Optimizing Mesh and CFD Simulation Performance: A Multivariate Analysis Approach

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Abstract. The Design of Experiments (DOE) methodology plays a fundamental role in the parameterization of Computational Fluid Dynamics (CFD), especially in mesh optimization and simulation accuracy. Using DOE, researchers can identify which mesh parameters influence flow quantities, leading to better numerical accuracy and design decisions based on CFD results. Within DOE methodologies, Response Surface Methodology (RSM) is used for experiment planning and response analysis, allowing optimization of process parameters and providing a systematic approach to designing experiments and analyzing results. Multiobjective optimization (MOP) was carried out, using weight assignment strategies based on the Design of Mixtures of Experiments (MDE) to understand the behavior of the functions. The systematic approach adopted the planning of experiments, assessment of significance between independent variables, identification of individual optimal points and use of the Payoff matrix. This approach made it possible to identify how each function operates from the perspective of weighing needs, validating the methodology.

Keywords: Design of Experiments,Computational Fluid Dynamics, Mixture Design Experiments, Response Surface Methodology.

1 Introduction

The Design of Experiments (DOE) methodology plays a fundamental role in the parameterization of Computational Fluid Dynamics (CFD), particularly when dealing with mesh optimization and simulation accuracy.[1], [2], [3], [4], so that by using DOE, researchers can identify which mesh parameters can influence flow quantities, leading to better numerical accuracy and design decisions based on CFD results[1]. Thus, this methodology has been applied in various fields, such as optimizing turbomachinery design, investigating optimal pump designs, and predicting solid particle erosion in pipe elbows through CFD simulations and DOE techniques.[2], [3]. Therefore, the integration of DOE with CFD allows the efficient use of computational power to predict flow effects, cavitation, optimize port layouts for combustion systems and determine the ideal lengths of tube sections, both thermodynamically and hydraulically. ultimately improving the overall performance and efficiency of the systems under study[3], [4], [5].

Within DOE methodologies, Response Surface Methodology (RSM) is a statistical and mathematical technique used for planning experiments and analyzing responses[6], [7], [8]. RSM allows researchers to optimize process parameters by relating independent input variables to the response, providing a systematic approach to designing experiments, analyzing results, and approximating variable-based responses. RSM's basis in principles of regression and variance analysis allows the development and optimization of processes or products with satisfactory accuracy, making it a valuable tool for various fields of engineering and statistics[8], modeling through responses to functions defined as objectives.

With a group of functions, a multiobjective optimization problem (MOP) is given, so that the resolution of all functions is required, which in practice does not occur. In normal situations, the improvement of one response directly affects the others, especially when the directions of improvement are opposite, such as maximization and minimization. In this way, the weight attribution strategy based on the Design of Mixtures of Experiments (MDE) is used, so that, as suggested by Das and Dennis[9]that the number of subproblems that must be solved in Normal Boundary Intersection depends on the objective functions considered in the MOP problem and the uniform spacing used between the weights. Therefore, defining the weights helps the decision maker to choose the best strategy for each situation.

Thus, the study aims to present new parameterization and mesh analysis tools, to promote the accuracy of results with lower process costs, focusing on the choice of objective functions suitable for multiobjective optimization (MOP). In order to use advanced techniques, such as the Response Surface Methodology (RSM), the Normal Boundary Intersection (NBI) and the Design of Mixture Experiments and analysis of optimal results, we seek to develop methods that allow a more accurate analysis and efficient analysis of meshes and post-processing responses, taking into account a multivariate or multiobjective analysis. This approach seeks to significantly improve the quality of the solutions obtained, in addition to offering a better understanding of the trade-offs between different objectives.

2 Theoretical Background

When dealing with planning of experiments (DOE) methodologies, there are several arrangements that use factors with upper and lower limits to facilitate mapping of the solution region, with techniques including full factorial arrangements, fractional factorials, Taguchi and surface methodology. response (RSM)[10]. RSM is a method that creates approximate quadratic functions through a sequence of experimental setups to identify areas of curvature[11], so that, after the modeling and experimentation phases, the developed functions are incorporated into non-linear optimization algorithms, with or without restrictions.

Thus, a complete second-order quadratic polynomial, described in eq. (1), is the most used option for nonlinear stochastic models[12]. To reduce complexity, it is advisable to limit the number of independent variables chosen to up to 5, in addition, the models can be used with optimization algorithms to determine the ideal conditions to maximize or minimize the system response.

$$f(\mathbf{x}) = \beta_{0p} + \sum_{i=1}^{k} \beta_{ip} x_i + \sum_{i=1}^{k} \beta_{iip} x_i^2 + \sum\sum_{i<j} \beta_{ijp} x_i x_j + \varepsilon \quad \forall p = 1,2,\dots,r \tag{1}$$

Where k is number of independent variables; β_0 the function-independent term; β_i the coefficients referring to the linear effect; β_{ii} the coefficients referring to the quadratic effect; β_{ij} the coefficients referring to the interaction effects measured between the input variables x_i and x_j, and p denoting the number of objective functions considered.

In possession of the p objective functions, it is noted that the functions rarely present significant curvatures, promoting a search for these curvatures from linear models resulting in a multiobjective optimization problem with inequality restrictions, as presented in eq. (two).

$$Minimize\ f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_p(\mathbf{x}) \qquad Subject\ to: g_j(\mathbf{x}) \leq 0, j = 1,2,\dots,m \tag{2}$$

In general, the objective of optimization in this case is to determine the direction that leads to the region of maximum or minimum, as there is no single solution that minimizes all functions to be analyzed simultaneously, considering that a set of individual gradients helps to balance the directions of improvement of these responses by replicating the gradient vector method (GRG) for each individual response.

Thus, the concept of Pareto Frontier (Figure 1) is often associated with MOP, being essential for carrying out equilibrium analysis, in which, according to its concept, it proposes that the frontier points are the set of non-dominated from objective space[13], so that one cannot be improved while the other is not worsened.

To draw the curve of Pareto-optimal points, the Normal Boundary Intersection (NBI) method, developed by Das and Dennis, is used.[9], which thoughtfully aggregates all objective functions through weights, considering specific targets and scaling individual functions, promoting the ability to present uniform and continuous boundaries regardless of the distribution of weights.

The individual optimal points, as well as the effects that these points have on related functions, are the targets of the model and are known as the results of the Payoff matrix. The utopia point, or optimal point of a function in bold, and the Pseudo-Nadir points (points contrary to utopia), are the anchor points of this matrix in Tab. 1, considering that we will work with more than two functions goal.

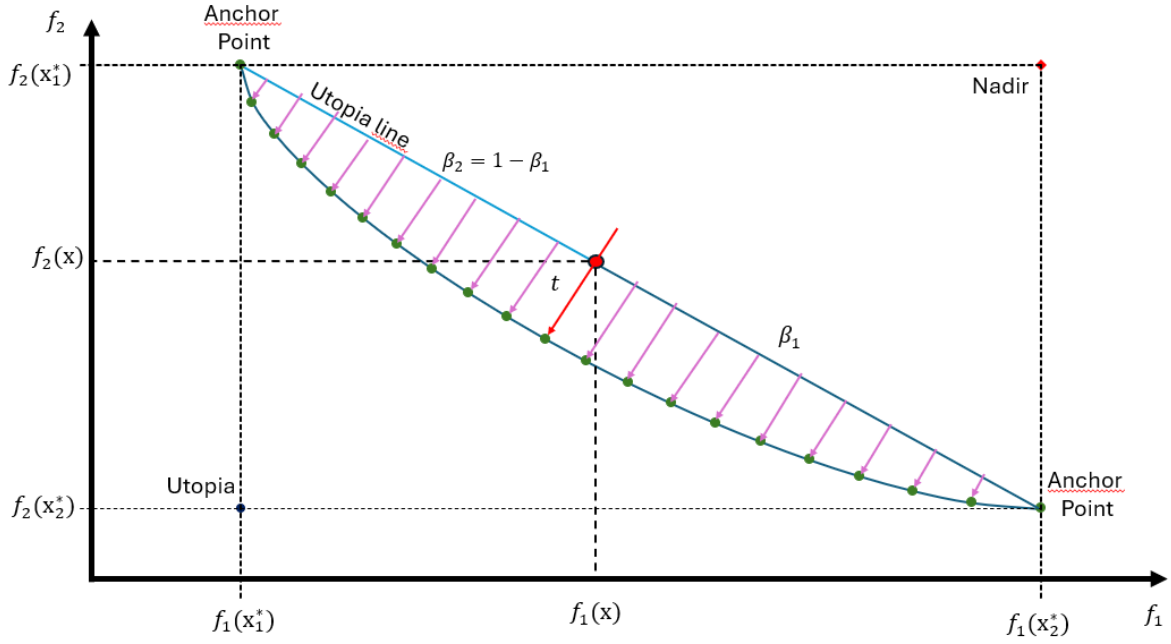

Figure 1. Pareto Frontier.

Table1. Payoff Matrix.

$$\begin{vmatrix} f_{11}^{U}(\mathbf{x}) & f_{12}^{PN}(\mathbf{x}) & f_{13}^{PN}(\mathbf{x}) \\ f_{21}^{PN}(\mathbf{x}) & f_{22}^{U}(\mathbf{x}) & f_{23}^{PN}(\mathbf{x}) \\ f_{31}^{PN}(\mathbf{x}) & f_{32}^{PN}(\mathbf{x}) & f_{33}^{U}(\mathbf{x}) \end{vmatrix}$$

Considering then that the values in Tab. 1 refer to the results of individual optimizations, it is necessary to use multiobjective optimization (MOP) approaches. The approach presented here considers the analysis of the multivariate Mahalanobis distance between a vector of functions f($\mathbf{x}$) and a centroid vector of individual targets ($\mathbf{\Phi}$), so that, relating the response vector ($\mathbf{z}(\mathbf{x})$), the matrix $\mathbf{X}$ and the variance-covariance matrix ($\mathbf{\Sigma}$), forming a global function F($\mathbf{x}$).

$$Minimize\ \mathrm{F}(\mathbf{x}) = \{[\mathbf{f}(\mathbf{x}) - \mathbf{\Phi}]^T\{[\mathbf{z}^\mathbf{T}(\mathbf{x})(\mathbf{X}^\mathbf{T}\mathbf{X})^{-1}\mathbf{z}(\mathbf{x})\mathbf{\Sigma}]^{-1}\}[\mathbf{f}(\mathbf{x}) - \mathbf{\Phi}]\}^{1/2} \quad (3)$$
$$Subject\ to\text{: } \mathrm{g}(\mathbf{x}) = \mathbf{X}^\mathbf{T}\mathbf{X} \leq \rho^2$$

Where: ρ is the radius of the solution region.

To define the centroid vector targets, the use of a special arrangement called the Experiment Mixture Arrangement (MDE) is considered, in which the arrangement is generated through independent factors that are considered as proportions of different components. For the case study, the independent factors will be defined by the Payoff matrix, and the arrangement will define with which weights (w_1, w_2 and w_3) that the mixture of functions will promote better results.

3 Case Study on Parametric Mesh Analysis Using MOP and MDE

3.1 Model of Simulation

This study is based on the model developed by Azevedo[14]which involved the modeling of the entire test bench combined with the design of a hydraulic machine adaptable to the bench, seeking the best performance. The author designed several interconnected domains, considering input elbows, regularization duct according to IEC 60193[15], inlet bulb, distributor, rotor, shaft outlet, and reservoir return outlet elbow, however for this work, only the inlet piping to the bulb will be used, as shown in Fig. 2.

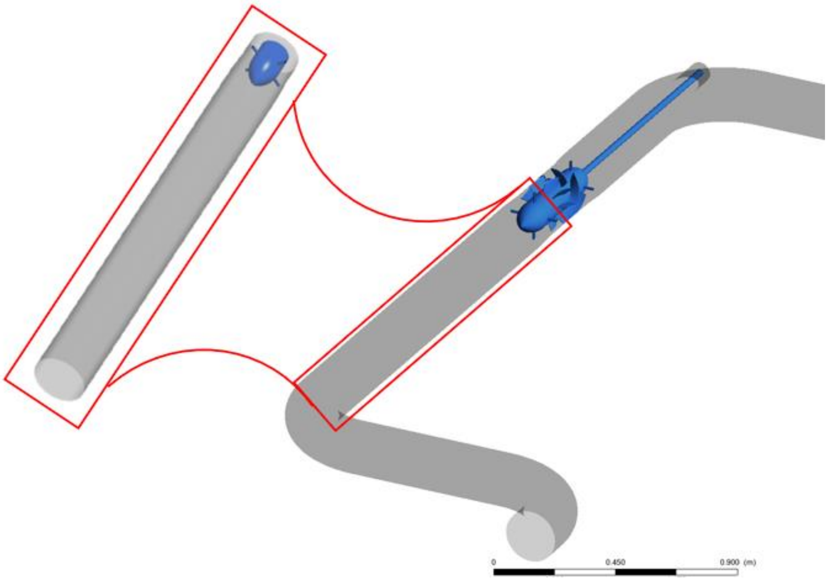

Figure 2. Virtually modeled experimental test bench.

To reduce simulation time, and because it is a symmetric modeling, the study also planned to use only a quarter of a circle to generate the meshes, using a periodic one, which can be rotated to understand the complete flow.

3.2 Parameterization of Mesh Model

Following the experiment planning methodology, and more specifically, RSM, five independent variables were used in the study as input, being: the predefined size in millimeters for volume (MV), for the entrance surface (ME), exit surface (MS), inlet mass flow rate ($\dot{m}$) and residual convergence criterion by RMS (CC) in the simulation stage.

For the standard arrangement, due to the established limits, the radius of the solution region was changed to ρ=0.5, which defined the factorial, axial and central points of the model presented in table g. The parameterization model involved the use of Central Composite Design (CCD) structured with two levels and five parameters (2^{k-1}=16), incorporated by ten axial points (2k=10) and six central points (CP=6), considering three replicates, thus considering ninety-six total experiments.

Table 2. Independent variables.

Symbol	Unit	Experimental Levels				
		-0.500	-1.000	0.000	1.000	0.500
MV	mm	2.125	1.500	2.750	4.000	3.375
ME	mm	2.125	1.500	2.750	4.000	3.375
MS	mm	2.125	1.500	2.750	4.000	3.375
$\dot{m}$	kg/s	25.574	22.455	28.693	34.930	31.811
CC	[-]	$3.25\text{x}10^{-5}$.	1.00×10^{-5}	5.5×10^{-5}	1×10^{-4}	7.75×10^{-5}

3.3 Multiobjective Functions and Their Characteristics

The use of RSM results in a group of objective functions, given by eq. (1), for defined answers. In this work, pre-processing responses were used, considering the number of elements generated in the meshes (N_{el}); processing, considering the mesh generation and simulation time, given as total time (T_t); and post-processing, considering the Reynolds number (Re) as a response item, which involves specific mass library data, dynamic viscosity, exit velocity and pipe diameter.

The initial result of these analyzes results in the objective functions of each response, and from this it is possible to find the Payoff matrix of their individual optimal functions, analyzing how each optimal response affects the adjacent ones, with the numbers in bold being the Utopia points, and the others, the Pseudo-Nadir, checking what was presented in the theory.

Table 3. Payoff matrix of functions

3.9154	10.8821	6.5341
1.8369	**4.8300**	2.7957
1.3239	1.3260	**1.4698**

Note: N_{el} (second line) and Re (third line) are presented with 10^6 and T_t (first line) with 10^1.

Note that the aim of the individual objectives is to minimize the execution time, so the utopia is 3.9154x10^1 minutes, maximizing the number of elements, with 4.8300x10^6 elements and maximizing the Reynolds number in the flow.

3.4 Mixture Arrangement for Analyzing Function Weights

With the Payoff matrix presented, it is now possible to define the target points that the mixture function will work on, and how the weights of each function affect the results. For this work, the Simplex-Lattice Design {3,2} with CP=1 was used for arrangement, and the target components presented in Tab. 3. The objective function is defined by eq. (3), in addition to the individual responses of each function, to understand how each weight affects the response. The data composition format was arranged as in Tab. 4., with weights of 0, 1, 0.5 and 0.33, for targets X1, X2, X3 that refers to Payoff Matrix.

Table 4. Example Mixture Arrangement.

w_1	w_2	w_3	X1	X2	X3	F(**x**)
0 to 1	0 to 1	0 to 1	3.9154 or 10.8821	4.8300 or 1.8369	1.4698 or 1.3260	

4 Discussion of Results

Objective functions, as they are quadratic functions, can have three types of specific concavities for statistical analysis, namely concave, convex or saddle. For a univariate function analysis, understanding its convexity allows you to understand the behavior of the variables, to prevent whether the study is a maximization, minimization or specific target problem. In Fig. 3, the contour plot of the three objective functions is presented, with hot colors being close to the plane while cold colors are moving away from the plane. Of the three functions presented, it is possible to note that Reynolds is a saddle function, while Time and Elements are convex functions.

Considering then a multiobjective analysis, that is, understanding the relationship that each of the objective functions has under the weight of a global function, it is possible to observe in Fig. 3, the behavior that the variation of these weights causes on these functions. In the case of a global minimization function, it is possible to note that the number of elements is more relevant, as is the simulation time.

Furthermore, understanding the space in which the solution is viable is of paramount importance, that is, because it is a problem with several functions, when projected under the same surface, and considering the upper and lower limits defined by the decision maker, A solution area is found that is the result of the convergence between the objective functions, presented in Fig. 4. This is the region in which it defines the capacity and possibility of working with the variability of the functions and defining the best optimum point of the problem. To solve the problem, one of the points of greatest predicted optimization of the problem, that is, minimization of F(x), contains the weights and functions presented in Fig. 3.

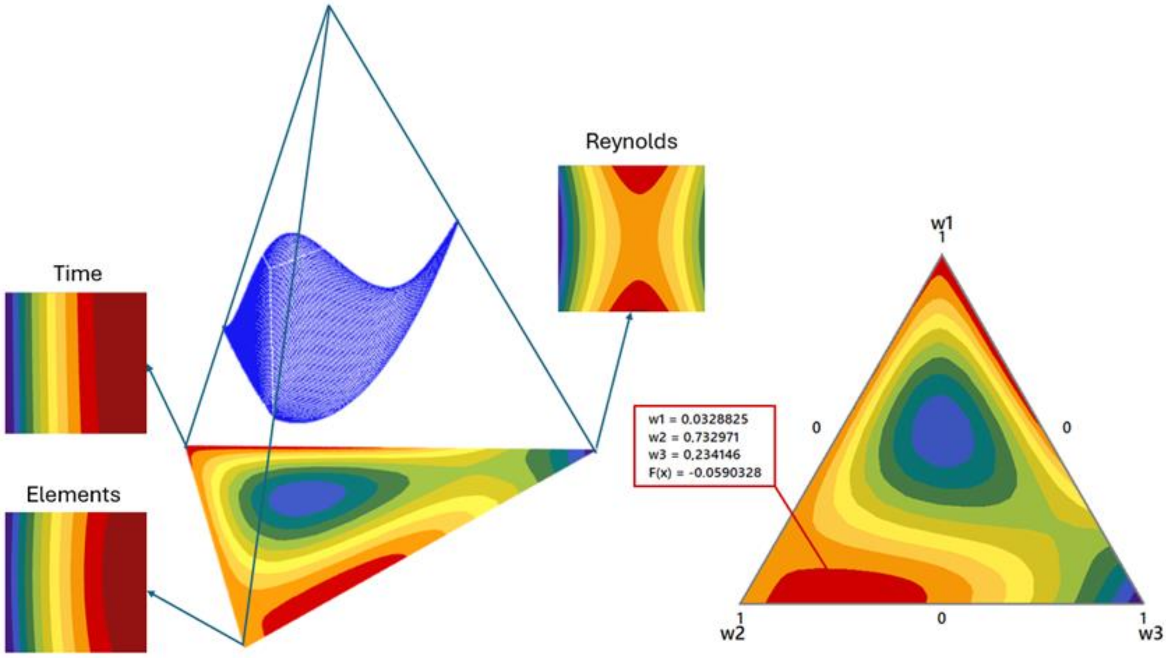

Figure 3. Mixture analysis results

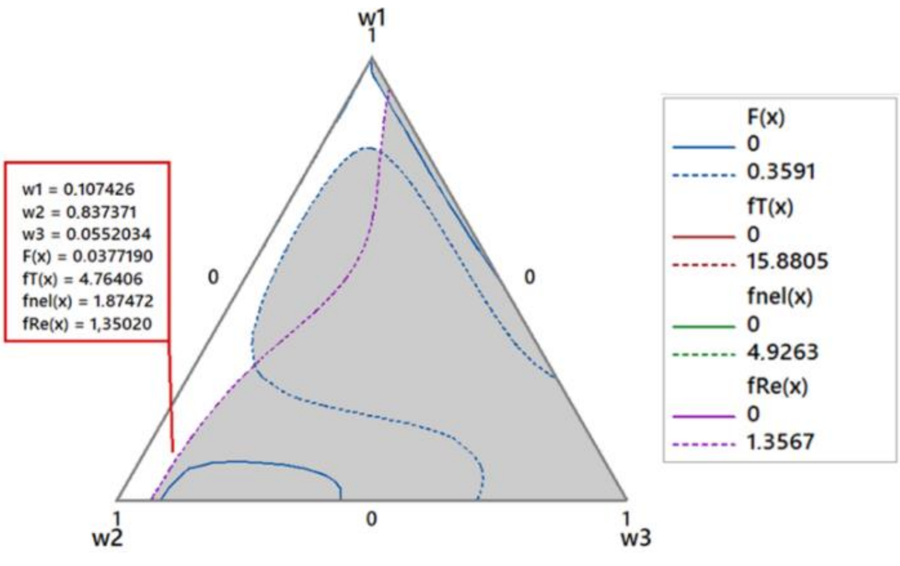

Figure 4. Overlaid Contour Plot.

5 Conclusions

The objective of this work was to describe experimental planning tools and more specifically, the response surface methodology for analyzing and parameterizing three-dimensional model meshes for simulation in Ansys-CFX.

Furthermore, the aim was to understand the behavior of the meshes, directly linked to the number of elements.

The processing time and the Reynolds number as a post-processing response influenced the precision capacity with shorter processing time.

The tools, in turn, present the possibility of analyzing the behavior of functions, promoting a gain for simulation engineering in terms of forms of processing study, cost reduction, increased precision and more conscious decision-making.

Therefore, understanding this behavior allows the construction of a strategy that best suits the needs of companies, consultants and engineers in general.

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