

Flexibility Assessment via Affine Bounds Evaluation

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ABSTRACT

Process design deals with the problem of finding the best process set-up, subject to a set of constraints defining the design space (D_{Sp}). This selection is guided primarily by economic considerations. Flexibility may also play an important factor in process design, since it embodies “how far” from the design space’s bounds are the candidate optimal designs, which in some cases may lead to off-spec products. This work proposes a novel approach for flexibility assessment. In design problems where the design space is constrained by a set of affine bounds, flexibility may be expressed either as the minimum or the maximum distance with respect to the feasible (design) space bounds. For any point in the D_{Sp}, the minimum distance provides a good indicator on the minimum flexibility, as the direction that represents the highest risk of violating the constraints. An analogous conclusion can be drawn between the maximum distance and maximum flexibility. These distances can be computed exactly via geometrical approaches, enabling the calculation of a minimum-based and maximum-based flexibility metrics for all points in the D_{Sp}. This class of problems are in fact multiparametric programming problems as the goal is to obtain comprehensive flexibility maps, rather than investigating unique points in the D_{Sp}. In the case of minimum flexibility, their solutions comprise: (i) a set of critical regions defining a convex hull within the D_{Sp} (each associated with a unique nearest bound of the feasible space), (ii) the corresponding optimizer functions (projection at nearest bound), and (iii) objective functions (minimum distance). A novel framework is under development for this class of problems. It enables a new paradigm for flexibility assessment, which can be applied to design problems of any dimension. Complexity is significantly reduced in comparison with the classic multiparametric programming approaches, since only a limited number of active sets need to be considered during solution calculation.

Keywords: Process Design, Flexibility, Multiparametric Programming

INTRODUCTION

Process design is inherently complex, often requiring the need for balancing conflicting objectives across different operational levels. Engineers must navigate physical constraints and specifications which delineate the feasible space within which design decisions can be made [1]. Within this context, process feasibility can be defined as the adherence to a set of predefined constraints during operation. To ensure processes designed are capable of adhering to the constraints, a quantitative measure for process flexibility is required. Swaney and Grossmann (1985) [2] initially addressed this by defining the flexibility index problem, which quantifies the ability

of a process to operate within the feasible region under uncertainty. The flexibility index problem aims to identify the size of the largest hyperrectangle that can be inscribed within the feasible space. This concept serves as a crucial metric for determining how robust a process design is against variability in operational parameters and external conditions.

Numerous works have built upon the flexibility index problem to solve complex design and operational challenges. For example, Pistikopoulos and Mazzuchi (1990) [3] introduced a stochastic framework for the flexibility index to quantify the impact of multivariate uncertainty distribution on process flexibility. Kabatek and Swaney (1992) [4] proposed an improved branch-and-bound

algorithm to identify how control actions can compensate for the worst-case scenario problems. In recent years, more work has focused on identifying the full feasible space directly – known as design space identification (DSI). Banerjee and Ierapetritou (2005) [5] proposed to use geometrical envelopes (alpha shapes) for DSI based on the feasibility function. Sachio et al (2023) [6] developed three strategies for constructing alpha shapes, integrating process knowledge and data-driven interpolation to reduce computational effort.

To reduce the computational demand from model simulation, several works have proposed to use data-driven approaches to directly approximate the feasibility function. In this way, the design space is represented by the binary classifier function which indicates the feasibility of an input combination. For this, kriging-based surrogate modelling [7], adaptive sampling techniques [8], and artificial neural networks [9] have been proposed to approximate the classifier function. Such approaches are applicable to high dimensions; however, they do not provide a quantitative measure of process flexibility.

This work builds upon existing foundations in design space identification and feasibility analysis. Specifically, we highlight two key aspects: the process-specific nature of flexibility boundaries, which may not align with box-like assumptions, and the need for flexibility metrics that quantify not just the distance to boundaries but also the variation of process flexibility with this distance. To address these challenges, we propose a novel methodology that leverages multiparametric programming (mp) to integrate design space identification with flexibility analysis. To our knowledge, this is the first application of a mp formulation for this combined problem. Additionally, we introduce two types of flexibility metrics to assess constraint sensitivity and the dependency of average process flexibility on boundary proximity.

METHODOLOGY

In this work, we consider design spaces defined via a set of affine inequality constraints:

$$Ax \leq b \quad (1)$$

where x is the vector of design variables of size n , and where A and b are a constant matrix and vector, respectively, defining the m bounds of the feasible space. It is assumed that Equation 1 defines a closed convex hull. We denote any design x satisfying Equation 1 as θ , and the full set of θ as the design space Θ .

The goal of this work consists of computing the minimum and maximum distances between all θ in Θ and the corresponding points at the bounds of Θ . Each of these distances are directly related to the minimum and maximum flexibilities: the former/latter concerns the nearest/furthest point at the bounds of the design space with

respect to a given θ , and represents, in principle, the highest/lowest risk of violating its bounds.

For design spaces formulated as a set of linear bounds as in Equation 1, the nearest point to a given θ is found when a single bound is active; conversely, the furthest point is found at a corner of the design space. A geometrical motivation is depicted in Figure 1.

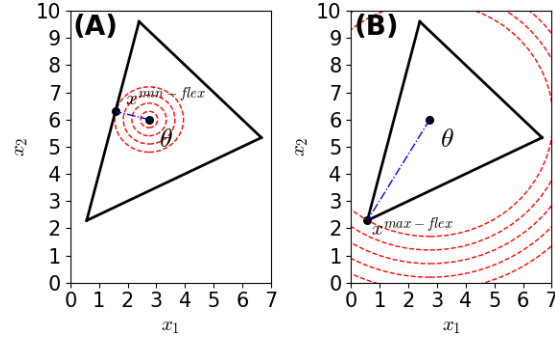


Figure 1: 2D illustration of minimum (A) and maximum (B) distances between a given design θ and the bounds of the feasible space as flexibility indicators.

The nearest point to θ (Figure 1A) is obtained by defining the smallest hypersphere centered on θ , such that it includes a unique point – $x^{\min\text{-flex}}$ – at a single bound of the design space. At $x^{\min\text{-flex}}$, the hypersphere is tangent to the single active bound, or, in other words, the normal vector connecting θ to $x^{\min\text{-flex}}$ captures the minimum distance to the bounds. Any combination of the single active bound with one or more bounds of Θ defines a more constrained subspace and cannot contain any point nearer to θ . As a result, the nearest point to any θ at the design space's bounds must conform to this scenario.

The furthest point is obtained by defining the largest hypersphere with center in θ , such that n bounds of Θ are simultaneously active at $x^{\max\text{-flex}}$ (Figure 1B). By relaxing this condition to include a smaller number of bounds, a less constrained subspace is obtained which necessarily includes points nearer to θ . As a result, the furthest point to any θ must conform to this scenario.

These two extreme scenarios concerning flexibility and a mathematical framework for their calculation are discussed in sequence.

MINIMUM FLEXIBILITY

Minimum flexibility is defined in this work as the minimum distance between a given θ and the bounds of Θ . The route for its calculation relies on the calculation of all minimum distance functions to each of the m bounds of the feasible space individually. These are defined as the partial minimum flexibilities.

Partial minimum flexibilities

For design spaces bounded consistently with

Equation 1, the partial minimum flexibilities are computed using simple geometric arguments. Given a design θ and the j^{th} bound of the design space – denoted as $A_j x \leq b_j$ – the nearest point to θ at the j^{th} bound is found via projection:

$$x^{\text{proj},j} - A_j' l^j = \theta \quad (2)$$

$$A_j x^{\text{proj},j} = b_j \quad (3)$$

where A_j is the j^{th} row vector of A and A_j' is the transpose of A_j (column vector), $x^{\text{proj},j}$ is the point at the j^{th} bound of Θ projected from θ along a normal vector to this bound. l^j is a multiplicative factor in Equation 2 defining the depth of the projection. Equation 3, enforces that $x^{\text{proj},j}$ is at the j^{th} bound to obtain the unique nearest point.

Equations 2 and 3 may be written equivalently in a matrix form (Equation 4), and an explicit solution for $x^{\text{proj},j}$ and l^j (Equation 5) is obtained as follows:

$$\begin{bmatrix} I & -A_j' \\ A_j & 0 \end{bmatrix} \begin{bmatrix} x^{\text{proj},j} \\ l^j \end{bmatrix} = \begin{bmatrix} \theta \\ b_j \end{bmatrix} \quad (4)$$

$$\begin{bmatrix} x^{\text{proj},j} \\ l^j \end{bmatrix} = \begin{bmatrix} I & -A_j' \\ -A_j & 0 \end{bmatrix}^{-1} \begin{bmatrix} \theta \\ -b_j \end{bmatrix} \quad (5)$$

The inverse of the symmetric matrix in Equation 5 may be computed numerically or analytically. In this work we focus on the calculation of l^j since it enables a path for minimum distance calculation. For brevity, only the last row of this inverse matrix (at row $n+1$) is shown:

$$\left[\begin{array}{c|c} I & -A_j' \\ \hline -A_j & 0 \end{array} \right]_{n+1}^{-1} = \frac{[-A_{j,1} \dots -A_{j,n} \ -1]}{\|A_j\|^2} \quad (6)$$

Since l^j is defined as a multiplicative factor along the direction of the normal vector, it follows that the minimum distance between θ and the j^{th} bound of the design space – $d^{\text{min},j}$ – is obtained from the product of l^j and the norm of A_j . Combining Equations 5 and 6:

$$d_j^{\text{min}}(\theta) = \frac{[-A_{j,1} \dots -A_{j,n} \ b_j] \begin{bmatrix} \theta \\ 1 \end{bmatrix}}{\|A_j\|}, j = 1, \dots, m \quad (7)$$

Computation of minimum flexibility

For any given θ , and consistently with the analysis above, the minimum flexibility – d^{min} – is in fact the minimum of all partial minimum flexibilities. Mathematically:

$$d^{\text{min}}(\theta) = \min\{d_1^{\text{min}}(\theta), \dots, d_m^{\text{min}}(\theta)\} \quad (8)$$

In this work, a solution of this problem for all θ in Θ is required. This is achieved by enforcing the space of parameters via Equation 9 on Equation 8 to deliver a new problem statement. Together, they define a mp problem.

$$A\theta \leq b \quad (9)$$

This formulation is non-conventional in the context of mp, since m candidate optimal objective functions (per each of the m bounds of Θ) are enumerated a priori in

Equation 8, instead of a single objective function. This formulation is enabled by the analysis presented earlier, which narrows the optimal candidate active sets for minimum distance calculation to the m single constraint active sets and the corresponding distance functions via Equation 7. The authors are not aware of any algorithm for this class of problems, and the development of a more formal framework will be the subject of future work.

Yet, this problem formulation implicitly suggests a solution strategy as described in sequence. Firstly, we note that explicit expressions for the optimizer functions per optimal active set are not strictly required, though they can be obtained directly from Equation 5. All candidate optimal objective functions of the mp problem are calculated explicitly via Equation 7. To deliver the full solution of this problem it suffices to obtain the critical regions for all m single-constraint active sets. This is achieved via a set of optimality conditions and a set of feasibility conditions. The first kind of conditions results directly from Equation 7: by comparing all partial minimum flexibilities this can be achieved as follows:

$$d_{j_1}^{\text{min}}(\theta) \leq d_{j_2}^{\text{min}}(\theta), j_2 = 1, \dots, m, j_2 \neq j_1 \quad (10)$$

where $d_{j_1}^{\text{min}}$ corresponds to the minimum distance to the j_1^{th} bound, which must be lower than or equal to the minimum distances to the remaining bounds. This ensures that the subset of all θ in Θ via Equation 10 yield the minimum distance to this bound. Feasibility conditions must also be defined for critical region construction, which in this case match the bounds of Θ .

MAXIMUM FLEXIBILITY

Maximum flexibility is defined in this work as the maximum distance to the bounds of the design space for any given θ . The individual distances to all corners of Θ are the relevant candidates for the maximum flexibility, which are defined as the partial maximum flexibilities.

Partial maximum flexibilities

Given a design θ and the k^{th} corner of the design space – denoted as $\theta^{c,k}$ – the distance between them is computed trivially using the Euclidean norm:

$$d_k^{\text{max}}(\theta) = \|\theta - \theta^{c,k}\|, k = 1, \dots, t \quad (11)$$

where t denotes the total number of corners of Θ , which must be computed beforehand. For convenience the square of the partial maximum flexibilities is also presented below, where θ' denotes the transpose of θ :

$$\begin{aligned} (d_k^{\text{max}}(\theta))^2 &= \theta' \theta - 2\theta' \theta^{c,k} + (\theta^{c,k})' \theta^{c,k}, \\ k &= 1, \dots, t \end{aligned} \quad (12)$$

Computation of maximum flexibility

For any θ , the maximum flexibility – d^{max} – is the

maximum of all partial maximum flexibilities:

$$d^{max}(\theta) = \max\{d_1^{max}(\theta), \dots, d_t^{max}(\theta)\} \quad (13)$$

By combining Equations 9 and 13 a mp problem is defined: it must deliver the maximum distance to the bounds of Θ for all θ in Θ . Similarly to the case of minimum flexibility, the candidate optimal objective functions for each of the t corners are enumerated explicitly in Equation 13. To solve this problem, it suffices to compute the corresponding critical regions. The feasibility constraints are the bounds of Θ (Equation 9), and the optimality constraints are defined conceptually as follows:

$$d_{k_1}^{max}(\theta) \geq d_{k_2}^{min}(\theta), k_2 = 1, \dots, t, k_2 \neq k_1 \quad (14)$$

where $d_{k_1}^{min}$ corresponds to the maximum distance between θ and the k_1 th corner, which must be greater than the distance to all remaining corners of Θ . This would define a non-linear analytical statement for critical regions construction consistently with Equation 11; to restore linear dependence on the definition of critical regions, it suffices to use the square of the distance functions, enabling a fully equivalent, and more convenient condition (square terms θ cancel each other):

$$\theta' \theta - 2\theta' \theta^{c,k_1} + (\theta^{c,k_1})' \theta^{c,k_1} \geq \theta' \theta - 2\theta' \theta^{c,k_2} + (\theta^{c,k_2})' \theta^{c,k_2}, \quad k_2 = 1, \dots, t, k_2 \neq k_1 \quad (15)$$

RESULTS

To illustrate the calculation of the minimum and maximum flexibility maps, two 2D design spaces are presented next. Some notes on high-dimensional problems are presented at the end of this Section.

Square

We consider the following square design space:

$$\begin{bmatrix} -1 & 0 \\ 1 & 0 \\ 0 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leq \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \quad (16)$$

Minimum flexibility map

Firstly, the partly minimum flexibilities are calculated for each of the four bounds of the design space:

$$\begin{bmatrix} d_1^{min} \\ d_2^{min} \\ d_3^{min} \\ d_4^{min} \end{bmatrix} = \begin{bmatrix} 1.000 & 0.000 & 0.000 \\ -1.000 & 0.000 & 1.000 \\ 0.000 & 1.000 & 0.000 \\ 0.000 & -1.000 & 1.000 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ 1 \end{bmatrix} \quad (17)$$

Secondly, by comparing each of these distance functions (optimality conditions) and incorporating the bounds of the design space (feasibility conditions), the maps of critical regions for this problem are obtained.

Table 1: Critical regions for minimum flexibility in first example ($CR^A \theta \leq CR^B$).

Critical region	Active bound	$[CR^A \mid -CR^B]$
1	$\theta_1 = 0$	$\begin{bmatrix} -1.000 & 0.000 & 0.000 \\ 1.000 & -1.000 & 0.000 \\ 1.000 & 1.000 & -1.000 \end{bmatrix}$
2	$\theta_1 = 1$	$\begin{bmatrix} 1.000 & 1.000 & -1.000 \\ -1.000 & -1.000 & 1.000 \\ -1.000 & 1.000 & 0.000 \end{bmatrix}$
3	$\theta_2 = 0$	$\begin{bmatrix} -1.000 & 1.000 & 0.000 \\ 1.000 & 1.000 & -1.000 \\ 0.000 & -1.000 & 0.000 \end{bmatrix}$
4	$\theta_2 = 1$	$\begin{bmatrix} -1.000 & -1.000 & 1.000 \\ 1.000 & -1.000 & 0.000 \\ 0.000 & 1.000 & -1.000 \end{bmatrix}$

The map of critical regions is shown in Figure 2 (A). The flexibility in the full design space is also plotted as a heatmap (B). For this purpose, a grid of points within the design space were selected and the minimum distances calculated from the solution of the mp problem.

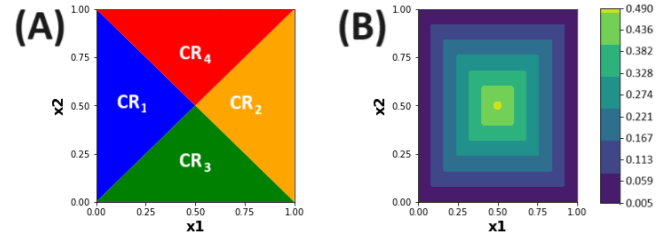


Figure 2: Map of critical regions (A) and flexibility design map (B) for minimum design flexibility - first example.

Note that, as expected, all critical regions are in the vicinity of the corresponding nearest bound. This map is useful to identify the nearest bound to any design; yet, by combining this information with the partial minimum distances in Equation 17, the resulting flexibility map (Figure 2B) provides very valuable insight into flexibility. For those points near the bound, the minimum distance is very low; conversely, for those points at the center of the design space, the minimum flexibility becomes increasingly higher. The largest value of the minimum flexibility is found at the center of the box ($\theta = [0.500, 0.500]$), where $d^{min} = 0.5$ for all active sets.

Maximum flexibility map

All corners of the feasible space are calculated from the interception of pairs of bounds. These are found at:

$$\begin{bmatrix} \theta^{c,1} \\ \theta^{c,2} \\ \theta^{c,3} \\ \theta^{c,4} \end{bmatrix} = \begin{bmatrix} 0.000 & 0.000 \\ 0.000 & 1.000 \\ 1.000 & 1.000 \\ 1.000 & 0.000 \end{bmatrix} \quad (18)$$

Then, the distance between θ and each of these corners is computed using Equation 11:

$$\begin{bmatrix} d_1^{max} \\ d_2^{max} \\ d_3^{max} \\ d_4^{max} \end{bmatrix} = \theta' \theta \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + \begin{bmatrix} 0.000 & 0.000 & 0.000 \\ 0.000 & -2.000 & 1.000 \\ -2.000 & -2.000 & 2.000 \\ -2.000 & 0.000 & 1.000 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ 1 \end{bmatrix} \quad (19)$$

At last, the critical regions for all corners are computed via Equations 14 and 15, as listed in Table 2.

Table 2: Critical regions for maximum flexibility in first example ($CR^a \leq CR^b$).

Critical region	Corner	$[CR^a -CR^b]$
1	$\theta = [0, 0]$	$\begin{bmatrix} 0.000 & -2.000 & 1.000 \\ -2.000 & 0.000 & 1.000 \\ 1.000 & 0.000 & -1.000 \\ 0.000 & 1.000 & -1.000 \end{bmatrix}$
2	$\theta = [0, 1]$	$\begin{bmatrix} 0.000 & -2.000 & -1.000 \\ -2.000 & 0.000 & 1.000 \\ 1.000 & 0.000 & -1.000 \\ -1.000 & 0.000 & 0.000 \end{bmatrix}$
3	$\theta = [1, 1]$	$\begin{bmatrix} 2.000 & 0.000 & -1.000 \\ 0.000 & 2.000 & -1.000 \\ -1.000 & 0.000 & 0.000 \\ 0.000 & -1.000 & 0.000 \end{bmatrix}$
4	$\theta = [1, 0]$	$\begin{bmatrix} 2.000 & 0.000 & -1.000 \\ 0.000 & -2.000 & 1.000 \\ -1.000 & 0.000 & 0.000 \\ 0.000 & 1.000 & -1.000 \end{bmatrix}$

The maps of critical regions and maximum design flexibility are illustrated in Figure 3.

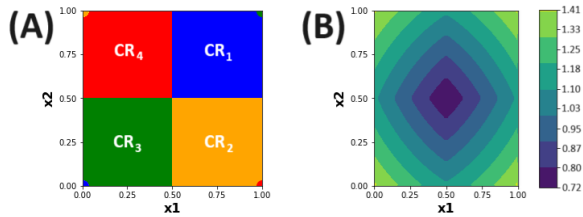


Figure 3: Map of critical regions (A) and flexibility design map (B) for maximum design flexibility - first example.

For each corner, the corresponding critical region is in the vicinity of the opposite corner as expected (all corners are highlighted in the same color as the matching critical region in Figure 3A). By combining this information with the partial maximum flexibilities in Equation 18, the maximum flexibility map is delivered as a heatmap in Figure 3B. This is continuous quadratic function of θ . Note that the contours in all critical regions are centered in the opposite, most distant corners. The highest maximum flexibilities are found at the corners, where the maximum distance to the bounds of the feasible space correspond to the opposite corners, as expected ($d^{max} = \sqrt{2}$).

Hexadecagon

We consider a second 2D example defined via a total of 16 bounds. Its shape will become clear from the analysis of Figures 4 and/or 5.

Minimum flexibility map

The partial minimum flexibilities were computed for all 16 bounds and the matching critical regions obtained by comparing them. For brevity, these are not listed, and only the maps of critical regions and minimum flexibility are shown in Figure 4.

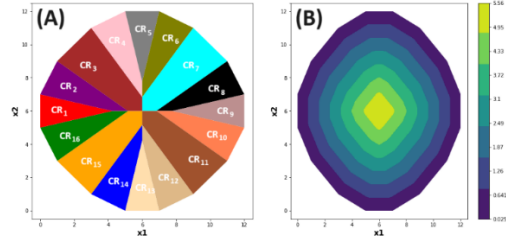


Figure 4: Map of critical regions (A) and flexibility design map (B) for maximum design flexibility - second example.

All critical regions extend from the corresponding nearest bound to the boundaries where the partial minimum distances equate those of a neighboring critical region. The minimum design flexibility is null at the bounds of the design space, and as expected increases towards the center of the convex hull. Closer to the center of the convex hull the contours progressively resemble more like a square which is consistent with critical regions 3, 7, 11 and 15 delivering the minimum distance in the vicinity of $x = [6.000, 6.000]$.

Maximum flexibility map

The partial maximum flexibilities and the corresponding critical regions for all corners were then calculated. For brevity, only the critical region and maximum flexibility maps are shown in Figure 5.

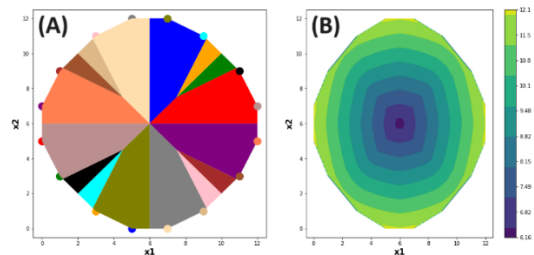


Figure 5: Map of critical regions (A) and flexibility design map (B) for maximum design flexibility - second example.

For convenience all corners are highlighted with the same color as the corresponding critical regions. A quick analysis confirms all regions are effectively the most distant to the matching corners. The flexibility map shows that the maximum flexibility increases from the center towards the bounds of the convex hull. Since there are a total of 16 corners, the contours are made of the individual quadratic contours, yielding a more complex, yet fully continuous, map.

Hypercubes (1D to 10D)

This methodology is particularly attractive for 2D design problems, for which heatmaps can be obtained to provide useful insights on design flexibility. However, it is not constrained by the size of x or even the number of constraints defining the feasible space. The same principles are directly applicable for any design space defined consistently with Equation 1, for which solutions in the format of Equations 17-19 and Tables 1 and 2 are obtained. In this case, for any given θ , the matching critical region must be identified and the minimum or maximum flexibilities determined to provide insights for design.

A total of 10 examples defining boxes between 1D and 10D were defined. These have been defined with the same structure as presented in the first example (Equation 16): restraining the design space between 0 and 1 in the relevant axes. All were successfully solved and validated by the methodology developed.

CONCLUSIONS AND FUTURE WORK

A new methodology for flexibility assessment in design spaces defined via a set of affine bounds is proposed in this work. The minimum and maximum design flexibilities have been defined as the minimum and maximum distances between a given design and the bounds of the feasible space. This information is useful for design purposes since it quantifies the risk of a given design not complying with the defined design space.

Minimum flexibility is closely related to the distances of individual bounds, while maximum flexibility is associated with the distances to the corners of these convex hulls. Based on this analysis a mathematical framework has been developed to solve problems of this class. Since flexibilities must be computed for all points in the design space, this kind of optimization problem is in fact a multiparametric programming problem. To solve it, the explicit functions for the partial minimum and maximum flexibilities must be calculated, from which the critical regions can be obtained from their comparison. Collectively, these partial flexibilities and the matching critical regions define the flexibility maps, which provide useful information for design. In 2D problems this is particularly relevant since these maps can be shown as heatmaps for effective assessment of flexibility in the full design space.

While the key principles of this methodology have been illustrated in practice, a formal theoretical framework including also the development of algorithms is required. Furthermore, we note that starting with the partial minimum and maximum flexibilities, it is possible not only to calculate the minimum and maximum flexibilities but more broadly, the minimum, average and maximum of these flexibilities, which correspond to a total of 6 potentially flexibility metrics complementing each other. A more detailed examination of the merits and usefulness of these cases will be addressed in our future work.

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