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HEAT TRANSFER OPTIMIZATION OF A RIBBED SURFACE USING SURROGATE-ASSISTED GENETIC ALGORITHMS

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Abstract. *Over the last years, complex design and optimization engineering problems became more and more demanding in computational time. Despite the advances made in computer science, these demands are prohibitive in some cases, in many engineering fields such as fluid mechanics and heat transfer. Aiming to alleviate this, surrogate response models are introduced and coupled with optimization drivers to deliver cheaper and accurate optimization results. The present paper investigates the performance of various surrogate-assisted optimization schemes applied to a heat transfer modeling problem of a ribbed surface. In this study, performance of different surrogate models such as Kriging, Co-Kriging and Support Vector Regression in different evolutionary optimization schemes are assessed. These schemes employ the aforementioned surrogate models coupled with different infill strategies depending on the availability of an uncertainty measure for the prediction. The results show that Co-Kriging model provides accurate results in comparison with the other metamodels while the computational time is reduced by more than 50%. It is illustrated that the combination of multi-fidelity approaches and sophisticated infill strategies can provide accurate predictions at a reduced computational cost.*

1 INTRODUCTION

Design and optimization problems in various engineering fields, are becoming more complex. The growing need of taking into account the highest number of design variables possible, stretches the capabilities of the existing computational systems. In this context, the Curse of Dimensionality is an important issue that has to be addressed. Use of surrogate evaluation models, is a well-known practice to alleviate the computational time of expensive response models. Surrogates can mimic the underlying behaviour of the response function providing a cheap and alternative evaluation tool. The prediction quality of these models relies on their effective training process and the proper selection of the respective training samples. The coupling of those models with optimization schemes, called Surrogate Based Optimization (SBO), results in more computationally efficient strategies.

The seminal study of Jones et al. [1] used Kriging models as a predictor during the optimization cycles. The validation of the surrogate model is crucial during the optimization process to assess the results derived and it is thoroughly discussed at [1]. Emmerich et al. [2] described an SBO scheme for both single and multi-objective optimization problems. The proposed scheme in that study employs Gaussian Random Field Meta-models (GRFM) and a novel procedure of selecting the infill training points from the offspring generated. It should be noted here that this infill strategy requires an uncertainty measure of the surrogate model's prediction. Particularly for the multi-objective problems, the Expected HyperVolume Improvement (EHVI) suggested, uses balanced exploration and exploitation of the metamodel in order to screen out the less promising individuals during the generational process. Thus, the proposed scheme results in a more computationally efficient optimization strategy. Building more on the EHVI concept, Hupkens et al., in studies [3, 4], suggest a faster computational procedure for the calculation of the EHVI scores which replaces the initial Monte-Carlo integration technique. Empirical comparisons showed that this new implementation results in minimum five times faster computations for two or three dimensional objective spaces. It is worth to mention here that the Couckuyt et al. [5] algorithm remains the fastest one for the computation of hypervolume-based Probability of Improvement in higher dimensional objective spaces (more than three dimensions).

The use of SBO schemes for heat transfer modeling problems is of great importance, since the application range is very wide and the numerical response models can be relatively costly. Particularly, the heat transfer optimization of ribbed surfaces is important for the cooling performance of turbine blades. The wide application field of turbomachinery justifies the rigorous research activity, aiming to define the optimal geometrical and operational configuration of these ribbed surfaces. Labbé [6] described the flow topology and heat transfer performance of a ribbed surface with constant-sized ribs using Large Eddy Simulation. Recirculation zones on the top and behind the rib were identified while the enhancement of heat transfer performance is maximum in front of the ribs, as a result of the highly unsteady secondary eddies. The numerical optimization of a ribbed channel was performed in Yang and Chen study [7], where Response Surface Method (RSM) and evolutionary-based optimizer were coupled in order to derive the optimized scenarios. The design variables used in the study were the height and thickness of the ribs and the pitch of the channel while the formulated objective was based on the Nusselt number distribution and the pressure drop. Results showed an apparent increase of the channel's performance particularly for the staggered ribs design scenario. Xie et al. [8] investigated numerically five different configurations of variable sized ribs in a three-dimensional internal cooling channel flow. The different scenarios employ half-sized and same-sized ribs aiming to define the configuration that results in the maximum Nusselt number distribution and the minimum pressure drop. Despite the fact that no optimizer is used in this study, the numerical investigation provides useful insights for the ribbed surface set up and a detail description of the heat transfer modeling case.

In the present study, a nominal geometrical configuration based on [8] is used to build a SBO test case and investigate its performance using CFD evaluations and different surrogate models. Thus the purpose of this research study is twofold: investigate and assess the performance of the SBO in heat transfer problems and derive further optimized configurations of the ribbed surface under examination. Therefore, the suggested optimization framework will be first described and validated against a well-known analytical test case. Then, the numerical optimization results regarding the heat transfer test case will be presented and thoroughly discussed.

2 A SURROGATE-BASED OPTIMIZATION FRAMEWORK

The implementation of the optimization test cases is based on the development of a modular SBO framework. Each of the implemented modules performs a specific group of tasks. The modular approach enhances the flexibility while it makes easier the addition of new features. The necessary modules are enlisted in Table 1 along with a short description.

Modules	Short Description
Base module:	Co-ordinates the actions of different modules
Parameters module:	Defines the input parameters for the selected test case
Evaluation module:	Implements the proper fitness function for the selected test case
Sampling module:	Performs the initial sampling plan
Optimize module:	Implements the optimization schemes. Contains the optimizer as well
Infill module:	Implements different infill strategies
Surrogate module:	Implements the training, activation and assessment actions of different surrogate models

Table 1: Short description of the SBO framework modules.

The developed framework can function in two basic modes: the offline and the online meta-model training modes. The simpler offline training strategy uses an initial Design of Experiment in order to train the surrogate model and uses it instead of the expensive fitness function during the optimization cycles. The method does not use infill points to update the metamodel. Thus, the quality of the predictions and the final optimization outcome is based on the sampling technique and the initial amount of samples. This primitive strategy is simple to implement and suitable for very low dimensional problems. The more sophisticated and currently used online mode is starting with a Design of Experiment (DoE) which serves as the population of the first generation as well. These design samples are calculated then, employing the exact response. The resulting data is used as input training data for the respective surrogate model. The trained meta-model is activated during the optimization cycles, aiming to calculate the fitness values of the offspring created. An infill strategy, such as EHVI [2], is employed to assess the offspring and to choose the best individual which will be evaluated through the expensive response. Afterwards this individual is added to the training database and the metamodel is updated. In this way the model evolves during the optimization cycles which results into better prediction at the regions of interest (near the optimum). This strategy is based on a smaller initial DoE and it is depending strongly on the performance of the infill strategy.

The described task-flow of the framework is based on the implementation of specific techniques for each modules. Starting from the sampling strategy, the Optimal Latin Hypercube Design [9] was used due to its improved space-filling properties. A simple genetic algorithm is used to maximize the Morris-Mitchell criterion and derive the optimized sampling plan. The optimizer employed in all the test case is the extensively used Nondominated Sorting Genetic Algorithm Type-II (NSGA-II) [10], which is suitable for multi-objective problems. The respective algorithm was created with the Distributed Evolutionary Algorithms in Python (DEAP) library [11]. The infill strategy used here is the classical Expected Improvement (EI) in case of a single-objective problem and the described EHVI [2] method for the bi-objective problems. A hypervolume-based indicator is used as well in order to be coupled with specific metamodels. The combinations of the surrogates and the infill strategies are explained in the next paragraph. The surrogate model part contains models such as Kriging [12] and its variant Co-Kriging [13] and Support Vector Regression [14]. The implementation of the Co-Kriging model was based on the work of Le Gratiet et al. [15] as it was implemented originally at the Open Multidisciplinary Design Analysis and Optimization (OpenMDAO) [16] framework in Python. The use of Co-Kriging requires the definition of variable levels of fidelity. The model is based on the correlation of those levels which eventually bring advantages in computational efficiency.

Finally it should be mentioned that the different surrogate models are capable to work with specific infill strategies. This is resulting in two different optimization schemes for the online mode. The Kriging and Co-Kriging models are combined with EHVI [2-4] infill criterion which accounts balanced exploration and exploitation of the surrogate models. The SVR metamodel is combined with the hypervolume indicator which in the case of a bi-objective problem translates to the area of the produced Pareto front and purely exploits the surrogate model. The reason behind those choices is that, unlike the SVR models, the Gaussian metamodels can easily provide an uncertainty measure of their prediction. Thus the balance between exploration and exploitation of the surrogate is allowed.

3 TEST CASES DESCRIPTION

3.1 Analytical Test Case

The implementation of different techniques and its coupling is not a trivial task. In order to ensure the proper functioning of those techniques, a validation test case should be implemented. Therefore, the DTLZ2 [17] bi-objective analytical test case is chosen to validate and assess the performance of the multi-objective SBO framework. The mathematical formulation of the test case is described as follows:

$$\begin{aligned} f_1(\vec{x}) &= (1+g(\vec{x}))\cos x_1 \frac{\pi}{2} \\ f_2(\vec{x}) &= (1+g(\vec{x}))\sin x_1 \frac{\pi}{2} \end{aligned} \tag{1}$$

where:

$$g(\vec{x}) = \sum_{x_i \in \vec{x}} (x_i - 0.5)^2 \tag{2}$$

$$0 \leq x_i \leq 1, i = 1, 2, \ldots, N_{dimensions}$$

3.2 Heat Transfer Test Case

3.2.1 Design Variables and Computational Domain

The heat transfer test case aims to improve the heat transfer modeling of a surface with variable-size ribs placed in an internal cooling passage. The detailed description of this test case is based on [8], where five different geometric configurations are investigated. The configuration selected to be further optimized is demonstrated in Fig. 1(one-pitch length).

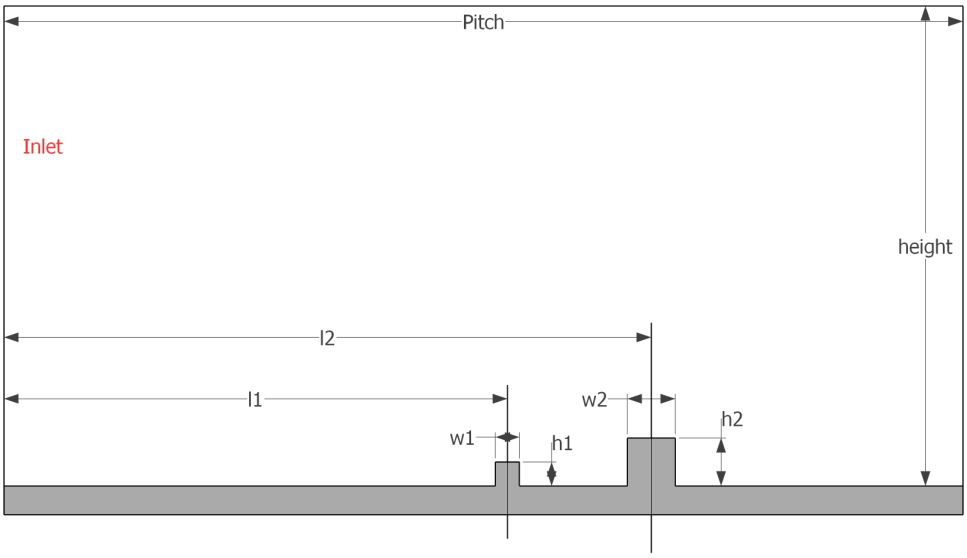

Figure 1: Nominal geometric configuration.

As shown in Fig. 1, the design variables of the test case are the height, width and placement length of the ribs resulting in a six-dimensional design space. The height and the pitch of the ribbed channel are 50 mm and 100 mm in respect, with a hydraulic diameter of 50 mm as well. The computational domain is restricted in one-pitch length in order to decrease the mesh size and accelerate the numerical evaluations. The proper definition of the periodic boundary conditions based on [8] ensures the quality of the CFD results.

3.2.2 Overview of the Numerical Procedure

The CFD evaluations aim to calculate the Nusselt number distribution on the ribbed surface and the pressure drop between the inlet and the outlet of the channel. A two-dimensional, steady and turbulent flow process is assumed to calculate these values. The standard k-ϵ turbulence model with standard wall-function is selected. It should be added that the selected model is not the most suitable for the heat transfer problems. The present study though focuses more on the performance of the SBO scheme. Therefore, the balance between the quality of the results and the simplicity of the model is deemed proper for these purposes. The pressure-velocity coupling is achieved through SIMPLE method, while second order schemes are used for the spatial discretization. Finally the absolute convergence criterion is set at 10^{-6}.

3.2.3 Boundary Conditions

As it was stated previously periodic boundary conditions are used for this problem. The periodicity is defined at the inlet and the outlet of the channel. The mass flow rate is used as a parameter. In order to mimic the heat transfer in an internal cooling passage, constant heat flux of 1000 W/m^2 is applied to the entire walls of the channel, including the ribs. The air enters the passage at a temperature of 300K and a Reynolds number of 20000. The turbulence intensity level is defined as 5% at the inlet.

3.2.4 Definition and Validation of Different Fidelities

As it was mentioned in section 2, the multi-fidelity approach is employed in order to use the Co-Kriging model and benefit from its advantages. Therefore, it is important to describe two different levels of fidelity which serve as a cheap and expensive response. The first cell distance is defined as the basic criterion to derive the alternative levels of fidelity, since the heat transfer phenomena are intense at the boundary layers. Table 2 summarizes the main aspects of the two defined fidelities.

	Lower Fidelity	Higher Fidelity
First Cell Distance [m]	1e-04	1e-05
Mesh Size	15500	32000
Computational Time* [min]	7	30

**The computational time was defined on an 4-cores Intel Xeon E3-1200*

Table 2: Main characteristics of the various fidelities.

In addition, the distributions of Nusselt number on the ribbed surface and the pressure drop along the vertical axis are presented in Fig. 2. It is apparent that the lower fidelity simulations overpredict Nusselt number distribution while the pressure drop is underpredicted.

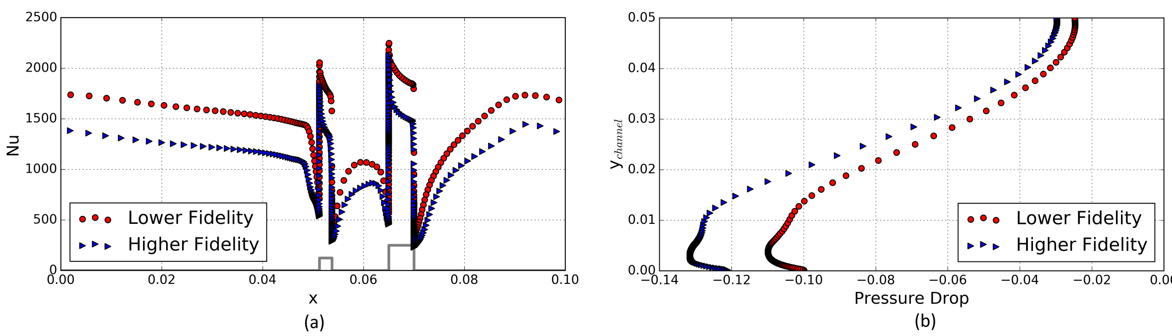

Figure 2: Nusselt number (left) and pressure drop distribution (right) for different fidelities.

In the extent of this definition, the numerical approaches used are validated against the velocity profiles obtained from [8]. An indicative comparison plot is shown in Fig. 3. The overall agreement is good. The underprediction of the velocities is due to the fact that the present study employs a two-dimensional simulation while [8] uses a three-dimensional approach.

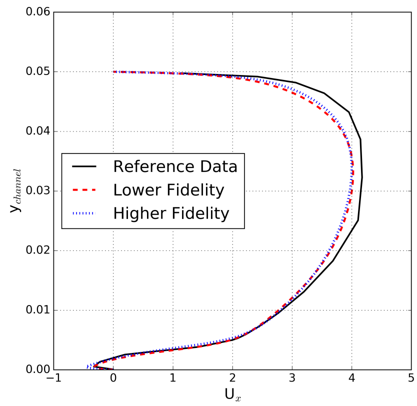

Figure 3: Comparison of derived velocity profiles to the reference CFD data.

4 RESULTS AND DISCUSSION

4.1 Analytical Test Case Results

The DTLZ2, bi-objective analytical test case is used mainly to test and validate the function of the developed framework. The validation is performed using a six-dimensional version of the DTLZ2 problem (same size of the design space as the heat transfer test case), while one surrogate model per objective is used. It is reminded that the results presented are obtained using the combinations of Kriging metamodel with the EHVI strategy and SVR surrogate model with the hypervolume-based indicator. The Co-Kriging model is not used in this test case since the definition of variable levels of fidelity does not lead to any actual computational time differences. The model will be investigated in the heat transfer test case where the different levels of fidelity are properly defined.

A reference Pareto front of the optimized DTLZ2 test case without surrogates employed is obtained. Fig. 4 compares the Pareto fronts obtained by the described surrogate models against the reference one. The results presented are obtained after 20 generations. The Kriging

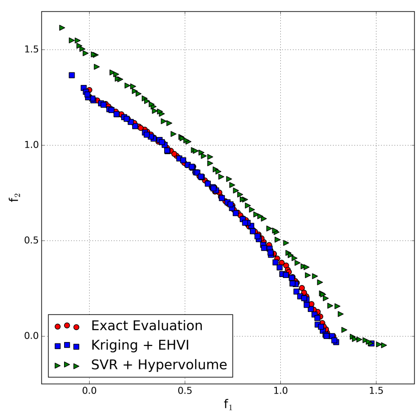

Figure 4: Optimal Pareto fronts obtained with the different optimization schemes.

surrogate model coupled with the EHVI technique managed to derive an optimal Pareto front similar to the reference one by calculating 95% less samples. The SVR model along with the hypervolume-based selection of infill points results in a Pareto front clearly dominated by the reference Pareto. The reason behind this difference is the infill strategy used. The hypervolume-based selection only exploits the surrogate model. Thus, the improvement of the surrogates performance is slower. It is expected that the higher number of samples in the training database will finally increase the prediction quality. Indeed, the Pareto front obtained for SVR models trained with higher number of samples is closer to the reference Pareto as it is presented in Fig. 5. It should be mentioned that in this case the SVR training database is 36% bigger than the Kriging training database.

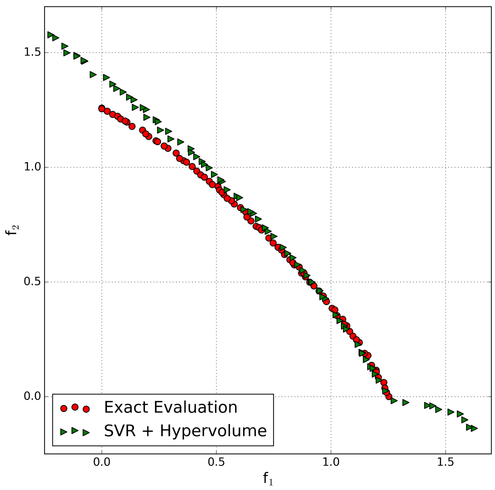

Figure 5: Reference and SVR obtained Pareto fronts.

The implementation of the analytical test case with the developed framework provides a fast way to assess different optimization schemes. Therefore, the comparison between the offline and online training schemes of the surrogate models is described within this test case. The NSGA-II optimizer with a constant number of twenty generations was employed, while the Kriging model is selected for the surrogate evaluations. The online training mode allows the surrogate to start from a small training database and enrich it during the optimization cycles by selecting the most appropriate infill points. On the contrary, during the offline training mode the metamodel is trained a priori, with a constant higher number of samples and then is used as the fitness function. This fact results to the calculation of unnecessary samples which decreases the overall computational efficiency. The superior performance of the online training mode is illustrated at Fig. 6.

The online training mode outperforms the offline one in terms of accuracy for almost the same number of samples. Further increase of the size of the training database, which is translated to more computational time, will improve the performance of the surrogate trained with the offline mode. It is proved that the proper selection of the new points, added in the training database is essential for the performance of the surrogate as a fitness function and for the reduction of the final computational cost. The pre-definition of the training database using solely the initial DoE results in less computationally efficient SBO schemes. The efficiency decreases

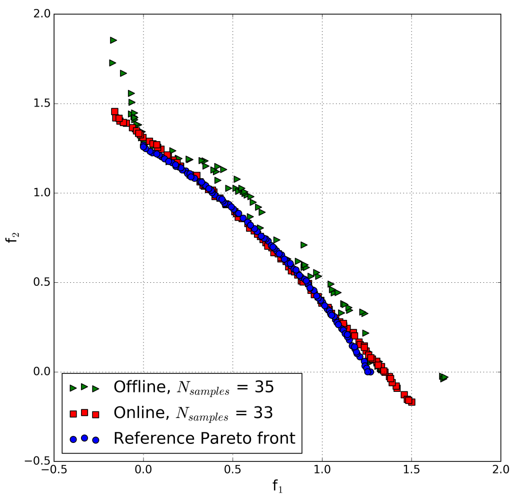

Figure 6: Comparison of online and offline surrogate training modes for the DTLZ2 test case.

more intensively for higher dimensional test cases. Moreover, the prediction accuracy in offline mode depends more strongly on the morphology of the response. Thus, the use of the online training mode is clearly recommended.

4.2 Heat Transfer Test Case Results

The goal of this test case is the heat transfer modeling of a ribbed surface placed in an internal cooling channel. First a reference solution based only on CFD evaluations only is obtained. This solution is considered as the baseline to determine the most efficient scheme among the different SBO approaches. One surrogate model per objective approach is employed in this test case as well. The online training mode of the surrogate is used due to its profound advantages described in the previous section. The definition of various levels of fidelity for this test case (section 3.2.3) allows the meaningful assessment of a multi-fidelity surrogate such as Co-Kriging.

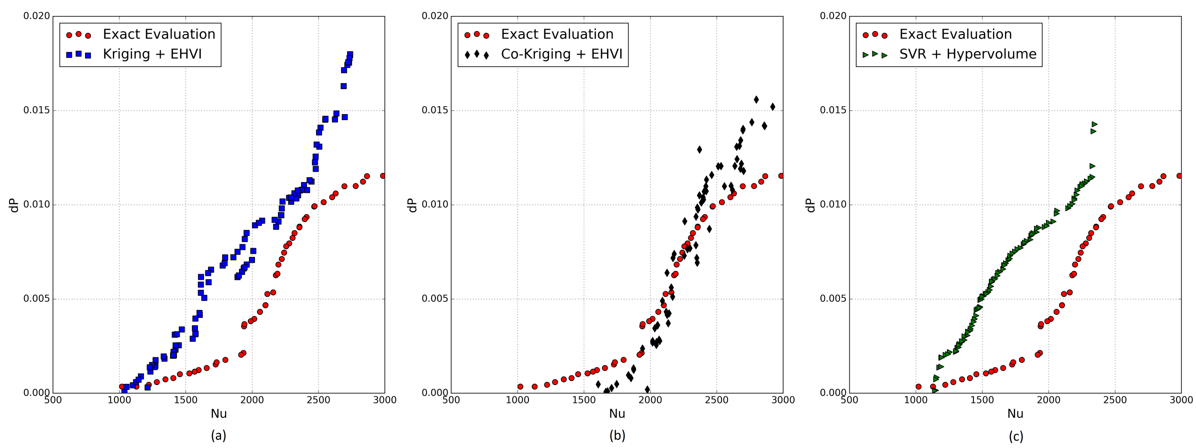

Figure 7: Optimal Pareto fronts obtained with the various surrogate models: a. Kriging, b. Co-Kriging, c. SVR.

In all the cases, optimal Pareto fronts are well formed and tend to follow the same trends as the reference Pareto. The Co-Kriging metamodel manages to derive the optimal Pareto front closer to the reference one. Particularly, the lower part of this Pareto contains individuals which dominate the respective individuals at the reference front. Those configurations indicate further improved designs of the ribbed surface. Among Kriging and SVR surrogate models, the latter present the less dominant Pareto front due to the use of the less efficient hypervolume-based infill strategy. This is justified from the selection process of the infill points as it was described for the analytical test case. The points defined from the DoE and the different infill strategies are presented for each surrogate in Fig. 8.

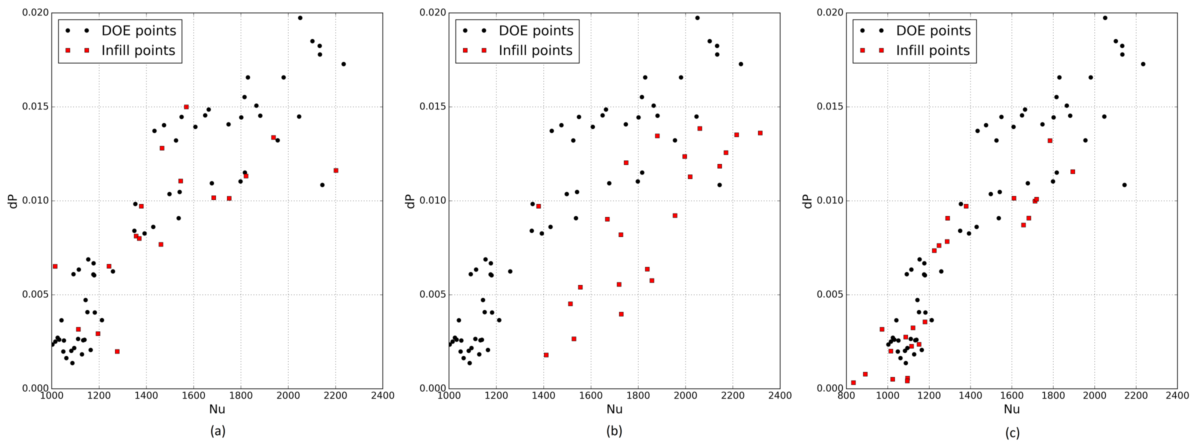

Figure 8: DoE and Infill design sites: a. Kriging. b. Co-Kriging, c. SVR.

The Co-Kriging metamodel coupled with the EHVI technique manages to capture far more infill points placed closer to the reference Pareto (towards bottom-right of Fig. 8b) front than the other two metamodels. Thus, the surrogate model improved its prediction capabilities at the region of interest, at a reduced computational cost due to the multi-fidelity approach. As it was expected the SVR model capture the least points at the region of interest. It is clear that more generations are needed in order to obtain a dominant Pareto front. The additional calculation time though will lead to a further decrease of the computational efficiency.

Finally, the prediction accuracy of the surrogate models are tested. For each optimal Pareto front obtained, 30 points are randomly selected to be evaluated through CFD simulations. Then, the coefficient of determination (R^2) is calculated to determine the quality of the prediction:

$$R^2 = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2} \tag{3}$$

Table 3 summarizes the prediction performance along with the number of samples in the training database and the respective computational time.

The computational cost of Co-Kriging surrogate is reduced by 57% and 61% compared to the Kriging and SVR model respectively. The huge decrease of computational time is due to the multi-fidelity approach. Among the approximately one hundred samples only twelve of them are calculated using the higher fidelity. The computational efficiency of the Co-Kriging is dramatically increased since the lower fidelity simulations require 75% less time. Thus, the Co-Kriging model coupled with the EHVI method capture the most efficient infill points

	Number of Samples	Computational Time [min]	R^2_{Nu}	R^2_{dP}
Kriging	76	2280	0.8775	0.84915
Co-Kriging	101	983	0.8925	0.8603
SVR	83	2490	0.8205	0.9403

Table 3: Performance metrics of the surrogate models.

by consuming the least time. Moreover the performance of the Kriging and SVR models in terms of computational time is quite close since the size of the final training database is similar. The quality of the infill points though from the optimization standpoint, is reduced for the SVR model. Finally, the generalization error for all the surrogate models is sufficiently good. Further increase of the training database size will improve the quality of the predictions.

5 CONCLUSIONS

The present study described the development of a Surrogate-Based Optimization framework capable of implementing different optimization strategies. The framework then was used to optimize the heat transfer modeling of a ribbed surface of an internal cooling channel.

The proper functioning of the model was validated through a benchmark multi-objective analytical test case. The superior performance of the online surrogate training mode against the corresponding offline mode was proved as well. The results for both test cases showed that the algorithm is able of approximating the real optimal Pareto front particularly for the case of the Gaussian models coupled with the Expected HyperVolume Improvement infill strategy. Furthermore, among the Gaussian models, Co-Kriging showed sufficient good prediction capabilities while the computational time needed was 57% less than the Kriging surrogate model. Thus, the multi-fidelity surrogate models coupled with a sophisticated infill strategy, which allows balanced exploration and exploitation of the metamodel, were considered as the best option in the present study.

Further investigation of the Support Vector Regression (SVR) models regarding the uncertainty measures of their predictions will improve their performance within an optimization framework. This is suggested as a subject of future research since the performance of the SVR models within this study and their capabilities in general are quite promising.

REFERENCES

[1] D. R. Jones, M. Schonlau, W. Welch, Efficient Global Optimization of Black Box Functions. *Journal of Global Optimization*, **13**(4): 455-492, 1998.

[2] M. T. M. Emmerich, K. C. Gianakoglou, B. Naujoks, Single and Multiobjective Evolutionary Optimization Assisted by Gaussian Random Field Metamodels. *IEEE Transactions on Evolutionary Computation*, **10**(4): 421 439, 2006.

[3] I. Hupkens, M. Emmerich, A. Deutz, Faster Computation of Expected Hypervolume Improvement. *arxiv:1408.7114v1[cs.Ds]*,2014.

[4] I. Hupkens, A. Deutz, K. Yang, M. Emmerich, Faster Exact algorithms for Computing Expected Hypervolume Improvement. *In Proc. Part II EMO Conf.*,Guimares, March, 2015.

[5] I. Couckuyt, D. Deschrijver, T. Dhaene, Fast Calculation of Multio-bjective Probability of Improvement and Expected Improvement Criteria for Pareto Optimization. *Journal of Global Optimization*, **60**(3): 575-594, 2014.

[6] O. Labb, Large-eddy-simulation of flow and heat transfer in a ribbed duct. *Computers and Fluids*, **76**, 23-32, 2013.

[7] Y. T. Yang, P. J. Chen, Numerical Optimization of Turbulent Flow and Heat Transfer Characteristics in a Ribbed Channel. *Heat Transfer Engineering*, **36**(3): 290-302, 2015.

[8] G. Xie, S. Zheng, W. Zhang, B. Sundn, A Numerical Study of Flow Structure and Heat Transfer in a Square Channel with Ribs Combined Downstream Half-Size or Same-size Ribs. *Applied Thermal Engineering*, **64**(2): 289-300, 2013.

[9] M. D. Morris, T. J. Mitchell, Exploratory Designs for Computer Experiments. *Journal of Statistical Planning and Inference*, **43**(3): 381-402, 1995.

[10] K. Deb, A. Pratap, S. Agarwal, T. Meyarivan, A fast and Elitist Multi-Objective Genetic Algorithm: NSGA-II. *IEEE Transactions on Evolutionary Computation*, **6**(2): 182-197, 2002.

[11] F. A. Fortin, F. M. De Rainville, M. A. Gardner, M. Parizeau, C. Gagn, DEAP: Evolutionary Algorithms made Easy. *Journal of Machine Learning Research*, **13**, 2171-2175, 2012.

[12] D. G. Krige, A Statistical Approach to Some Basic Mine Valuation Problems on the Witwatersrand. *Journal of the Chemical, Metallurgical and Mining Engineering Society of South Africa*, **52**(6): 119-139, 1951.

[13] A. I. J. Forrester, A. Sobester, A. J. Keane, Multi-fidelity Optimization via Surrogate Modeling. *Proceeding of the Royal Society A*, **463**(2088): 32513269, 2007.

[14] A. J. Smola, B. Schlkopf, A Tutorial on Support Vector Regression. *Statistics and Computing*, **14**(3): 199-222, 2004.

[15] L. Le Gratiet, J. Garnier, Recursive Co-Kriging Model for Design of Computer Experiments with Multiple Levels of Fidelity. *International Journal for Uncertainty Quantification*, **4**(5): 365-386, 2014.

[16] J. Gray, K. T. Moore, B. A. Naylor, OPENMDAO: An Open Source Framework for Multidisciplinary Analysis and Optimization. *In Proc. AIAA/ISSMO Conf.*, Atlanta, June, 2014.

[17] K. Deb, L. Thiele, M. Laumanns, E. Zitzler, Scalable Multi-objective Optimization Test Problems. *In Proc. CEC 02 Conf.*, Honolulu, May, 2002.