0200]$	





• A new multifidelity metamodel:

- RBF-based
- Optimization method extended to multifidelity framework
- Validation on a real engineering design problem

• Perspectives:

- Test on a higher dimensional problem
- Adapt other RBF-based optimization method to multifidelity framework.

Forecasting and optimization are complex



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