UNIVERSIDAD POLITÉCNICA DE MADRID

ESCUELA TÉCNICA SUPERIOR DE INGENIERÍA AERONÁUTICA Y DEL ESPACIO

**Efficient Design and Analysis of Multi-Fidelity Experiments for
High Dimensional Aerodynamic Data Space**

Doctoral Thesis for
Ph.D. in Aerospace Engineering

Guy Raoul Yondo Mine
Aeronautical Engineer

Madrid, September 28, 2018

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Departamento de Matemática Aplicada a la Ingeniería Aeroespacial

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Dr. Esther Andrés and Prof. Eusebio Valero

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Abstract

The critical impact of aerodynamic phenomena on the design and performance of modern transport aircrafts calls for their accurate numerical predictions. Until the advent of numerical methods and computing facilities, mainly wind-tunnel measurements and empirical methods were used, leading to fairly reasonable predictions, except in the transonic flight regime; a flight regime critical for high performance, known to encompass one of the most efficient regimes of flight and characterized by large shock motion for small Mach number variations. One of the most important requirement for aeronautical applications of computational methods in fluid dynamics being the capability to predict the steady flow past a configuration, it is therefore important to be able to calculate steady solutions of aerodynamic flows in transonic regime, where the formation of shock waves lead to the onset of drag rise and a drastic deterioration of the lift to drag ratio as we approach the sonic boom. While computational fluid dynamics solvers have accurately mimic the trends of the full-order aerodynamic models of a complete aircraft in all flight regimes, the associated high computational budget has prevented conceptual designers to fully integrate them into routine analysis loops. The simultaneous development of numerical methods and high performance computing algorithms has then suggested the use of alternative fast and cheap to evaluate approximations, reduced-order models, capable of retaining the dynamics and characteristics of the original full-order model behavior over the parameter space, while neglecting irrelevant features. Progresses in the field have triggered the interest of aircraft aerodynamicists because of the possibility to achieve numerous query analyses but also to combine different sources (CFD, wind tunnel and flight tests, empirical methods, etc), the idea being to achieve large speedups while maintaining an acceptable level of accuracy.

The primary aim of this research is to build hybrid surrogate model frameworks, combining multi-fidelity and projection-based surrogates, that would be efficient when applied to high dimensional nonlinear 'target' aerodynamics problems. Two single-fidelity and two multi-fidelity POD-based reduced order models are implemented in this thesis. Other contributions include the evaluation of two approaches of low-fidelity models generation and the problem posed by the ROM adaptation. To illustrate the use of the various algorithms, applications to the 2D NACA64A010 airfoil and 3D NASA Common Research Model are presented respectively for two and one design parameters. The results demonstrate that the choice of the snapshot matrices/sets (size and locations), the 'perturbations' in the snapshots (in partially converged CFD simulations when fusing data from different fidelity) influence the POD basis functions and therefore contribute to the error in the performance of the POD-based ROMs predictions (model

quality/accuracy). Moreover, the thesis underlines the necessity to monitor the convergence of the greedy procedure and to automatically detect the level of correlation between the full order models and the low models for a better performance of the ROMs.

Resumen

El impacto crítico de los fenómenos aerodinámicos en el diseño y el rendimiento de las aeronaves modernas de transporte requiere de predicciones numéricas precisas. Hasta aparición de los métodos numéricos y los equipos informáticos, se utilizaron principalmente mediciones de túnel de viento y métodos empíricos, lo que condujo a predicciones bastante razonables, excepto en el régimen de vuelo transónico; un régimen de vuelo crítico para el alto rendimiento, caracterizado por grandes cambios en las ondas de choque pequeñas variaciones en el número de Mach. Uno de los requisitos más importantes para las aplicaciones aeronáuticas de los métodos de dinámica de fluidos computacional es la capacidad de predecir el flujo constante en una configuración, por tanto, es importante poder calcular soluciones de flujos aerodinámicos en régimen transónico, donde la formación de ondas de choque conducen al aumento de la resistencia y a un deterioro drástico de la sustentación a medida que nos acercamos al estallido sónico. Mientras que solucionadores las herramientas software de dinámica de fluidos computacionales han imitado con precisión las tendencias de los modelos aerodinámicos de un avión completo en todos los regímenes de vuelo, el alto presupuesto computacional asociado ha impedido que los diseñadores conceptuales los integren completamente sus procesos de diseño. El desarrollo simultáneo de métodos numéricos y algoritmos informáticos de alto rendimiento ha sugerido el uso de alternativas rápidas y baratas para evaluar mediante aproximaciones, modelos de orden reducido, capaces de conservar la dinámica y las características del comportamiento original del modelo completo en el espacio de parámetros, mientras se desprecian las características irrelevantes. Los avances en este campo han despertado el interés de los ingenieros aerodinámicos debido a la posibilidad de realizar numerosos análisis pero también combinar diferentes fuentes con distinto nivel de fiabilidad y coste asociado (CFD, túnel de viento y pruebas de vuelo, métodos empíricos, etc.), con la idea de lograr grandes reducciones del tiempo mientras se mantienen un nivel aceptable de precisión.

El objetivo principal de esta investigación es construir un framework híbrido de modelos surrogados de multiple fidelidad, que serían eficientes cuando se aplican a problemas de aerodinámica no lineal y alta dimensión. En esta tesis se implementan dos modelos de orden reducido basados en POD de fidelidad simple y dos de fidelidad múltiple. Otras contribuciones incluyen la evaluación de dos enfoques de generación de modelos de baja fidelidad y el problema planteado por la adaptación ROM. Para ilustrar el uso de varios algoritmos, se presentan casos de validación para el perfil 2D NACA64A010 y el modelo de investigación común 3D de la NASA con dos y un parámetros de diseño respectivamente. Los resultados demuestran que la

elección de las matrices/conjuntos de muestras (tamaño y ubicaciones), las 'perturbaciones' en las instantáneas (en simulaciones de CFD parcialmente convergentes cuando se fusionan datos de diferente fidelidad) influyen en las funciones básicas de POD y contribuyen al error en el rendimiento de las predicciones de ROM basadas en POD (calidad / precisión del modelo). Además, la tesis subraya la necesidad de controlar la convergencia del procedimiento y detectar automáticamente el nivel de correlación entre los modelos completo y los modelos de orden reducido para un mejor rendimiento de los ROM.

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Guy Raoul Yondo Mine,

Madrid, September 28, 2018

Dedication

To my late sister **Christelle Marcelle Yondo**, who passed away at the beginning of my PhD.

As each day passes, I still sit and wonder why? why you were taken without a chance to say goodbye. Though I feel very weep inside of me, with tears running down my cheeks, quite difficult to simply say life goes on.

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Chapter 1

Introduction

1.1 Background and motivation

Designing complex aerodynamic systems is one of the challenges in aircraft engineering that demand significant resources allocation (computational budget, personnel, high performance computing environment, etc) as well as great amount of various analyses to help decide in the concepts that satisfy the design objectives and constraints, the technical requirements and best practices, the customer needs, etc. Aerodynamics in the design process typically impacts and need to be considered in the feasibility, concept, definition and development phases. High dimensional aerodynamic design problems (discretization in more than 3 spatial dimensions) require time consuming and computationally expensive simulations or physical experiments to evaluate the complex objectives functions and constraints for analysis, parametric studies or optimization. Moreover due to the broadness of the flight envelope while designing a new aircraft, the computational resources needed to support advanced-decision making in aerodynamic teams at the conceptual design phase is prodigious; The related aerodynamic systems can easily reach (and even exceed) an order of $\mathcal{O}(10^6)$ degrees of freedom (independent variables or parameters - dimension) for a full aircraft Navier-Stokes flow simulation, requiring wall-clock times in the order of hours or days (even on the latest computer clusters); therefore the need of robust/efficient (rapid/accurate) and reliable methods to be able to screen multiple aircraft configurations (cruise/high lift, control surface deflections, etc), flow solutions and flight conditions (Mach number, Angle of attack, etc), in order to pare down the curse of dimensionality, to gain a better insight into problems and identify the most genuine ones for further analysis in subsequent design stages.

Figure 1.1: Common research model.

Recent progresses in aircraft aerodynamics have witnessed the introduction, in real-time and many-query analyses, of surrogate-based approaches as rapid and cheaper to simulate models that address the challenges posed by the above-mentioned high dimensional aerodynamic models (High Dimensional Aerodynamic Model (HDAM), also known as full order aerodynamic models - Full Order Aerodynamic Model (FOAM)) and the restrained allocated computational budgets (time and storage). The many-query setting arises when the system is solved repeatedly for many different parameters and for various configurations, as occurs in design optimization, optimal control, multi-scale simulation and uncertainty analysis. The real-time scenario is often desired when the solution of the problem needs to be known very quickly under limited resources for a previously unknown parameter (example of routine analysis, control and nondestructive evaluation/parameter estimation). A relevant classification of surrogate models is given by Eldred and Dunlavy[1] who cluster them as data-fit (Data-Fit Model (DFM)), multi-fidelity (Multi-Fidelity Model (MFM)) and projection-based (also known as reduced-order models, Reduced-Order Model (ROM)) models. However, it is not clear from the literature review[2, 3, 4, 5, 6, 7, 8, 9] if the above-mentioned surrogates taken solely are suitable for aerodynamic analysis and optimization, and could fit the needs of the aircraft industry; therefore the need for hybrid frameworks encompassing advanced design of experiments, novel/efficient optimization cheap-to-evaluate hybrid surrogates characterized by a dimensionality reduction of the underlined system, with the governing equations (state variables) of the HDAM being projected onto a low-dimensional subspace that spans the main features (physics and dynamics) of the FOAM. Moreover, those hybrid surrogates shall take advantage of redundancies (in space/time/parameters), calibrate and/or fuse aerodata of different sources (Computational Fluid Dynamics (CFD), wind tunnel and flight tests, empirical methods, etc) and be able to model the complexity of major aerodynamic functions while preserving a satisfactory level of

accuracy.

1.2 Literature review

1.2.1 Terms definition and ground explanations

Following are defined and basically explained common terms that compose the vocabulary in design of experiments and surrogate modeling:

- **Experiment:** a test or a series of tests in which purposeful changes are made to the input variables or parameters of a system so that one may observe and identify the reasons for changes in the output response(s). Experiments are conducted in the field of engineering to minimize the time to develop new designs/products, to improve the performance/design/reliability of existing products, minimize the time spent in gathering data (speeding up a design process), screen the keys design parameters that significantly affect the performance, etc.
- **Design of experiments (Design of Experiments (DoE)):** the methodology of planning experiments so that appropriate data can be analyzed using methods that results in valid, objective and relevant conclusions. DOE allows experimenters to develop mathematical models that predict simultaneously the individual and interactive effects of input variables on output variables or responses in a process or system. Originally develop to construct response surfaces and to obtain a maximum amount of information from fewest experiments, DoE has evolved with the advent of numerical methods and computing facilities and nowadays encompasses simulation-based experiments (also known as design and analysis of computer experiments (Design and Analysis of Computer Experiments (DACE))).
- **Design space:** or parameter space is a subset of a dimensional space consisting of the set of all possible (constrained) values of the input variables or design parameter(s), which are allowable in a particular model. It characterizes the allowable parameter values and combinations of parameter values; therefore sometimes understood as or set of all possible design options
- **Design variable:** is a numerical input whose value can be freely varied by the designer to define a designed model.

- **Sampling:** a procedure that specifies a method used to generate samples. Each combination of generated parameter values is referred to as a sample or sample point.
- **Tuning:** code tuning or calibration of a computer model is the process of matching the computer model to the observed data by adjusting the unknown constants (or parameters) in the computer model
- **Black box:** a function for which the analytical form is not known and is generally assumed to be computationally expensive; also known as 'original' or objective function, full order model or high-dimension model. Typically a black-box function can be evaluated to obtain value, definiteness, (approximate)gradient, etc.
- **Surrogate model:** are 'cheap-to-evaluate' (static or dynamic) mathematical approximations that mimic the deterministic computationally expensive response or behavior of an original system over the complete or part of the design space. Building a surrogate model is posterior to performing an analysis at certain sample points in design space. Contrary to a static surrogate model, a dynamic surrogate model is based on past evaluations and is updated periodically.
- **Design optimization:** is the process of finding the best design parameters that satisfy the product design/process requirements (i.e. providing the necessary tools to move efficiently toward a design that is superior to all other alternatives). Engineers typically use design of experiments (DOE), statistics, and optimization techniques to evaluate trade-offs and determine the best design under given constraints.
- **Model selection:** estimating the performance of different models in order to choose the (approximate) best one.
- **Model assessment:** having chosen a final model, estimating its prediction error (generalization error) on new data.
- **Design:** consist in determining design parameters that lead to the best 'performance' of a product or system.
- **Cost:** or budget is any measure of the resources required to evaluate the black-box function(s). Cheap functions requires not much than ~ 1000 calls of the objective function. Expensive functions can only be evaluated few times, $\ll 200$ evaluations).
- **Training & validation set:** A model is fit on the training set and the fitted model is used to predict the responses for the observations in the validation set. In the validation

approach, only a subset of the observations, those that are included in the training set rather than in the validation set, are used to fit the model.

- **Curse of dimensionality:** refers to the problem of finding structure in data embedded in a highly dimensional space. In rough terms, the 'Curse' refers to the apparent impossibility of making calculations in situations where the number of design variables and possible outcomes is so large that it seems futile even to try to comprehend the problem in the first place. It can be understood as, in the absence of simplifying assumptions, the sample size needed to estimate a function of several variables to a given degree of accuracy (i.e., to get a reasonably low-variance estimate) grows exponentially with the number of variables.
- **Fusion:** allows to construct surrogate models using data of variable (levels of) fidelity.
- **Verification:** The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model (estimating the numerical solution error, etc). Verification provides evidence that the computational model is solved correctly and accurately.
- **Validation:** provides evidence that the mathematical model accurately relates to experimental measurements. Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.
- **Test error & training error:** the test error is the average error that results from using a statistical learning method to predict the response on a new observation, one that was not used in training the method. In contrast, the training error can be easily calculated by applying the statistical learning method to the observations used in its training. But the training error rate often is quite different from the test error rate, and in particular the former can dramatically underestimate the latter. The validation-set error provides an estimate of the test error. The validation estimate of the test error can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set. This suggests that the validation set error may tend to overestimate the test error for the model fit on the entire data set.
- **Fidelity:** denotes the degree to which a model captures the physics of a phenomenon of interest.
- **Objective function:** A criterion for best design (or goodness of a design) design variables or parameters that are chosen to describe the design of a system.

- **Constraint:** Constraints are important to the design process because they limit the size of a design space by forcing the designer to meet a well defined set of requirements. Constraints enable us to reject unacceptable alternatives, while objectives enable us to select among design alternatives that are at least acceptable a limit or restriction on the design's behaviors or attributes.
- **Dimensionality reduction:** projects points in a manifold of lower dimensional space while preserving the structure, a meaningful representation of reduced dimensionality. Ideally, the reduced representation should have a dimensionality that corresponds to the intrinsic dimensionality of the data (minimum number of parameters needed to account for the observed properties of the data). Dimensionality reduction mitigates the curse of dimensionality and other undesired properties of high-dimensional spaces. As a result, dimensionality reduction facilitates, among others, classification, visualization, and compression of high-dimensional data.
- **Model inadequacy:** accuracy of the mathematical model with respect to the truth physics.
- **High Dimensional Models (High Dimension Model (HDM)):** are constructed a priori, using local polynomial basis functions which do not know much about the dynamical system of interest
- **Parametric ROM:** are constructed using global basis functions which embody a posteriori information gathered from exercising the HDM offline to compute solution snapshots

1.2.2 Design of experiments

In the early beginnings, experiments were planned using[10]

- either the one factor/variable at a time (One Factor/Variable at a Time (OFAT or OVAT)) approach that not only failed to consider the interaction among the design variables (factors), but also appeared to be very expensive because of the significant amount of runs/tests required
- or the likely indefinite 'trial and error' approach, based on an attempt to find best guesses or sample points locations, with no guarantee to attain the latter.

As an alternative to bypass these limitations, DoE was originally introduced by Fisher and al.[11] in the beginning of the 20th century to plan and conduct experiments with the aim of understanding the probabilistic behavior of agricultural crops systems. At first, DoE[10, 12, 13] were only concerned with physical experiments, for which the basic principles of DoE (randomization, replication, and blocking)[10] established by Fisher for controlling noise and bias are applicable. Physical experiments means an experimenter 'physically' carries out the experiments (example of Wind Tunnel Testing - Wind Tunnel Testing (WTT)), that are more often corrupted by random errors ('noise') and consequently makes the data modeling complex.

With the advent of numerical methods and computing facilities, it became possible to design experiments through computer-based simulations. In contrast to physical experiments where the process looked into is stochastic, simulation-based experiments are deterministic, with no need of replication[10]. Sampling the design space, i.e. selecting a good set of data points (also called observations or training points or samples) became a key issue in computer-based simulations, with the prevailing goal of maximizing the amount of information gained from a limited number of samples. A detailed discussion on physical experiments versus simulation-based experiments is found in Kleijnen et al.[14].

Sampling techniques can be grouped into two main categories, namely Classical DoE (Classical Design of Experiments (CDoE))[10, 15, 16, 17, 18, 19, 20] and Modern DoE (Modern Design of Experiments (MDoE) or Design and Analysis of Computer Experiments - DACE in some literature)[11, 12, 17, 20, 21, 22, 23, 24, 25, 26]. Giunta et al.[27] and Gardner et al.[28] presented broad summaries of both CDoE and MDoE methods used in Aeronautics. Additionally, sampling points (also known as training points) selection strategies can be classified into domain-based (also known as model-free or non-adaptative, a priori, one-shot, off-line or single-stage) and response-based (also known as model-based, adaptative, a posteriori, sequential or online) approaches.

In domain-based approaches, training points are chosen based on the information available from the design space (e.g. distance between two training points); whereas in response-based approaches the training points are chosen based on the information provided by the surrogate models (e.g. mean squared error approach) to enhance their efficiency. Domain-based approaches are based on space-filling techniques[13, 17, 29], that try to spread the sample points uniformly throughout the design space (a possible guarantee for an eventually acceptable a priori global approximation of the surrogate model).

Generally, it is not possible in aircraft aerodynamics to select a priori the number of samples

for a given accuracy, mainly because of the non-linearities of the aerodynamic functions. Space-filling approaches (considering their effects on the surrogate models accuracy and eventually the global optimum) provide the opportunity to monitor the refinement of the initial surrogate model built offline; initial surrogate model that is adaptatively updated during the online phase by adding new sample points at locations of the parameter space that display large errors between the expensive and the surrogate models. Nevertheless, offline sampling approaches are quite often very expensive, especially for high dimensional aerodynamic problems; therefore the need for a trade-off between the offline and online sampling strategies in order to reduce the associated computational cost. A thorough introduction to response-based approaches is given in Forrester et al.[4], Forrester and Keane[5], Ahmed et al.[6], Koziel et al.[7], Leifsson and Koziel[9] or Rai et al.[30].

1.2.2.1 Classical design of experiments

Classical sampling techniques (CDoEs) have known an extensive use in aerospace engineering for various design improvement applications. Originally developed for planning physical experiments, they assume the existence of a random error term in the measured response and a non-repeatability of the latter, even with the use of the same sample during two different measurements; hence the use of replicated sampling. They are all based on similar statistical principles of analysis of variance (Analysis of Variance (ANOVA)) and regression analysis[10, 15, 16, 17]. CDoEs techniques presuppose a uniform distribution of the training points with the aim to have a fixed number of samples in the design space, so as to minimize the influence of the random error term in posterior simulations. Therefore, a significant number of samples tend to locate in the neighborhood or on the boundaries of the design space, with very few samples in the interior of the design space. A comprehensive review on the explanation/causes of such samples spread is given by Myers and Montgomery [31]. Though they could lead to sound outcomes when combined with adequate engineering knowledge, CDoEs only provide guidelines as to the reliability and validity of the results[10]. Some of the CDoEs can be used to plan simulation-based experiments, sometimes arising in good enough approximations of the objective functions[17, 20, 22, 23]. Commonly used classical sampling techniques in Aerospace engineering are:

- Full and Fractional-Factorial designs (also known as grid designs)[10, 17, 20],
- Central Composite designs[20, 32, 33],

- Box-Behnken designs[34, 35, 36],
- Optimal designs[37, 38, 39],
- Orthogonal arrays designs often referred as Taguchi designs[40, 41, 42].

1.2.2.2 Modern design of experiments

Modern Design of Experiments (MDoE - also known as space-filling or exploratory designs)[13, 17, 20, 21, 43, 44, 45, 46] have known a comprehensive development in parallel to the evolution of computer science and ease access to computing facilities[17, 20]. Contrary to physical experiments, these simulation-based experiments are deterministic, i.e. not only samples with the same input setting produce the same outputs but also no measurements inaccuracies inherent to randomness occur. MDoE have become a substitute to CDoE when the latter are infeasible or too costly[47]. MDoE sampling techniques tend to locate much more training data points in the interior of the design space, with the aims to find an approximate model and to minimize the bias errors - local gaps between the true response trend and its estimated trend (surrogate)[4, 5]. Therefore, MDoE sampling techniques require different approaches than CDoE techniques in their development.

A theoretical justification in the use of most CDoE lies on their space-filling nature. Though widely used by many experimenters, the term **space-filling** is in itself very ambiguous because its various definitions are subject to the criteria or property used to spread the sample points. Originally concerned with randomness (full, pseudo or quasi) only, statisticians have developed many space-filling strategies, uniformity measures, etc to address different design space exploration demands in terms of spread and to ensure a reasonable coverage of the design space[4, 17]. Vazquez and Bect[48] proved that numerous space-filling designs of experiment outperform most of other non-space-filling designs. The class of MDoE is quite broad. Following is a 'global' classification of simulation-based experiments, though certain sampling methods may display features from two or more groups:

- Random samplings (simple random samplings[17, 49, 50], monte carlo methods[51, 52, 53]),
- Quasi-random samplings (Quasi-monte carlo designs[54, 55, 56], Sobol designs[54, 57, 58], Faure sequences, Hammersley and Halton sampling methods[54, 59, 60] or Niederreiter sequences generators[54, 58, 61]),

- Projections-based designs, mainly Nearly orthogonal arrays based design (NOAs)[22, 62, 63],
- Uniform designs(Statistical measures-based designs[17, 64, 65], Euclidean distance-based designs[66, 67, 68]),
- Miscellaneous and hybrid designs (Latin hypercubes samplings[13, 17, 69]), Latin hypercubes based designs[17, 29, 70, 68].

1.2.2.3 Future in advanced design of experiments for aircraft aerodynamic applications

Till date, there is no rule of thumb or efficient guidance in the choice of a specific sampling strategy for aircraft aerodynamics design and analysis purposes. Building an initial data set remains quite a complex task when thinking of issues posed by the nonlinearities of the aerodynamic functions, their high dimensionality or possibilities to investigate stall/buffet boundaries problems or beyond flight envelope designs. Selection of locations where to a priori spread the sampling points depends on our interest in design space exploration or design space exploitation, on the type of query analyses to be achieved, etc. Suitable DoE strategies may in any case consider greedy sampling techniques[71, 72] or a partition of the design space into different regions[73, 74] within which appropriate DoEs shall be applied to improve local predictions. Furthermore, they should be able to address the hardship posed by the sampling of non-rectangular bounded regions (also known as slid-rectangular regions)[75, 76] such as the flight envelope, for which existing adaptative sampling methods cannot be utilized[77, 78]. Nonetheless, some authors have introduced some hints or comparative studies on DoEs. The papers from Loeppky et al.[79] and Looss et al.[80] gave hints on how to select the size of the training set in order to build an accurate surrogate model; a small number of design points leading to erroneous approximations inside optimal regions. Younis et al.[81] & Cavazzuti[82] presented the pros & cons of various classical and modern DoEs. Younis et al.[81], Romero et al.[68], Rosenbaum et al.[83], Swiler et al.[84], Looss[85] or Yondo et al.[86] studied the effects of a priori sampling and sample size on the accuracy of various surrogate models. They came to the conclusion that an increase in the number of samples at the offline stage may not necessarily decrease the global or local error; different error measures could lead to opposite error trend estimations, due not only to the type of error measures selected but also to the sampling techniques used during the design. Burkardt et al.[87] suggested the combined use of Proper Orthogonal Decomposition (POD)-Centroidal Voronoi Tessellation (CVT) (proper orthogonal decomposition-centroidal voronoi tessellation) as

a reduced-order model surrogate, to approximate the solution of the Navier-Stokes equations at low Reynolds numbers. Crombecq et al.[88] introduced the LOLA-Voronoi sampling technique, a hybrid approach between exploitation-based and exploration-based sampling methods that is suitable for various types of problems, with a satisfactory coverage of the design space, but do not always guarantee the model accuracy.

1.2.3 Single and multi-fidelity surrogate modeling approaches

Numerous aircraft aerodynamic design analysis and optimization problems require running computationally intensive and complex simulation codes, such as Navier-Stokes CFD solvers, to be able to screen multiple aircraft configurations (cruise/high lift, control surface deflections, etc), flight conditions (Mach number, Angle of attack, etc), etc[89, 90]. Despite the availability of advanced computing capabilities, the excessive computational cost makes it absurd to exclusively rely on expensive simulations (also known as high-fidelity simulations) for the purpose of aero data production, aerodynamic shape optimization, design space exploration, etc. An attempt to circumvent the computational budget restrictions was introduced by Box and Draper[91], Kleijnen[92] through the use of surrogate models(also known as metamodels, emulators, proxy models, predictors, interpolators or response surface models). Surrogate models are 'cheap-to-evaluate' mathematical approximations that mimic the deterministic computationally expensive response or behavior (black-box) of an original system over the complete or part of the design space[17]; once constructed, a surrogate is used in lieu of the expensive full-order model in order to predict the values of the objective functions at locations that do not belong to the set of points used during the fitting process or training phase. In other words, Surrogate modeling enables virtually instantaneous analyses to be run in real-time by approximating computer-intensive functions or models across the entire design space with simpler mathematical ones. Additionally, these techniques yield insight into the relationships between design variables (inputs) and responses (outputs), hence facilitating concept exploration and providing knowledge about the behavior of the system across the entire design space as opposed to a small region. Surrogate models presuppose a model of the form $y(\mathbf{x}) = \hat{y}(\mathbf{x}, \epsilon)$, where $y(\mathbf{x})$ is the black-box (a function for which the analytic form is unknown) to be approximated and ϵ the vector of undetermined parameters that has be assessed prior to apply the surrogate.

Deciding on a preference for a surrogate model remains quite an open issue though authors like Forrester [4], Booker[3], Sacks et al.[23, 24] or Benner et al[93] presented some guidelines. Both the selection and accuracy of such approximations depend not only on the nature of the

Figure 1.2: Basic surrogate model framework.

underlying problem (e.g. of aerodynamic optimization) but also on the industrial common practices and designer experience (e.g. of the a priori knowledge of the related physics and of the features provided by certain surrogate models)[4]. Ostensibly, to attain an acceptable preliminary approximation (that may not be necessary for a local modeling), it is recommended to make use of space-filling samplings with a minimal number of calls of the high dimensional model, while retaining most of underlying features. This is generally not trivial in aerodynamic design, since there is few or no a-priori knowledge of the trends of the modeled (sometimes highly nonlinear) functions. Furthermore, the use of surrogate models depends on the type of analyses to be achieved (real-time or many-query)[94], on an interest either in improving the global accuracy over the entire domain (global modeling or design space exploration) or in an approximation of the optimum to locally improve the current design (local modeling or design space exploitation)[4, 95]. General and detailed reviews on surrogate models employed in fluid mechanics and aerospace engineering are given throughout the various subsections.

A wide variety of predictors have been introduced into aircraft aerodynamic design (flow control, estimation of aerodynamic coefficients, data calibration and fusion, aerodynamic shape optimization, etc.). Two major criteria allow to categorize the surrogate modeling techniques[6]:

- the nature of the design variables that group surrogates as parametric, semi-parametric or non-parametric. Parametric surrogate models such as polynomial regression, multivariate adaptive regression splines or kriging approximates the original high-dimensional model over a range of design parameters and presuppose a global functional relationship between the training set and the corresponding responses[96, 97]. Moreover, parametric surrogates may combine local information (obtained from a partition of the design space into different regions) with an interpolation method [93]. Unlike parametric ones, non-parametric surro-

gates such as radial basis function, neural networks or support-vector regression implicitly use a combination of local information to construct an overall surrogate model[96]

- the methodology use to build the surrogates: interpolation, regression, projection, etc.

Surrogate models used to mimic the full order aerodynamic models in many-query analyses or flow predictive control are often subjected to various kind of uncertainties that generally compromise their performances. Such types of uncertainty could enclose CFD code uncertainties, model parameter uncertainties, residual variations, model inadequacy, etc[98]. Bayesian model calibration, that represent uncertainties as probability distribution functions and further consider the quantified uncertainties while attempting to correct for the model inadequacy, is beyond the scope of this review. Nevertheless, Kennedy and O’Hagan[99], Le Gratiet[100], Boon et al.[101], Frangos et al.[102], Cui et al.[103], Allaire and Willcox[104] are interesting releases on a bayesian approach to surrogate models, in the framework of aerodynamics.

A relevant classification of surrogate models is given by Eldred and Dunlavy[1] who cluster them as data-fit (DFM), multi-fidelity (MFM) and projection-based (also known as Reduced-Order Models, ROM) surrogate models.

1.2.3.1 Data-fit surrogate models

Primarily developed to assess physical experiments results[91], data fit surrogate models are parametric and non-parametric regression-based or interpolation-based approximations generated from data arising from few calls of the full order model. They are identified as non-physics-based approximations, i.e. no attempt is made to ensure that the surrogate model the flow physics[9]. Examples of data-fits surrogate models are response surface model (Response Surface Model (RSM), polynomial regressions), Gaussian process regression also known as Kriging, splines, artificial neural networks (Artificial Neural Networks (ANN)), radial basis functions (Radial Basis Functions (RBF)), stochastic spectral approximations (Stochastic Spectral Approximations (SSA)), etc. Fang et al.[17], Younis et al.[81], Ahmed and Qin[6] or Peter et al.[105] presented some pros and cons of the most popular data-fit surrogate models. Jin et al.[106], Wang and Shan[107], Alvarez[108], Paiva et al.[109] and Chen et al.[11] reviewed or compared different data-fit surrogate model types.

Following introduced some common data fit surrogate models employed in aerodynamics:

- RSM - Polynomial regressions[10, 17, 110],

- Multivariate adaptive regression splines[106, 111, 112],
- Gaussian process regressions - Kriging[4, 5, 24, 113, 114, 115],
- Radial basis functions and artificial neural networks[116, 117, 118, 119, 120],
- Support vector regressions[121, 122, 123, 124, 125].

1.2.3.2 Reduced-order models

High Dimensional Aerodynamic Models (HDAM, also known as Full Order Aerodynamic Models - FOAM) present large-scale systems[126] of complex equations arising from discretization of (parametric) partial differential equations (PDE - example of Navier-Stokes equations) describing the models of interest. Such HDAMs can be expressed in the form:

$$\begin{cases} \frac{d}{dt} \mathbf{w}(t) = \mathbf{f}(\mathbf{w}(t), t) \\ \mathbf{y}(t) = \mathbf{g}(\mathbf{w}(t), t) \\ \mathbf{w}(0) = \mathbf{w}_0 \end{cases} \quad (1.1)$$

where $\mathbf{w} \in \mathbb{R}^q$ is the vector of state variables, $\mathbf{y} \in \mathbb{R}^p$ the vectors of output variables (with $p \ll q$), $\mathbf{y}(\cdot, \cdot) \in \mathbb{R}^q$ defining the full equations and $\mathbf{w}_0$ the initial condition. The large dimensionality of these models often leads to excessive computational efforts and data storage management that need to be kept down to a reasonable level. The global objective is, de facto, to solve the following initial boundary value problems:

- for general PDEs

$$\begin{cases} \mathbf{R}(\mathbf{w}, \mathbf{x}, t) = 0 \\ \mathbf{B}(\mathbf{w}_{\text{BC}}, \mathbf{x}, t) = 0 \text{ (associated boundary conditions)} \\ \mathbf{w}_0(\mathbf{x}) = \mathbf{w}_{\text{IC}}(\mathbf{x}) \end{cases} \quad (1.2)$$

- for parameterized PDEs

$$\begin{cases} \mathbf{R}(\mathbf{w}, \mathbf{x}, t; \boldsymbol{\mu}) = 0 \\ \mathbf{B}(\mathbf{w}_{\text{BC}}, \mathbf{x}, t; \boldsymbol{\mu}) = 0 \text{ (associated boundary conditions)} \\ \mathbf{w}_0(\mathbf{x}) = \mathbf{w}_{\text{IC}}(\mathbf{x}; \boldsymbol{\mu}) \end{cases} \quad (1.3)$$

with $\mathbf{w} = \mathbf{w}(\mathbf{x}, t) \in \mathbb{R}^q$ being the vector of state variables, $\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^d$, $d \leq 3$ the vector of space variables, $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^p$ the parameter vector and $t \geq 0$ the time variable.

Established and expanded by numerical mathematicians and specialists in statistical inference, model order reduction (Model Order Reduction (MOR), Fig. 1.3) were introduced in the eighties [127, 128, 129, 130] with the aim to alleviate this computational burden by generating low-order (low-dimensional) models (reduced-order models - ROMs) that are fast and cheap to evaluate approximations capable of retaining the dynamics and characteristics of the original large-scale model behavior over the parameter space, while neglecting irrelevant features. In other words, the goal is to obtain a model such that

$$\begin{cases} \frac{d}{dt} \mathbf{w}_r(t) = \mathbf{f}_r(\mathbf{w}_r(t), t) \\ \mathbf{y}(t) = \mathbf{g}_r(\mathbf{w}_r(t), t) \end{cases} \quad (1.4)$$

where $\mathbf{w}_r \in \mathbb{R}^k$ is the vector of reduced state variables, $\mathbf{y} \in \mathbb{R}^p$ the vectors of output variables and $\mathbf{y}_r(\cdot, \cdot) \in \mathbb{R}^k$ defining the reduced equations.

Figure 1.3: Model order reduction.

In recent years, progresses in the field have triggered the interest of aircraft aerodynamicists, making it more computationally affordable to solve complex steady/unsteady-state aerodynamic problems, to run near real-time analyses (model predictive control, routine analysis or aero-data production) and many-query analyses (optimal control, aero-data production/reconstruction, uncertainty quantification, high dimensional inverse problems or optimization) [131].

Surrogate-Based ROMs do not require data from different fidelities and are based only on the discretized governing equations of the high-fidelity model, early referred to as HDAM. The

scope of these HDAM remain quite limited for applications that require numerous evaluations of the objective functions due to the associated high computational costs (example of aero-data production for routine analysis or parametric studies); therefore, only carefully selected training points based on designers knowledge of the model and experience from previous aircraft campaigns have served as a guideline in the past. Though sometimes quite code intrusive[132, 133, 134], surrogate-Based ROMs via MOR bring an added value to data fits models as they offer the possibility to model high dimensional functions while handling their dynamical evolutions. One other feature of surrogate-Based ROMs is their capability to permit a rigorous framework for deriving system-theoretic error bounds and error estimates between the high-dimensional model and the reduced-order model solutions[93, 135, 136, 137].

As previously mentioned, most ROM strategies are characterized by a dimensionality reduction of the system, with the governing equations (state variables) of the HDAM being projected onto a low-dimensional subspace that spans the main features (physics and dynamics) of the HDAM. The major differences among these various strategies lie on the way the state variables are defined/determined and the projection matrix or the set of reduced basis vectors (Lagrange, Hermite or Taylor bases) or transfer function is constructed[93, 138, 139]. Surrogate-based ROMs cover an extensive spectrum of methodologies whose problem-solving suitability depends on the available computational cost, the targeted accuracy, the dynamics of the aerodynamic model under investigation, the parameters of interest or the need to include analytical or (sometimes noisy) experimental data while building the surrogate. Advances in the development of ROMs allow to group them[93, 138, 140, 141, 142] based on the types of systems encountered (linear, weakly linear or non-linear, steady or time-invariant or time-varying, parametric or non-parametric) or based on the analyses of the HDAM with respect to frequency or time (time-domain and frequency-domain ROMs). Unlike non-parametric methods that generate the surrogate model from the data only, parametric methods use the data to mimic the full-order model (Full Order Model (FOM)) by solving for the design parameters that minimizes the error between the surrogate and the data.

The construction and applications of linear non-parametric time-invariant (with few inputs/outputs) dynamic systems in science and engineering have already reached a considerable level of maturity[93]. Moreover, for many aircraft engineering applications, the FOMs depend on a set of deterministic or stochastic parameters (system geometry, system configuration, initial or boundary conditions, etc); therefore the need to generate parametric ROMs capable of approximating the original full-order dynamical system with high fidelity over a range of design parameters[140, 141].

Though the understanding of the term **surrogate-based ROMs** by some authors include all type of surrogate models, it is used within this survey to label the class of projection-based (surrogate) ROMs. Continuous progresses have been noticed in the field of linear and nonlinear parametric ROMs, with the emergence of numerous and novel methods, that can be grouped[93, 138, 140, 141, 142] as krylov-based (system-theoretic methods, rational interpolation also known as moment matching, etc), Reduced Order Basis (ROB) (Reduced Order Bases)-based (Proper Orthogonal Decomposition, greedy reduced order basis, etc), Tensor-based ROMs, Truncated-based ROMs, Hankel-norm MORs, etc. Despite the fact that many of these methods are not yet implemented in aircraft aerodynamics (very few, mainly in subsonic flow regime), the present subsection however introduces the most popular of them that have been employed within the general field of fluid mechanics, providing some of their pros and cons. Surveys and theoretical notes on the topic are found in [93, 94, 138, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149, 150, 151]. Kevin Thomas Carlberg addressed the challenges posed by the use of ROMs in the SIAM (Society for Industrial and Applied Mathematics) online news of March 2016[152]. Other interesting MOR-related websites are the ones of the MIT Willcox Group[153], of the Stanford University Farhat Group[154] and the extensive MOR Wiki[155], an exchange platform that gather together experts in model order reduction and pages introducing different types of MOR.

ROMs for linear aerodynamic systems

A high number of aircraft aerodynamic applications often result in parametric linear steady or unsteady time-dependent models. However, under certain circumstances, it is possible to reduce linear parametric models by interpolating between linear non-parametric time-independent models. In that case, the structures and physical properties of the models could be proven to depend only on the state variables, yielding linear time-invariant systems.

Linear time-invariant PDE models whose discretization in space result in linearized Ordinary Differential Equation (ODE) (for example through the transformation of the state variables, discontinuous Galerkin method, finite difference method, finite element method or spectral methods) have been solved using Low-rank Gramian approximants, Singular Value Decomposition (SVD)-based (Truncated Balanced Approximation, Singular Perturbation Approximation, etc), Pade approximants (Moment Matching) via Krylov subspaces (whose basis are generated by means of Arnoldi or Lanczos process) or Fourier decomposition (non-linear harmonic)[93, 138, 140, 141, 142, 150, 155, 156, 157, 158, 159]. Recent developments have led to hybrid methods that combine Krylov subspace methods with Gramian-based approaches. Contrary to most

Krylov-based ROMs that require some post-processing to achieve a certain level of stability, most gramian-based approaches present the advantage not only to provide a global error bound between the reduced-order model and the original model, but also to guarantee the stability of the reduced-order model. However, both methods have mainly been developed for low-dimensional aerodynamics problems[160].

Another method found in aeronautical literature is ROB-based ROMs techniques. They reduce the dimension of the governing equations by projecting the full order model onto a manifold of lower dimension spanned by the reduced bases. The state of the full order model is expressed as a linear combination of the basis vectors that must be selected carefully in order to attain a ROM with high performance. Most ROB-based ROMs have shown not to be robust with respect to physical parameters, boundary or initial conditions variations[143, 157, 161] because their robustness and accuracy are strictly related to the reference parameters from which the modes have been derived; which implies that the ROB has to be reconstructed every time the configuration/parameters is/are changed, a scenario not recommended to avoid a too large offline cost.

Two ROB-based ROMs approaches are found in literature[93, 131, 138, 141], namely a global approach that considers the construction of a single ROB to reduce the dimension of the full order model and the local approach that partitions the parameter space into multiple subspaces, each of them being associated to a local ROB. Global approaches keep some redundant dimensions during online computations and generally lead to high simulation times. In the latter approach, a local ROB is chosen at each time step of the ROM simulation based on the current state of the system, resulting in small and accurate surrogate models. For large parameter space, that implies an extensive truncation of the full-basis, global ROB-based ROMs have most often resulted in inefficient surrogates unable to reconstruct the flow features, especially in portions of the parameter space outside of the manifold of lower dimension spanned by the reduced bases. Attempts to remedy to this drawback include sampling a large size of values of the parameters of interest or make use of multiple local ROB.

Numerous methods to derive the reduced basis matrices exist, among which the proper orthogonal decomposition (POD), balanced truncation or the rational interpolation methods(moment matching, pade approximants, tangential interpolation, etc). POD-based ROMs and related interpolation methods are incontestably the most used projection-based reduction techniques in aircraft aerodynamics[162, 163, 164, 165, 166, 167, 168, 169, 170, 171]. Also known as Karhunen-Loeve decomposition or principal component analysis (Principal Component Analysis (PCA))

or singular value decomposition (Singular Value Decomposition (SVD), the discrete version of POD) and concurrently developed by Lumley[172], Kosambi[173], Karhunen[174], Loève[175], Obukhov[176] and Pougachev[177], POD provides a set of optimally ordered orthonormal basis vectors for modal decomposition of an ensemble of experimental or computational data. In the area of fluid mechanics, one of the key advantage of POD lies in the fact that only few POD modes are required to reconstruct the flow (in terms of kinetic energy) and to capture its dominant features. Originally, two versions of POD were found in the literature, namely the Lumley classical POD (also known as direct method) that computes the eigenproblem in the spatial domain and the **snapshot** POD (introduced by Sirovich[129, 130] for high-dimensional problems) that construct a ROB from few a priori computed flow solutions in the temporal domain. It is worth mentioning that a similar POD discretization can also be done in the frequency domain[178], in the case for example of linear time invariant systems, assuming simple harmonic solutions and replacing the data at discrete time steps with data at discrete frequencies over a frequency range of interest. Such an approach has been used for example when solving unsteady aerodynamics problems (example of CFD-based aeroelastic ROMs), by constructing a parametric ROM that approximates the time-accurate governing equations under small approximate periodic perturbations[179]. With the aim to deal efficiently with the computational burden (especially in terms of data storage, data compression and memory management), a scalar version of the classical POD (scalar POD) was developed by Cordier and Bergmann[180], whose principle is to retain the relevant POD modes to rebuild the flow realizations that can later be used for example in the snapshot POD analysis. The implementation of POD[181] presents numerous challenges, among which solving the eigenvalue problem (that is generally intractable because of the large dimension and density of the matrix) or the optimality of the POD method that is often violated because the snapshots used to create the basis may not related (in certain cases) to the design variables of interest during the online phase.

Originally developed within the aerodynamic controls community, balanced POD (Balanced Proper Orthogonal Decomposition (BPOD))[182, 183, 184, 185] has arose to be an optimal POD/ROM approach that combines the methods of balanced truncation and POD. It is tractable for large dimensional problems and generates better ROMs than POD, that have an approximate cost close to POD computations. Nevertheless, BPOD has shown not to absolutely guarantee the stability of the resulting ROM. Additional POD versions were introduced in the field of aircraft aerodynamics, such as Zonal POD presented by Iuliano et al.[186], the Continuous POD introduced Volkwein [187] mainly for nonlinear systems, the Compact POD established by Carlberg et al.[131], the variable by variable POD[188] or the Jack POD tool[189] developed

in 2008 by the CFD team of a French research lab CERFACS. Further readings, discussing of the application of POD to turbulent flows, may include the publications of Holmes et al.[190], Volkwein[191], Pinnau[192], Allery et al.[193] or Berkooz et al.[194].

Binding POD (with or without Galerkin or Petrov-Galerkin projections) to an interpolation method (POD+I) [134, 195, 196, 197, 198, 199, 200, 201] with the aim to determine the coefficients of the POD basis modes or building a local RSM for each capability POD coefficient[202], have been widely used in both in linear and nonlinear aerodynamics. Apart from the a priori known drawbacks linked with the expensive off-line computational cost, POD+I surrogates optimally represent the most energetic modes contained in the set of state solutions (previously referred to as snapshots) and therefore generally result in good objectives predictions with regards to the interpolation of the POD coefficients[93, 203, 204]; which is not the case when considering extrapolation, because the resulting ROM hardly queries the underlying FOM away from the training configurations[205].

POD + Interpolation methods often pose issues in the sense that the snapshots derived therein are not obtained from the original model[206]. These methods attempt to construct more accurate ROMs during the online phase compared to numerous global basis based approaches; the major limitation being the accuracy of the interpolation, that mainly depends on the methods and the data. It is worth mentioning that generally it may not be possible to obtain good approximate for the error bounds using such methods.

POD-based techniques are a posteriori reduced-order model surrogates that require to generate some snapshots of the flow. Keeping in mind the continuous computational cost reduction trend, a couple of ROMs have been developed, considering no a priori knowledge of the flow solution; among them the a priori model reduction (A Priori Model Reduction (APR))[207, 208] or the proper generalized decomposition (PGD)[209, 210, 211, 212, 213], a generalization of POD that look for solutions in a separated form involving the use of space, time or any other parameter of the underlying problem.

One of the major barriers to the spread of ROM-based surrogates among the engineering and industrial communities is undeniably their lack of accuracy. To circumvent the flaws associated with ROMs and improve the accuracy towards robust parameterized ROMs, numerous strategies have been introduced. Among them, suitable sampling strategies[87, 93, 152, 214, 215] for ROMs optimization that entail iterating between the offline and online computations in favor of trust-region approaches[93, 152, 202, 216, 217], combination of ROMs with residual minimization schemes[218, 219], calibration of the models based on the Tikhonov regularization[220, 221],

or using various adaptation schemes[161, 214, 215] or sensitivities[93, 152] (active subspaces, parametric gradients of the ROM basis functions or adaptative strategy based on the gradient of the Lagrangian) to lessen the dimensionality of the parameter space. Known approaches[161, 222, 223] to address the ROM adaptation problem involve enriching the snapshot matrix with solutions corresponding to different values of the varied design parameters (Global POD), the subspace angle interpolation scheme, the method of direct interpolation of the reduced-order basis vectors, the method of interpolation on a tangent space to a matrix manifold, interpolation on a tangent space to the Grassmann manifold.

The offline-online strategies cited previously are convenient for real time analysis problems, especially in the framework of surrogate based optimization where the parameter space is sampled and the reduced basis computer a priori to generate a ROM (offline stage); computationally tractable ROM that is used a posteriori during the optimization phase to approximate the FOM over a large range of parameters values (online stage). Unlike optimization, other many-query analyses required a different approach when sampling the parameter space, which often means querying the model over a range of parameter values and therefore introduced the need of scalable methods capable of reducing the cost of the offline phase.

ROMs for nonlinear aerodynamic systems

Several methods[93, 142, 224] have been employed or developed for the reduction of nonlinear and parametric models, among which the popular data-fits quadratic methods, the bilinearization method or variational analysis-based methods. However, one of the most efficient approach has been to use multiple local predictors, each of them associated with a subdomain of the state space, the time interval space or the parameter space. A run-through of the existing physics-based approaches in the area of fluid flows allow to globally classify them into three major groups[93, 142]:

- Linear and weakly-linear methods

The use of linear projection-based ROMs in the approximation of nonlinear dynamical models and parametric models results from the possibility to represent a FOM as a linear or non-parametric global model, or as an interpolating superposition of linear or non-parametric local models, to which is/are applied a reducing projection scheme. Volterra series operators with kernels[225, 226, 227, 228] and local ROB-based approaches are among linear ROM approaches extensively used to approximate nonlinear and full order parametric aerodynamic models. Silva[229] identified some limitations in the use of

Volterra series and restrained their suitability to weakly nonlinear aerodynamic problems. Numerous authors[230, 231, 232, 233, 234, 235] established that the use of multiple local ROB in lieu of a (single) global ROB could lead to computationally efficient and accurate surrogates, especially in the field of fluid flows where the regime map in various parts of the parameter space is composed of different flow patterns (flow regimes); flow patterns to which are assigned appropriate local ROB that allows to capture more effectively the model local behaviors[171]. Another approach consists in associating a local ROB at each time step of the ROM simulation, based on the current state of the system (time-dependent models).

POD has been largely used to construct the reduced order bases through the method of snapshots and it has been a commonplace to do the model reduction through Galerkin or Petrov-Galerkin projections. Moreover numerous combinations of POD with data fit surrogates have been tested. However, due to the nonlinear nature of aircraft aerodynamics characteristics (especially in transonic regime with some unsteady or steady-state aerodynamic problems), these methods have sometimes shown to be poor surrogates to the FOMs mainly because they may lead to quite large extrapolation errors and the associated computational costs scale linearly with the dimension of the FOMs. Application of POD to nonlinear parametrized PDEs presents a number of challenges among which dealing with the high dimensionality of the parameter space, the computation of the reduced-order nonlinearities and system matrices in the state variable during the online phase or the validity of the basis across the parameter space. Numerous methods that could overcome the above-mentioned shortcomings were proposed in Paragraph 1.2.3.2 and are applicable in the construction of nonlinear ROMs. Alternative methodologies include trajectory-based ROMs such as the trajectory piecewise linear approximation (Trajectory Piecewise Linear Approximation (TPWL))[236, 237] that linearize the nonlinear FOM at multiple locations in the state space or the maniMOR[238, 239] that constructs, via projection, a low-order nonlinear manifold in the state space and unlike TPWL, make use of local reduced bases. Though the online phase of these two approaches is not code intrusive and does not scale with the size of the FOM, they however still required many parameters to be adjusted.

- Hyper-reduction methods

Most often, the implementation of nonlinear projection-based ROMs requires at least one operation per iteration whose computational complexity scales with the size of the underlying FOM. Hyper-reduction techniques[235, 240, 241, 242] were introduced as offline approaches that enable to eliminate this hinder, in order for the ROM to achieve

large speedups while maintaining an acceptable level of accuracy. Established by Everson and Sirovitch[243, 244], Gappy POD is undoubtedly the most implemented hyper-reduction technique in aircraft aerodynamics to reduce the complexity associated with solving the nonlinear reduced-order model. It makes use of POD orthogonal modes to reconstruct incomplete flow solutions or recover gappy wind-tunnel data. Other classes of hyper-reduction methods include the missing point estimation (Missing Point Estimation (MPE))[166, 245], function-sampling methods[246], Gauss-Newton with approximated tensors (Gauss Newton with Approximated Tensors (GNAT))[246, 247], POD-GNAT[246, 247], the Empirical Interpolation Method (EIM)[248, 249] and its variants the discrete empirical interpolation method (Direct Empirical Interpolation Method (DEIM))[250, 251] or the POD-DEIM[252] approach. Mostly, hyper-reduction techniques have shown to be robust with respect to deviations from the original training trajectory. Though the cost of the online phase in these methods does not scale with the size of the FOM, hyper-reduction methods are code intrusive during the online phase and required many parameters such as the ROB's size to be adjusted.

- Nonlinear manifold learning methods

Manifold learning methods encompass a group of algorithms whose purpose is to map a high-dimensional dataset onto a manifold of low dimension in a way to preserve the intrinsic properties. They can be clustered as local (local linear embedding, laplacian eigenmap, etc) and global manifold learning approaches (isomap, kernel PCA, multidimensional scaling, etc). They have found applications in many fields including linear and nonlinear dimensionality reduction, pattern recognition, data compression, machine learning, etc. Dealing with the high-dimensionality of the parameter space, the large number of features including the nonlinearities found in fluid flows (some of which might be irrelevant), represent a real burden in many engineering problems. For the past decades, nonlinear manifold learning has gained some interest among aircraft aerodynamicists as an alternative solution, especially in the area of transonic flows characterized by a formation of shock waves and known to encompass one of the most efficient regimes of flight. Among all the manifold learning methods used in aircraft aerodynamics, isometric mapping (Isomap) is perhaps the most well-known alternative to classical manifold learning such as POD (not to confuse with POD as a ROM). Isomap is a nonlinear generalization of classical multidimensional scaling (MDS)[253] that maps the original N high dimensional space onto a n low-dimensional manifold ($n \ll N$). Verveld et al.[254] presented the requirements to be fulfilled by any parametric ROM in order to use Isomap for CFD

applications. Franz et al.[255] combine Isomap with an interpolation model (Isomap+I) to predict steady transonic computations for a 2D NACA airfoil and a 3D wing. Unlike POD+I, Isomap+I achieved quite a good prediction of the location of the formation of the shock waves and their shapes. Verveld et al.[254] considered a POD+Isomap+I approach in order to predict the static aerolelastic loads in a multidisciplinary design and optimization (MDO) framework. The methodology appeared to be significantly time-saving and allowed to rapidly span the flight envelope, generating accurate enough aerodynamic loads and noticeably enhancing the selection of critical loads. Numerous other nonlinear manifold learning techniques that could be applicable exist. However, numerous aerodynamicists are still reluctant in applying those advanced methodologies, being of the opinion that it would result in shifting forward the difficulties presently encountered with POD. One of the main downsides with reduced-order models is their limited range of validity. For example in aircraft aerodynamics, a ROM may be valid for specific Mach numbers, velocities, dynamic pressures or flight conditions based on which those models were built. In other words, ROMs are merely valid for the set of parameters and initial conditions that were used to generate them. However, such a statement render unnecessary the use of ROMs since a new ROM will have to be generated for each set of parameters and initial conditions, implying a call of the full order model. Adaptive/Sequential sampling algorithms enable to improve the performance of the ROMs; which introduce the possibility to enlarge the range of validity of ROMs. Notwithstanding, there are some models, for example trust-region-based models, whose range of validity is 'automatically/naturally' restricted. More on the range of validity of ROMs can be read in [93, 254, 256].

1.2.3.3 Multi-fidelity models

Originally developed for gradient-based optimization[257, 258, 259], multi-fidelity models (MFM) find their roots in attempts to solve, for high-speed and low-cost, expensive high-fidelity optimization problems, by combining data from different levels of fidelity[4, 9, 260, 261, 262, 263, 264, 265, 266]; fidelity denoting the degree to which a model captures the physics of a phenomenon of interest. Though some authors have considered a three-level of fidelity classification (high, medium and low), the present survey will only retain the low and high levels of fidelity.

Routine analyses, uncertainty quantification, inverse problems or optimization for aircraft aerodynamic design are disciplines that demand thousands or even millions of repeated expensive evaluations of the FOMs (high fidelities). They are unfortunately inconceivable to

afford due to various computational or experimental cost constraints. With the availability of less-accurate cheap-to-evaluate aerodynamic data (low fidelities), multi-fidelity modeling (also known as data fusion, data merging) has emerged as a numerical alternative to reconstruct the FOM, fusing a large amount of low-fidelities with only few high-fidelities. Combining for example the limited amount of experimental (wind-tunnel) and/or flight tests data with numerical (CFD) data can sometimes be quite laborious due the dissimilarity of the parameter spaces; therefore the naming Variable-Complexity Model (Variable Complexity Model (VCM)) was given to qualify these types of multi-fidelity models. Low-fidelities can be obtained by the means of one or a combination of the following[9, 260]:

1. data-fits models
2. projection-based models
3. simplified models that encompasses:
 - variable-fidelity models (Variable Fidelity Model (VFM)) that substitute the governing equations of fluid dynamics with streamlined equations (example replacing the Navier Stokes equations by Euler equations, the potential theory or even empirical methods),
 - variable resolution models (Variable Resolution Model (VCM)) that use the same fluid-flow model as in the FOM, but with a coarser computational grid,
 - or variable accuracy models (Variable Accuracy Model (VAM)) that relax the convergence either by reducing the maximum allowable number of iterations and/or reducing the convergence tolerance - example of evofusion.

In aircraft aerodynamics, model hierarchies from low to high, include empirical methods, potential flow theory, Euler equations, (unconverged) Reynolds Averaged Navier-Stokes (Reynolds Averaged Navier-Stokes Equations (RANS)), large eddies simulations (Large Eddies Simulations (LES)), direct numerical simulations (Direct Numerical Simulations (DNS)), wind-tunnel testing (WTT) and flight testing (Flight Testing (FT)). Calibration-based methods[260, 262, 267, 268, 269] (also known as correction methods, bridge or scaling functions) are undeniably the most used multi-fidelity models. Typically, they can be local or global and the low-fidelities are scaled using an additive, a multiplicative or a joint/hybrid additive-multiplicative approach. Though additive methods have shown to outperform their multiplicative counterparts, most often the choice in the correction method has turned towards hybrid methods because of the additional flexibility they offer and the possibility to represent the complex interrelationships or correlations between

low-and high-fidelities.

Another MFM that has been widely applied in aircraft aerodynamics is Cokriging and its extensions. Originally developed in the field of geostatistics as an extension of the kriging surrogate model for multivariate functions[270, 271, 272], Co-kriging formulations for aircraft aerodynamics applications have evolved with the development of CFD codes, especially due to the possibility for example to include information such as cheaper-to-evaluate gradients. Chung and Alonso[273], Kennedy and O'Hagan[99], Craig et al.[274], Higdon et al.[275], Forrester et al.[4], Görtz et al.[261] or Da Ronch et al.[276] largely expanded on the theoretical aspects of Co-kriging for routine analysis or optimization. Qian and Wu[277], Cumming and Goldstein[278], Robert[279] or Le Gratiet[100] extensively discussed a Bayesian approach to Cokriging for uncertainty quantification or statistical inference. Laurenceau and Sagaut[280] discussed ways to build efficient response surfaces of aerodynamic functions using Kriging and Cokriging. Han et al.[281] developed an alternative cokriging approach, applicable to aerodynamics many-query problems and that could address the challenges posed by the construction of the covariance matrix; construction that represent one of the major hardships associated with the use of co-kriging. With the aims to reduce the number of total model tuning parameters and to enforce or control the level of correlation between the low- and high-fidelities, Zimmermann and Hua[282] suggested a simplified cross-correlation estimation, assuming both low- and high-fidelities sample values are treated as realizations of underlying random processes, each given by a regression model.

Han & Görtz[283] introduced hierarchical kriging, a substitute approach modeled on the external drift kriging(External Drift Kriging (EDK))[284, 285], suitable for engineering problems, that does not require modeling the cross correlation between the low- and high-fidelity functions. Relevant advantages of hierarchical kriging over co-kriging include a reduction in model complexity and a correlation matrix of much smaller size. Latterly, Han et al.[286] presented a new hybrid approach in the construction of bridge functions that fully exploit the trend underlying the low-fidelities. Le Gratiet[287] altered the original co-kriging model to generate a new multi-fidelity approach based on a recursive formulation. Peherstorfer et al.[288] introduced the concept of multi-fidelity importance sampling (Multi-Fidelity Importance Sampling (MFIS)) that combines (rather than replaces) a full order model with a surrogate model. Efficiently (in terms of space-fillingness and computational budget allocation) sampling the parameter space for MFM, building surrogate models with s -level of fidelities ($s \geq 3$) and fusing numerical simulation-based models

(CFD) with physical models (wind tunnel or flight test models) are some of the challenges posed by the use of MFM in aircraft aerodynamics.

Interesting MFM technical notes and applications in aircraft aerodynamics optimization are found in most of the publications listed in this subsection. Recently, Peherstorfer et al.[260], Fernández-Godino et al.[289] published reviews on MFM. Likeng et al.[290] presented a research on multi-fidelity aerodynamic optimization methods. Leifsson and Koziel[9] released a book fully dedicated to simulation-driven aerodynamics design using VFM.

1.2.4 Aircraft aerodynamic industrial applications of surrogate models: use, limitations and future perspectives

The following analyses mainly arose from journal and book releases, experience learned from joint university-aircraft industries projects, informal talks on identified drawbacks and judgments on the importance of DoEs and Surrogate Model (SUMO)s within some aircraft industry manufacturers flight physics teams in Europe, mainly in the areas of real-time and many-query procedures. Due to the sensitivity of the topic, only authorized or made-public references are quoted. The use of surrogate models in aircraft industry can be traced back from the time of OFAT wind tunnel practitioners and the introduction in the mid-nineties of modern design of experiments[291, 292, 293]. The complex requirements associated with the development of future aircrafts have boosted the industrialists interest[294, 295, 296, 297, 298, 299] in numerous surrogates to the highly expensive existing methodologies.

Figure 1.4: DLR-F12 wind tunnel model.

The present chapter introduces some of the known uses, limitations and future perspectives concerned with DoEs and SUMOs in industrial aircraft aerodynamic design. The chapter also addresses the difficulties surrounding the applicability within the industry of methodologies developed by the aerodynamics research community.

Changing, complex requirements and environment

Industrial aircraft aerodynamics analyses and designs pose numerous challenges when considering designing for example a new aircraft, though having gathered experiences from previous designs. Unlike within the academic or research centers communities, constant industrial test cases are infrequent, with objectives, constraints, aircraft parts, design and analysis tools or IT environments being modified frequently. Aeronautical industrialists and other type of researchers have different mindsets. While the first think of robust, reliable and 'convincing' methods that can be applied to complex cases within reasonable time frames, industrial best practices and various airworthiness regulations, others are in general mainly interested in generating 'original' methods with a high innovation rate. Moreover, within an industrial context, the common technical language with regards to DoEs or SUMOs could be hard to understand and may vary among engineers or from one company to another, with numerous information difficult to access (due to company internal privacy policies or administrative burden). Introducing new methodologies in the process chains may pose some problems because numerous aircraft manufacturers are reluctant to intrusive methods and the added capabilities should be able to wrap around with existing in-house processes. Moreover, new ways of working require to train the engineers, to change plenty of things that still need to be compatible with the company best practices and airworthiness procedures; actions that very few industrialists are ready to take, especially in the middle of ongoing projects whose budgets and time frames have priorly been set.

Computational budget allocation

Navier-Stokes simulations of certain flight configurations and queries such as aerodynamic optimization can be hard to achieve and computationally expensive in terms of CPU time and heavy memory storage. Important factors to assess the performance are computational resources includes memory, bandwidth, etc and the CPU time. From an industrial point of view, time to deliver the results is a priority, and it is more favorable to utilize, whenever possible, significantly larger number of CPUs to complete optimization as soon as possible, rather than utilizing the resources more efficiently but with longer delivery time (progress

with the design loop requires delivering optimization results no longer than a week after the task was formulated). Due to the large amount of data involved, the disk space limitations should be kept in mind. For example, it is sufficient to store flow variables values only on grid surfaces nodes, this approach requiring much less memory than handling a whole volume solution. A proper choice of samples location through advanced design of experiment methodologies, in conjunction with suitable surrogate modeling techniques will allow to attain an acceptable level of accuracy and help control the computational costs. However, the question on how to spend the allocated computational budget, in more low- and less high-fidelity simulations or just in high-fidelity ones when dealing with multi-fidelity surrogates, remains an open issue.

Design of experiments and Surrogate modeling in real-time and many-query analyses

For the past decades, random sampling and latin hypercube sampling have been the most popular design of experiments among aerodynamicists. Because they may lack some space-fillingness, both designs have failed to satisfy, in many cases, the needs of the designers. Furthermore, for real aircraft configurations (full aircraft, high-lift devices deployed, etc), evolutionary algorithms have theoretically shown to be extremely costly because of the large number of degrees of freedom of the models. Therefore, it becomes apparent that much work remain to be achieved in the construction of efficient algorithms tailored to aerodynamic design and to define strategies in the selection of suitable sampling techniques. The sample location determining the accuracy of the resulting surrogate model or influencing the targeted path to be taken by the optimization search, industrialist's interest lies on advanced space-filling and efficient sequential designs, convenient for non-rectangular bounded regions such as the flight envelope. There is a strong desire to improve available algorithms developed in the academia for effective models refinement, with the aim to enhance the sequential sampling algorithms, starting from best practices in computer experiments. Numerous authors proposed the use of uniform designs or orthogonal arrays for physical experiments, latin hypercubes, optimal designs or quasi-random designs for low to high-dimensional spaces. However, for complex routine analyses or optimization procedures mainly involving reduced-order models, Crombecq et al.[88], Burkardt et al.[87], Balajewicz et al.[300] respectively recommended the use of Latinized Centroidal Voronoi Tessellation (LCVT) and a goal-oriented greedy sampling approaches. The need for surrogate models can be explained from the early phase of the aerodynamic design, known to have large ranges of parametric variation with a relatively small number of design param-

eters; number of design parameters that increased as we move towards detailed designs where a large number of high fidelities are required. The computational cost associated with the generation of some of those high-fidelities (example of CFD computations of a wing with high-lift devices fully deployed) make it impossible to think of using them in routine analysis or optimization. Moreover, the complexity in the application of the surrogates strongly raises when facing the curse of dimensionality or the various nonlinearities. Data fit surrogate models have been extensively used in the industry, especially for modeling problems with low dimensional outputs (e.g. forces measurements during wind tunnel testing). They are applied as direct surrogates of aerodynamic coefficients and serve to estimate POD modal coefficients at different flow conditions other than those associated with the original snapshots. The use of multi-fidelity models have been quite limited and most of the applications have been mainly restricted to aero-data production, optimization of aerodynamic coefficients and calibration of high-fidelities CFD simulations to wind-tunnel models. Though high fidelity models have always represent a critical obstacle in the use of optimization algorithms, flight physics engineers have always wish to bring them in earlier in the design process, i.e. from the conceptual phase that encompasses many correlated disciplines. Consequently the research interest trend for the past years has been the development of multi-fidelity multidisciplinary optimization frameworks for aircraft integrated design that can investigate new design concepts, accommodate the increase in fidelity (high, medium, low), account for uncertainties and incorporate other challenges observed during the aircraft three-phases design process (conceptual, preliminary and detailed designs) or five major phases in the case of Airbus (Feasibility, Conceptual, Definition, Development and Series phases)[301]. Furthermore challenges on how to subsequently merge the flight test data with CFD and wind-tunnel data remain topical issues. POD-based ROM and its extensions are by far the most popular ROMs used in the aircraft industry and have been moderately employed for flow reconstruction, aerodynamic coefficients optimization, aerodynamic shape optimization and aerodata for loads prediction. Only global POD-based ROM methods have been implemented and they failed to produce surrogates that could accommodate turbulent flows or predict steady flows (one of the most important requirements for industrial aeronautical applications of CFD). The performances (accuracy and robustness) of those POD-based ROMs have suffered from numerous drawbacks:

- they are unable to accurately explore portions of the parameter space outside of the projection subspace
- they exclusively relied on high-fidelities and sometimes even on offline sampling pro-

cedures (which make them computational very expensive)

- Any change in the reference parameters from which the POD-ROM modes are derived will require a new computation of the POD bases.
- They are unable to substitute steady-state transonic ROMs that are difficult to construct and that are capable of modeling the aerodynamics nonlinearities.

Therefore the need for engineers to give a trial to new methodologies developed in the academia that circumvent such pitfalls. Enhancing POD-based ROM by exploiting the sensitivities is another field of interest, however facing the challenge posed by the use of adjoint methods. Other flight physics areas such as those involving real-time analyses (example of models predictive control) are still questioning themselves on the necessity of utilizing ROMs, benefiting by the way of rapid online evaluations of the associated aerodynamic objectives functions. Within those working groups, engineers are of the opinion that responding to real-time aero data impose them to continue tolerating the use of expensive offline computations. Furthermore it has been noticed in certain aerodynamic design optimization problems that the computational cost associated with solving for the FOM may not outweigh that much the one use to derive and employ a reduced model. Civil transport aircrafts in classical configuration are already well optimized in present days, which makes further progress arduous. Therefore, advanced optimization procedures that involve the complete aircraft should be introduced, in lieu of the actual *modus operandi* where parts of the aircraft are optimized separately (example of a clean wing optimized first and the engine integrated afterwards). Moreover, further improvements require flow around the aircraft to be calculated with high accuracy, with a drag count error estimated below 1%. For numerous aircraft manufacturers design groups, the new research directions concerned with POD-based ROMs involve:

- The development of advanced VFM and POD-based methodologies and tools,
- The development of a data model adaptation scheme, targeted towards an overall data changes (targeted data adjustment). For example the use of POD in the prediction of the aerodynamic flow field on a time-dependent deformed shape (wing aeroelasticity, etc.),
- Investigating the use of POD for interpolation between configurations in more complex conditions (high Mach numbers or angles of attack cases, compressible flows, turbulent flows etc.).

Another important requirement from an industrial point of view is the ability to reuse con-

structured surrogate models or solutions for different parameter values or posterior tasks, such as optimization problems with different objectives and constraints. Ideally, engineers wish to get nonlinear models at hands that could ensure the online cost associated with solving the reduced nonlinear equations does not scale with the dimension of the full order model. Quantifying and reducing uncertainties in predictions or solving high-dimensional aerodynamic inverse design problems with the use of surrogate models is significantly gaining importance among designers. One of the major goals of robust design is to evaluate and bound the uncertainties such that aerodynamic optimization can be implemented at reasonable computational cost, with increasing confidence. Industrial aerodynamic engineers are of the opinion that one way of attaining such a target is through the design of frameworks for robust aerodynamic optimization to quantify for uncertainties (computational noise or systematic errors) in CFD simulations, using MDO and surrogate models to smooth the data in order to span any 'gap' across the design space. Another key goal of robust design is to come to 'insensitive' optimum, considering a multi-point constrained design optimization. Obtaining a large number of snapshots sometimes represent a challenge in a process chain involving high fidelity data production. The objective being to have a fully automatized process, it is often necessary to have robust steps within the design process, running from geometry modifications, through mesh generations or deformations, job submissions to the computational clusters, CFD code evaluations, collection and results assessment, etc. The main drawback with existing robust designs is their high computational costs, linked to a large number of snapshots evaluations for uncertainty quantification; an example is the optimization of the wing in high speed cruise condition that should consider its high lift performances at lower speeds. Therefore, for robust design to be effectively and continuously applied in industrial aircraft aerodynamic design, there is need to for efficient 'cheap to evaluate' algorithms to quantify for uncertainties.

Geometry parametrization and shape optimization

The choice of the shape parameterization (Fig. 1.5) method is of significant importance in any aircraft aerodynamic design problems because it largely affects the efficiency of the underlying shape optimization. A successful parameterization scheme has to offer the capability to cover a large portion of the design space with a limited set of design variables, a large number of design variables generally arising in slow convergence rates; therefore the need of efficient screening and/or dimensionality reduction methods. Based on experienced gained, the parameterization strategies to be developed should:

- be easily implemented in any aerodynamic design problem and be able to tackle the issues posed by the 'curse of dimensionality' (reduced number of design variables) for a complete aircraft configuration, that is to be considered in future optimization processes,
- offer the possibility to include global parameters (e.g. angle of attack, wing sweep, etc.) as design variables, the advantages such as continuous gradients and the advantages to attain any geometry (be independent of the initial geometry),
- assess the deformations of aerodynamic surfaces, including intersections, excrescences or gaps,
- be able to handle geometric constraints methodically.

Figure 1.5: Example of shape parameterization of the NASA Common Research Model.

Moreover, the parameterization techniques should not limit the use of major numerical optimization schemes nor violate the assumption that the aerodynamic geometry surface should be continuous. Some interesting questions arose from aeroelastic engineers, such as how to calibrate the ROM in the context of shape optimization, how to define a POD basis that could be valid for a certain range of shape deformations or how to introduce an airfoil or a wing deformation in the ROM.

Grid deformations for small and large displacements - Adaptive mesh variations

Despite the knowledge gained and numerous meshing roundtables, the aircraft aerodynamic community is still demanding for new approaches and improvements related to the problem of mesh deformation algorithms, especially for large deformations. Mesh deformation algorithms are known to be expensive and at the industrial level, there is a need of more and more efficient but computationally cheap tools capable to cope with 3D grids of complete aircraft configurations with thick/fine boundary layers, nacelles, high-lift devices, etc. Designing algorithms to address the cost reduction have therefore be one of the main

Figure 1.6: Example of large displacement.

visions for the next years. In response to these large mesh deformations (Fig. 1.6), 'remeshing' the entire domain has been the solution proposed by some engineers and scientists. Howbeit, regenerating the mesh is extremely time consuming and may require manual adjustments for complex geometries. Therefore, it is desirable in aircraft aerodynamic optimization to develop robust and efficient mesh deformation methods for large displacements that not only lead to significant computational time savings (by automatizing the process) but also preserve a consistent mesh quality and could be applicable to a variety of mesh types. Furthermore, with the increasing interest in adjoint-based optimization, a particular attention should be put in the grid quality aspect because a poor grid will definitely have considerable effects on the gradients.

Concurrently, one of the industrial unresolved issues with regards to small deformations (Fig. 1.7) has been the definition of the validity of POD over a certain range of deformations; a concern with the use of reduced-order models being to develop some extensions of existing ones that could reliably handle the small deformations and their effects on the flow

Figure 1.7: Example of small displacement.

features. Adaptive Mesh Refinement (AMR) remains a concern when trying to improve the resolution of the flow features at reasonable computational cost.

Interactive process with inputs from engineering designers

Aerodynamicists are dealing with a large number of constraints not involve within the optimization process chains that may prevent them from gaining a full asset of the undergoing design. Moreover, 'manual' optimization till date remains the major strategy applied to industrial aircraft aerodynamic shape optimization. It provided the designer with a good understanding of the underlying physics and an awareness on how the aerodynamics is affected by the changes in geometry. The major disadvantages with such an approach are that it is time-consuming and laborious, it limits an efficient exploration of the design space and it largely depends on the designer expertise. Nevertheless, despite these drawbacks, many industrial aerodynamicists wish to have a control on the optimization process, that could be achieved through a 'decision support scheme'[264]. Such a decision support scheme could be efficient in the context of Surrogate-Based Optimization (SBO), within which few designers have a good expertise on when to stop the optimization process, without necessarily waiting for the allocated computational budget to run out; waste of computational resources that could be sometimes avoided if the designer had a possibility to enforce the process by computing snapshots at selected points of the parameter space close to the optimizer's path, based on engineering assumptions and experience acquired from previous aircraft campaigns.

1.2.5 A Review on existing nonlinear least-squares constrained optimization methods

For the past decades, numerous aerodynamic engineers and scientists have relied on the expensive direct optimization or on 'manual' optimization to attain better designs. Recent development of computational resources combined with the improvements achieved in numerical and stochastic methods, have altered the mindsets on simulation-based optimizations among the various design teams. Moreover, taking advantage of the numerous features displayed by surrogate models and the complexities of aircraft aerodynamic design problems (noise and inaccuracies in aero data, curse of dimensionality, competing multi-modal objective functions and constraints, non-linearities, computationally expensive simulations, etc), a novel optimization approach (SBO-Surrogate Based Optimization)[1, 2, 4, 5, 8, 302] based on surrogate models has gained popularity among the processes of rapidly and efficiently searching for optima (local or global) in the range of all possible solutions. SBO allows to gain a global insight into the design space of interest and offer the possibility to speed-up many routine analyses at lower computational costs, to facilely perform sensitivity analysis or parametric optimization, etc, sequentially sampling the design space with the aim of moving towards the optimal solutions.

The goal of an optimization problem can be recapped as a minimization or maximization of an objective function subject to constraints on its variables[303, 304]. The constrained optimization problems, that arise from models including explicit constraints on the variables, can be written as:

$$\min_{\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^d} f(\mathbf{x}) \text{ subject to } \begin{cases} c_j(\mathbf{x}) = 0, & j \in \mathcal{J} \\ c_k(\mathbf{x}) \leq 0, & k \in \mathcal{K} \end{cases} \quad (1.5)$$

can be reformulated as an iterative scheme[9] as shown below:

$$\mathbf{x}^{(i+1)} = \arg \min_{\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^d} s^{(i)} \mathbf{x} \quad (1.6)$$

where $\mathbf{x}^{(i)}, i = 0, 1, \dots$, is a sequence of approximated solutions to the FOM and $s^{(i)}$ the surrogate model at iteration i ; $\mathbf{x}^{(0)}$ being the initial design.

Constrained optimization algorithms are iterative. They begin with an initial guess of the optimal values of the design variables and generate a sequence of improved estimates until

they reach a solution. The strategy used to move from one iterate to the next distinguishes one algorithm from another. Most strategies make use of the values of the objective function, the constraints, and possibly the gradients and Hessians of these functions. Some algorithms accumulate information gathered from previous iterations, while others use only local information from the current point. Authors such as P.A. LeGresley & J.J. Alonso[170] or Zimmermann et al.[305] prove that ROM coefficients (Proper Orthogonal Decomposition in their case) of an approximate flow solution could be computed minimizing the associated CFD flux residual, evaluated using a full-order CFD flow solver. Dealing with steady aerodynamic cases, the optimization problem can be formulated as a nonlinear constrained (weighted) least-squares problem[306, 307, 308, 309, 310, 311, 312, 314, 315, 316] whose general form is:

$$\min_{\mathbf{x} \in \mathbb{R}^d} \frac{1}{2} \left\| \mathbf{W}^{\frac{1}{2}} \mathbf{f}(\mathbf{x}) \right\|_{L_2}^2 \quad \text{subject to} \quad \begin{cases} c_j(\mathbf{x}) = 0, & j \in \mathcal{J} \\ c_k(\mathbf{x}) \leq 0, & k \in \mathcal{K} \end{cases} \quad (1.7)$$

where $\mathbf{f} : \mathbb{R}^d \mapsto \mathbb{R}^m$ is a twice continuously differentiable nonlinear function and $\mathbf{W} = \text{diag}(\omega_1, \dots, \omega_m)$ a diagonal matrix with weights $\omega_i \geq 0$.

Since most nonlinear least squares problems are ill-conditioned, it is not recommended to solve eq.1.7 directly by a general nonlinear programming method. Nonlinear least squares problems can be solved by general optimization methods. Numerous related algorithms have been developed over the years and implemented in numerous coding languages (Python, Fortran, C/C++, etc). However, below are presented some special methods that have proven to be more efficient than others:

- The Gauss-Newton (GN) methods[311, 317, 318, 319], a class of 'classical' approaches to nonlinear least squares, are line-search methods in which the search direction at the current iterate minimizes a quadratic function.
- Corrected Gauss-Newton methods[311, 312, 313] that avoid shortcomings of Gauss-Newton (example of hybrid Gauss-Newton[315, 320, 321, 322] and BFGS (Broyden-Fletcher-Goldfarb-Shanno) Quasi-Newton[309, 323, 324] methods, altered line search algorithms with the search algorithm[311, 325, 326], or special Quasi-Newton methods[310, 312, 324, 327, 328]).
- The Levenberg-Marquardt (LM) methods[308, 329, 330, 331, 332] (where the Gauss-Newton quadratic model is minimized subject to a trust-region constraint) and Cor-

- rected/hybrid Levenberg-Marquardt methods[333, 334].
- Sequential Quadratic Programming (Sequential Quadratic Programming (SQP)) Methods[314, 335, 336, 337, 338, 339, 340, 341, 342, 343] that closely mimic Newton’s method for (un)constrained optimization, with an approximation of the Hessian of the Lagrangian computed at each major iteration, using a Quasi-Newton updating method.
 - Interior point algorithms[344, 345, 346, 347] such as Feasible Arc Interior Point (FAIPA) (feasible arc interior point algorithm)[348] that makes iterations in the primal and dual variables of the optimization problem to solve Karush-Kuhn-Tucker optimality conditions. Given an initial interior point, The defines a sequence of interior points with the objective reduced at each of the iterations.

1.3 Thesis objectives

The primary aim of this research is to build hybrid surrogate model frameworks, combining multi-fidelity and projection-based surrogates, that would be efficient when applied to equality constrained high dimensional aerodynamic systems.

Typical early-stage or conceptual design of a complex system is done using basic physical tools or empirical methods, but these tools may not capture important features, especially when new technologies are involved. Given the task to design a new wing or aircraft featuring certain prescribed aerodynamic characteristics, or facing a lack of relevant knowledge and data regarding a typical design problem (requirements, constraints, etc), the loads engineer require early on in the design stage an estimate of the corresponding aerodynamic loads. Moreover, having a fixed configuration at hand, engineers could assume (via engineering assumption or previous experience) that the final or quasi-final design may feature for example a certain lift and would like to have a first idea on how the corresponding aerodynamic loads distribution might look like. In other words, given some target lift, drag and/or pitching moment coefficients C_L^{target} , C_D^{target} or C_M^{target} to be met, the multi-fidelity frameworks to be designed will be applied to the flow over an airfoil, wing or fuselage to approximate the flowfield at untried locations (not used to generate the POD-ROM basis), to mimic global aerodynamic coefficients (as surrogate models) or to approximate local aerodynamic coefficients (by intra or extrapolation) via model order reduction. This may be useful to meet industrial needs in order to obtain and/or evaluate at lower costs more stable and realistic load cases. Such target aerodynamics tasks might be implemented in the early stages of the wing/aircraft design, where the number of design concepts to be

developed and examined is significant. The designed frameworks may be complementary to existing methodologies and could enable a rapid identification and selection of feasible and viable design concepts to be further developed and refined during detailed design; with the advantage to have a strong impact (decrease) on the overall design costs.

Though the use of high-fidelity simulations helps to reduce the need for costly redesigns due to a system not meeting performance targets or behaving unexpectedly, their computational costs remain very high. However in the early stages of aerodynamic design, it is important to rapidly evaluate a design so that numerous other configurations can be analyzed. This rapid turn-around is usually only possible with the append of low-fidelity analyses; the goal being to bring low-fidelity analyses earlier into the design process, without compromising the design requirements and objectives. A multi-fidelity POD basis algorithm attempts to lessen the problems posed by such a challenge. Two new multi-fidelity approaches are implemented in this thesis, namely a naive nonlinear multi-fidelity Least Square (LSQ) POD-Based ROM (an extension to multi-fidelity of the ROM developed by Zimmermann et al.[349]) and a novel Multi-fidelity POD+I algorithm. Additionally to the single-fidelity LSQ POD-Based ROM, the offline-online classical greedy POD based ROM is implemented to understand the influence of DoE in the construction of the ROB. The outputs of the various models are separately compared to those of the TAU solver, for the single-fidelity on one side and for the multi-fidelity models on the other side.

In both multi-fidelity approaches, an extended multi-fidelity offline POD basis is generated. In the case of the Multi-fidelity POD+I algorithm, the trend of the low-fidelity level projection coefficients will be mapped to their high-fidelity counterparts through an extrapolation at high-fidelity, based on Co-Kriging; with the difference (from similar methods) that the low-fidelity level outputs are projected on the truncated high-fidelity POD basis. While in the other approach, The POD-based multi-fidelity ROM approach is naively reformulated as a constrained weighted nonlinear least-squares optimization problem, restricted to the POD subspace, in order to accelerate the convergence at lower computational costs towards optimal high-fidelity designs. To enhance the accuracy of the multi-fidelity POD basis, a certain (minimum) level of correlation between the two different fidelities is expected. To generate the low-fidelity models, two approaches are impletended, all based on relaxed convergence.

One of the most important requirements for aeronautical applications of computational methods in fluid dynamics being the capability to predict the steady flows past configurations, this research will focus on the construction of nonlinear surrogate-based ROMs

suitable for transonic flow regime problems and capable of spanning the main features (physics and dynamics) of the Full Order Model(CFD solutions).

To summarize, the research objectives are:

- the smart selection of samples locations - The samples locations determine the accuracy of the multi-fidelity models, as well as the accuracy of the resulting POD-Based ROM in the entire parameter domain. In this thesis, the parameters are related to the flow (Mach number, AoA, Re number, side-slip angle, dynamic pressure, etc)
- the enrichment of the high fidelity computational domains (nodal values of pressure or velocity), reconstructing new data making use of model management strategies (data fusion, model correction, etc) - The goal is to leverage the cheap, but less accurate, simulations to speed up the convergence and to improve the prediction of aerodynamic coefficients. Another goal of the present research is to try to detect the level of correlation between the high and low fidelities through a simplified cross-correlation co-kriging approach or any other approach.
- build a global offline and an offline-only greedy reduced-order bases (POD - method of snapshots) that can capture the solutions in the entire parameter domain. The POD coefficients will be restricted to a 'physically reasonable' range. Applications of POD techniques and its extension to steady aerodynamics problems considered in this study, to the best of the author's knowledge, are not abundantly found in literature. These surrogates present fast and low-order models that accurately capture the variations in flow parameters. The steady state transonic flow solution for an arbitrary parameter in the case of the offline POD basis is obtained without any a posteriori calls of the expensive FOM (the CFD solver TAU); contrarily to the greedy approach that iteratively add new snapshots based on an a posteriori indicator of the error associated with the projection-based ROM. Globally, POD-based methods have shown to be promising in solving constrained design problems.
- One of the approach to compute the POD coefficients is the weighted nonlinear least square optimization. Optimization here refers to computing the best possible ROM approximations for a given aerodynamic shape and not to shape optimization; i.e. the quality of the ROM solution is optimized rather than the aerodynamic shape itself. The nonlinear weighted constrained LSQ POD-Based ROM optimization method is able to reconstruct the pressure field from the airfoil/wing surface pressure distribution for example; i.e in the case of the airfoil or the wing, the aerodynamic data field

is (re)created retaining only the pressure values on the airfoil/wing surface. With the knowledge of limited surface pressure data available, the complete pressure field (pressure contours) in the vicinity of the airfoil/wing can be predicted accurately with only few POD modes and shall be quite close to the exact contours computed with the

1.4 Thesis outline

This thesis is organized as follows: **Chapter 2** briefly reviews the fundamentals of aerodynamic design, steady and transonic aerodynamics. The steady formulation of the governing equations are presented, as well as the SMARTy toolbox and the DLR TAU flow solver. The latter is used to generate the various high- and low- fidelities (snapshots) required in the cokriging model and to build the POD basis for example. Challenges linked with the reduced-order basis will be enlightened. **Chapter 4** familiarizes oneself with the various sampling methodologies implemented in this thesis. Moreover, the chapter introduces the theoretical background on all the surrogate modeling techniques employed (cokriging, projection-based models, etc). **Chapter 3** accustoms the reader to methods for nonlinear least squares problems and discusses the parallel between them and the optimization of steady-state aerodynamic problems solutions. An emphasis will be put on algorithms for equality constrained nonlinear least squares problems and the major issues related to their application in large scale problems.

Chapter 5 introduces and discusses results from two aircraft steady aerodynamics applications. Those test cases encompass the prediction, in transonic regime, of local/global aerodynamic coefficients (intrapolation within and extrapolation out of the a priori training set) for the 2D NACA64A010 airfoil using two independent parameters (Ma, AoA) and the NASA Common Research Model (wing-body DPW4 A/C) for one parameter ROM. Furthermore, comparisons of the reconstructed pressure fields (pressure contours) to their counterparts obtained using the FOM (full TAU simulations) will be performed. Additionally, pressure coefficient plots comparisons are presented at 4 different (Ma, AoA) locations for the 2D airfoil and at 3 spanwise locations for the model aircraft case. Lastly, **Chapter 6** concludes the research work and offers leads for future work.

Chapter 2

Aerodynamics design and computational fluid dynamics

The present thesis is concerned with the design of a multi-fidelity LSQ POD-Based ROM framework for aerodynamic design of transport aircraft. The surrogate models involved, namely multi-fidelity and projection-based (POD), require the generation of snapshots that are aerodynamic flow field data collected over a number of time instances within the parameter space. These snapshots are obtained through flow computations, by performing numerical simulations using the DLR's hybrid unstructured CFD flow solver TAU[350] in RANS mode. The most important requirement for aeronautical applications of computational methods in fluid dynamics is the capability to predict the steady flow past a configuration s.t. key performance parameters such as lift to drag ratio (L/D) or $C_{L_{\max}}$ can be estimated. During aircraft maneuvers, the time scales of the motion are large compared with those of the flows, so that unsteady effects are in general secondary; this means the aerodynamic design should normally be based on the analysis of steady flows. Moreover, it is important to be able to calculate steady solutions of aerodynamic flows in transonic range (to be modeled by nonlinear methods for accurate results), where the formation of shock waves lead to the onset of drag rise and a drastic deterioration of the lift to drag ratio (as we approach the sonic boom) and because transonic aerodynamics is known to encompass one of the most efficient regimes of flight. Steady-state transonic ROMs are often more challenging to construct than unsteady ROMs (large shock motion for small Mach number variations). However, many well-established unsteady ROM methods are not directly transferable to steady case.

This study mainly focused on steady-state aerodynamics case studies. Moreover, features

of the DLR Surrogate Modeling for AeRo-data Toolbox (Surrogate Modeling for AeRo-data Toolbox (SMARTy))[255] are employed to deal with POD-based LSQ ROMs for equality constrained problems. The following gives a short introduction to the aerodynamic design of transport aircraft and presents the governing equations of fluid dynamics (including their steady formulation). Additionally, are introduced the DLR flow solver DLR Flow Solver (TAU) and its embedded SMARTy toolbox.

2.1 Aerodynamic design of transport aircrafts

'Design is a problem-solving activity that maps a set of requirements to a set of functions, leading to a set or series of decisions that contribute to the final description of a solution meeting particular needs'[298]. Specifically, design involves defining and exploring a vast space of possibilities that requires the building up of knowledge and a familiarity with the constraints and trades involved. Aerodynamic design is an important phase in aircraft design that concerned with the design and development of aircraft shapes, optimizing performances, manage qualities and loads. One of the main tools used for those aims is computational fluid aerodynamics (CFD), i.e. the capabilities to predict the flow at any location within the parameter space (flight envelope). Design activities involve an irrevocable allocation of resources (money, personnel, infrastructure) as well as a great amount of analysis to help choose an alternative that satisfies the strategic goals, product objectives, customer needs and technical requirements. New aircraft designs have increased in complexity and need to address numerous requirements. As a consequence, today's aircraft aerodynamic design has been greatly transformed and impacted with the advances in computing power, computational analysis and numerical methods; the way designs are conducted has been altered, with the introduction of surrogate modeling techniques that replace expensive codes and experiments[299].

Aircraft aerodynamic design globally encompasses three phases: the conceptual, preliminary and detailed design phases. The conceptual is the most important ones in terms of the number of designs to be developed and examined, the methods and tools to be considered, the feasibility studies to be conducted, etc. The conceptual phase having a strong impact on the overall design costs, it is therefore relevant to introduce optimal methods (such as the ones developed in the present thesis) to help the designers with the complexity of the problems, the lack of relevant knowledge and data encountered regarding those design problems. The main focus of preliminary design is to size the various design

variables optimally to obtain a design that meets requirements and constraints. This requires a multidisciplinary investigation that is out of this thesis. Consequently, though our algorithms could impact the designs in those two first aircraft design phases, the present study will be restricted to the conceptual phase.

2.2 The full order and steady formulation of the governing equations

The derivation of the principal equations of fluid dynamics (Navier-Stokes equations)[351] is based on the fact that the dynamical behavior of a fluid is determined by three conservation laws, namely the conservation of mass, the conservation of momentum, and the conservation of energy. Let an arbitrary finite region of the flow, bounded by the closed surface $\partial\Omega$ and fixed in space, defines the control volume Ω . Lets introduce a surface element as dS and its associated, outward pointing unit normal vector as $\mathbf{n}$. Casting all the conservation equations together yields (in the absence of a source term which comprises all volume sources due to body forces and volumetric heating):

$$\frac{\partial}{\partial t} \int_{\Omega} \mathbf{w} d\Omega + \oint_{\partial\Omega} \mathbf{F} \cdot \mathbf{n} dS = \mathbf{0} \quad (2.1)$$

where $\mathbf{w}$ given as

$$\mathbf{w}^T = (\rho, \rho v_1, \rho v_2, \rho v_3, \rho E) \quad (2.2)$$

is the vector of conservative variables, ρ is the density, E the total energy per unit mass, u, v, w are the components of the velocity vector $\mathbf{v} = (v_1, v_2, v_3)^T$ and $\mathbf{F}$ represents the fluxes through the boundaries of the control volume. the latter consist in the convective flux $\mathbf{F}^c((\mathbf{w})) = (\mathbf{f}_1^c(\mathbf{w}), \mathbf{f}_2^c(\mathbf{w}), \mathbf{f}_3^c(\mathbf{w}))$ and the viscous flux $\mathbf{F}^v(\mathbf{w}, \nabla \mathbf{w}) = (\mathbf{f}_1^v(\mathbf{w}, \nabla \mathbf{w}), \mathbf{f}_2^v(\mathbf{w}, \nabla \mathbf{w}), \mathbf{f}_3^v(\mathbf{w}, \nabla \mathbf{w}))$ whose components are respectively given as

$$\mathbf{f}_i^c(\mathbf{w}) = \begin{pmatrix} \rho v_i \\ \rho v_1 v_i + \delta_{1i} p \\ \rho v_2 v_i + \delta_{2i} p \\ \rho v_3 v_i + \delta_{3i} p \\ (\rho E + p) v_i \end{pmatrix}, \quad i = 1, 2, 3 \quad (2.3)$$

and

$$\mathbf{f}_i^v(\mathbf{w}, \nabla(\mathbf{w})) = \begin{pmatrix} 0 \\ \tau_{1i} \\ \tau_{2i} \\ \tau_{3i} \\ \sum_{j=1}^3 \tau_{ij} v_i - q_i \end{pmatrix}, \quad i = 1, 2, 3 \quad (2.4)$$

where δ_{ij} is the Kronecker symbol and p , $\tau = (\tau_{ij})_{i,j=1,2,3}$ and $\mathbf{q} = (q_1, q_2, q_3)^T$ respectively denote the pressure, the viscous stress tensor and the heat flux. In pure aerodynamics, it has been a commonplace to assume the working fluid to behave like a calorically perfect gas. Expressing the pressure in terms of conservative variables, the following formulation is obtained:

$$p = (\gamma - 1)\rho \left(E - \frac{v_1^2 + v_2^2 + v_3^2}{2} \right) \quad (2.5)$$

with $\gamma = 1.4$ in case the considered fluid is ambient air.

Reynolds Averaged Navier-Stokes (RANS) equations are considered in this thesis due to their popularity in engineering applications and to raise the fundamental difficulties associated with viscous or turbulent flows. This approach, which was presented by Reynolds in 1895, is based on the decomposition of the flow variables into mean and fluctuating parts, followed by time or ensemble averaging. By inserting the decomposed flow variables into the Navier-Stokes equations and averaging, the same equations for the mean variables are formally obtained with the exception of two additional terms: the Reynold stresses tensor and the turbulent heat flux vector that should respectively be incorporated the tensor of viscous stresses and the diffusive heat flux. Thus we can see that the solution of the Reynolds-averaged Navier-Stokes equations requires the modelling of the Reynolds stresses and the turbulent heat flux. The advantages of this approach are that consider-

ably coarser grids can be used compared to numerous other methods and that stationary mean solution can be assumed. More on RANS can be read from J. Blazeck[351], A. Jameson[352], Lomax et al.[353], J. Ferziger[354] or J. Anderson et al.[355]. The Spalart-Allmaras one-equation turbulence model [351] is considered in this thesis to model the turbulence.

Consider the Navier-Stokes equations, spatially discretized on a grid of size n_g for some aerodynamic configuration. Let n_v be the corresponding number of primitive mean-flow variables including the number of primitive variables associated with the turbulence model. The primitive mean-flow variables are the density ρ , the velocity components in all spatial directions (u_x, u_y, u_z) , and the total energy E . The number of primitive turbulence variables is subject to the chosen turbulence model. Let $n = n_v n_g$ denotes the total length of the discretized flow solution vectors. Given a finite volume spatial discretization scheme, the corresponding system of semi-discrete ordinary differential equations can be written as:

$$\frac{d}{dt} \mathbf{w}(t; \boldsymbol{\mu}) + \boldsymbol{\Omega}^{-1} \text{res}(\mathbf{w}(t; \boldsymbol{\mu})) = \mathbf{0} \in \mathbb{R}^n \quad (2.6)$$

where $t \in \mathbb{R}^+$ denotes the time, $\boldsymbol{\mu} \in \mathbb{R}^d$ the vector of input parameters, $\mathbf{w}(t; \boldsymbol{\mu}) \in \mathbb{R}^n$ the state vector of primitive variables and $\text{res}(\mathbf{w}(t; \boldsymbol{\mu})) \in \mathbb{R}^n$ the vector of flux residuals corresponding to the state solution $\mathbf{w}(t; \boldsymbol{\mu})$. $\boldsymbol{\Omega} \in \mathbb{R}^{n \times n}$ is a diagonal matrix with n_v sub-blocks, each containing the cell volumes $(vol_1, \dots, vol_{n_g})$ of the corresponding computational grid on the diagonal, stems from the spatial discretization of the flow problem and induces the discrete L_2 -metric. Denoting by $\mathbf{w}_{k,i}$ the value of the flow variable k corresponding to grid cell i and by $\text{res}_{k,i}(\mathbf{w})$ the flux residual of flow variable k in grid cell i , the system of Eq. (2.6) may be written in cell-wise form as

$$\forall k = 1, \dots, n_v \quad \forall i = 1, \dots, n_g : \quad \frac{d}{dt} \mathbf{w}_{k,i} + \frac{1}{vol_i} \text{res}_{k,i}(\mathbf{w}) = 0 \quad (2.7)$$

An equivalent formulation for conservative variables is found in [351]. The steady state is achieved if the time derivative drops out in Eqs. (2.6) & (2.7), or equivalently, if the CFD flux residual vanishes:

$$\mathbf{0} = \boldsymbol{\Omega}^{-1} \text{res}(\mathbf{w}(\boldsymbol{\mu})) \in \mathbb{R}^n \quad (2.8)$$

The weights matrix $\boldsymbol{\Omega}^{-1}$ stems from the spatial discretization of the flow problem. when

computing approximations to Eq. (2.8) restricted to a subspace of lower dimension, the weighting is significant.

2.3 The DLR flow solver TAU and the SMARTy toolbox

The following introduction of TAU is based on the description of TAU on the DLR website (<http://tau.dlr.de/code-description/>) and from the publication of Rossow et al.[350].

TAU is a leading modern high-performance software system for computational fluid dynamics (CFD), owned by the German Aerospace Center (DLR), that delivers fast, reliable and accurate solutions across a wide range of CFD applications. TAU is made up of libraries that enable developers and maintainers to easily accomplish multiple tasks ranging from adding new features, carry on maintenance on or reuse parts of the source code or its full content. Applications of TAU encompass the prediction of viscous and inviscid flows over complex geometries, within the low subsonic and the hypersonic flow regime, making use of hybrid unstructured grids. The various modules of TAU, below described in few words, can both be used as stand-alone tools with corresponding file I/O or within a Python scripting framework (TAU Python), that allows an inter-module communication using common memory allocation. TAU presents advanced parallel performance features and its optimization for cache processors through specific edge colouring procedures. The parallelization procedure is based on domain decomposition and on library specification for message-passing (Message Passing Interface (MPI)). The main uses of TAU comprises simulations of complex aircraft configurations within the flight physics context; though applications to chemical or space shuttle launch and re-entry aerodynamics have proven to exhibit satisfactory results.

Grid generation plays a key role in any scientific computing problem. Though TAU encompass grid adaptation and deformation modules, it does not provide a mesh generation utility. TAU uses both (block-) structured and hybrid unstructured grids. A dual mesh approach is possible to make the solver independent of the type of cells that the initial grid is made of and to better resolve the wake in traditional calculations about complex geometries. Numerous spatial discretization schemes are implemented within TAU, including several upwind methods or the central differencing scheme with artificial dissipation. A typical (primary) TAU code uses an explicit Runge-Kutta multistage scheme in combination with an explicit residual smoothing. Multigrid methods, based on the the

agglomeration of the control volumes of the dual grid for coarse grid computations, are embedded in order to accelerate the convergence of basic iterative methods within the code. Moreover, a grid adaptation algorithm for hybrid meshes based on local grid refinement and wall-normal mesh movement in semi-structured near-wall layers is implemented with the aim to efficiently resolve detailed flow features. TAU allows to deal with unsteady flows, arbitrary motion and grid deformation. A major reason for using implicit methods is to enhance the stability of the numerical schemes, allowing to take large timesteps, which is not possible with explicit methods. within TAU, a dual time stepping scheme is employed. To overcome the problem posed by the slow convergence of computations at low speed, a convergence acceleration technique, namely preconditioning is implemented.

Turbulence models allow to compute the mean flow without first calculating the full time-dependent flow field. The standard turbulence model in TAU is the Spalart-Allmaras model with Edwards modification. It has proven to yield highly satisfactory results for a wide range of aero applications, while maintaining a high level of numerical robustness. Beside this model, numerous others are incorporated among which several $k - \epsilon$ models with and without compressibility corrections, nonlinear explicit algebraic Reynolds stress models (EARSIM) and linearized LEA models. Additionally, rotation corrections for vortex dominated flows are available for the different models. TAU also allows to perform detached eddy simulations (DES) based on the Spalart-Allmaras model and few hybrid Large Eddy Simulations (LES) methods. with the advent of the idea of overlapping grids (subsequently named as Chimera grid after the mythical Chimera beast) and its proven capability to efficiently simulate aircraft manoeuvres, the chimera methodology was also embedded within TAU.

SMARTy stands for Surrogate Modeling for AeRo data Toolbox. It was developed at the DLR Institute for Aerodynamics and Flow Technology and is nowadays embedded within TAU. It is implemented in Python programming language and contains a significant number of modules that were designed in support of design of experiments, adaptive sampling, surrogate modeling (interpolation models), multi-fidelity modeling, ROM, dimensionality reduction, optimization, etc. SMARTy is flexible, parallelized in the core functionality and is integrated as a plug-in in the TAU CFD environment. SMARTy has been employed in target loads aerodynamics, data fusion, uncertainty quantification, acceleration of CFD computations, rapid loads prediction across the flight envelope or data compression. It ROM-based surrogate models have been applied in flow control, aeroelasticity or other couple simulations in lieu of full order expensive aerodynamic models. Several methods

Table 2.1: SMARTy features description.

Design of experiments, DoE	Full factorial, Quasi Monte Carlo, LHS, Halton
Sample selection algorithms	MSE-based, cross-validation-based, TAU residual-based EIF, manifold filling, combinations, adaptive
Surrogate model types	Radial Basis Functions, TPS Kriging (Simple, Ordinary, Universal, Hierarchical, Regression) Gradient-Enhanced Kriging
Correlation functions / kernels	Gaussian exp., Gaussian, cubic spline, TPS, power
Model-order reduction techniques	POD, incl. SVD update, Gappy POD, tKLE Isomap Low-rank approximation (cross-approx., low-rank EVD)
Model parameter optimization	Levenberg-Marquardt non-lin. LSQ Constrained Gauß-Newton (both parallelized)

employed to obtain ROMs for the prediction of steady and unsteady aerodynamic flows using low-dimensional linear subspaces as well as nonlinear manifolds and whose performances may be further improved by applying sampling techniques and hyper-reduction procedures are implemented in SMARTy. Table 2.1 summarized the features offered by SMARTy.

Chapter 3

Algorithms for constrained nonlinear least squares equality problems

Optimization is an important decision-making and system analysis tool in engineering sciences that can be, mathematically speaking, recapped as a maximization or minimization of an objective function subject to constraints on its parameters or variables that can be explicitly constrained [303, 341].

$$\min_{\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^d} f(\mathbf{x}) \text{ subject to } \begin{cases} c_j(\mathbf{x}) = 0, & j \in \mathcal{J} \\ c_k(\mathbf{x}) \leq 0, & k \in \mathcal{K} \end{cases} \quad (3.1)$$

The idea to consider specific solution methods for constrained nonlinear least squares problems, was born when designing an interactive software system for mathematical programming [449]. Generally, problems of the form 3.1 can be classified as discrete or continuous, or even according to the linear/nonlinear/convex nature of the objective functions and constraints, the smoothness of the objective functions (differentiable or non-differentiable), the type of solutions we are interested in (global or local optimization) or the number of design variables. Nonlinear problems tend to arise naturally in the physical sciences and engineering, and are becoming more widely used in aircraft aerodynamics. Nonlinear optimization (or nonlinear programming) [303, 341] is the term used to describe an optimization problem within which the objective or constraint functions are not linear, but not known to be convex. Till date, there is, to our knowledge, no robust or fully satisfactory methodology

for solving general nonlinear optimization problems. Solving problems with as few as 10 design variables can be extremely challenging; worse, problems with hundreds or more design variables can become intractable. The resolution of nonlinear optimization problems is based on multiple approaches, each of which involves some compromise. Least squares problems [446, 447] arise most often in the context of optimal control, parameter estimation or data fitting applications. It addresses the problem of minimizing the L_2 -norm of a multivariate or parametric function,

$$\min_{\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^n} \frac{1}{2} \|\mathbf{f}(\mathbf{x})\|_{L_2}^2 \quad (3.2)$$

where $\mathbf{f}(\mathbf{x})$ is a vector in $\mathbb{R}^n$ whose components are real-valued nonlinear functions with continuous second partial derivatives. We shall refer to the function $\frac{1}{2} \|\mathbf{f}(\mathbf{x})\|_{L_2}^2$ as the nonlinear least-squares objective function. Therefore least squares minimization aims at reducing the sum of squares of the errors between the snapshots (training points) and the original function through a sequence of updates to parameter values. If the fit function is non linear in the parameters, the least squares problem is nonlinear. Least squares problems have a number of statistical interpretations, e.g. as maximum likelihood estimation of a vector $\mathbf{x}$, given linear noisy measurements, with errors being Gaussian-distributed [4, 5]. Much research has focused on the development of efficient algorithms that attempt to exploit the structure of the nonlinear least-squares objective. Solving constrained nonlinear least squares problems is (in general) much harder than solving unconstrained cases; determining if a solution exists is hard, with no guarantee that it exist. Numerous algorithms exist for the solutions of linear and nonlinear least-squares problems, mainly for the unconstrained cases. A comprehensive introduction of algorithms for least squares problems is given in Björck [448]. Couple of nonlinear least-squares software exist. As an example, numerical software libraries such as SAS, programming environments or collection of software libraries such as IMSL, Mathematica, Matlab or Python contain nonlinear least-squares implementations. More efficient implementations include, for example DFNLP [449], MINPACK [450], NL2SOL [328] or ELSUNC and ENLSIP [451, 452], two software packages that respectively solve simple bounded and general equality constrained nonlinear least squares problems. The present research focus on algorithms solving constrained nonlinear equality that is finding the least squares minimizer of Eqn. 3.3, with equality constraints only introduced in the form of simple bounds.

$$\min_{\mathbf{a}_1, \dots, \mathbf{a}_{\tilde{m}}} \left\| \Omega^{-1} \text{res}(\mathbf{w}(\mathbf{a})) \right\|_{L_2}^2 = \sum_{k=1}^{n_v} \sum_{i=1}^{n_g} \frac{1}{\text{vol}_i} (\text{res}_{k,i}(\mathbf{w}(\mathbf{a})))^2 \quad (3.3)$$

As previously mention, solving the constrained nonlinear least squares equality (Constrained Nonlinear Least Squares Equality (CNLLE)) problems consists in finding the least squares minimizer of Eqn. 3.3 subject to the equality constraints. By prescribing that the curve should interpolate at some points we get an equality constrained curve fitting problem, that is

$$\min_{\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^d} f(\mathbf{x}) \left\{ \begin{array}{l} \text{subject to} \\ c(\mathbf{x}) = 0 \end{array} \right. \quad (3.4)$$

Though nonlinear least squares problems can be solved with the use of general optimization methods, this section presents two proficient methods:

- a block-wise inversion version of the hybrid Gauss-Newton method introduced by Gullikson et al. [453],
- and the Levenberg-Marquardt algorithm (also known as a damped least-squares method) [443], a robust pseudo-second order modification of the Gauss-Newton algorithm, proposed by K. Levenberg [329], that significantly outperforms gradient descent and conjugate gradient methods.

3.1 The hybrid block-wise inversion Gauss-Newton method

The choice of this method is motivated by the nature of the problem in Eqn. 3.3 (a constrained and weighted nonlinear least squares equality problem) and the known poor convergence performance of the classical Gauss-Newton method. Assume a number of n_c constraints given in the form of vector-valued function $g(\mathbf{a}) \in \mathbb{R}^{n_c}$ depending on the proper orthogonal decomposition (POD) coefficients, with the number of constraints is smaller than the number of POD basis modes ($n_c < \tilde{m}$); $n_c = 0$ meaning the optimization problem becomes unconstrained. Suppose we wish to approximate the flowfield at untried locations given, for example, some target global aerodynamic coefficients C_L^{target} , C_D^{target} or C_M^{target} to be met. g takes the form

$$g(\mathbf{a}) = \begin{pmatrix} C_L(\mathbf{w}(\mathbf{a})) - C_L^{\text{target}} \\ C_D(\mathbf{w}(\mathbf{a})) - C_D^{\text{target}} \\ C_M(\mathbf{w}(\mathbf{a})) - C_M^{\text{target}} \end{pmatrix} \quad (3.5)$$

where $\mathbf{w}(\mathbf{a})$ is the approximate ROM solution corresponding to the vector of POD coefficients $\mathbf{a}$ according to Eqn. 3.6.

$$\mathbf{w}^i(\mathbf{a}) = \bar{\mathbf{w}} + (\mathbf{U}_1, \dots, \mathbf{U}_{\tilde{m}})\mathbf{a} = \frac{1}{m} \sum_{j=1}^m \mathbf{w}^j + \frac{1}{\tilde{m}} \sum_{j=1}^{\tilde{m}} \mathbf{a}_j^i \mathbf{U}^j \quad (3.6)$$

Introducing the function $f(\mathbf{a}) = \text{res}(\mathbf{W}(\mathbf{a}))$, Eqn. 3.3 can be rewritten as:

$$\min_{\mathbf{a} \in \mathbb{R}^{\tilde{m}}} \left\| \Omega^{-1} f(\mathbf{a}) \right\|_{L_2}^2 = \min_{\mathbf{a} \in \mathbb{R}^{\tilde{m}}} \left\| \Omega^{-\frac{1}{2}} f(\mathbf{a}) \right\|_2^2 \begin{cases} \text{subject to} \\ g(\mathbf{a}) = 0 \end{cases} \quad (3.7)$$

By analogy, considering $\Omega^{-\frac{1}{2}}$ to be the weight matrix, the problem above can be solved using the publication of Gullikson et al. [453] on algorithms for constrained and weighted nonlinear least squares problems. All methods for non-linear optimization are iterative, that is starting from a spatial location $\mathbf{a}^0$, the method generates a sequence of location vectors $\mathbf{a}^1, \mathbf{a}^2, \dots$, that will (hopefully) converges to $\mathbf{a}^*$, a local minimizer for the given function. Assuming the function f to be twice continuously differentiable and that the weight matrix $\Omega^{-\frac{1}{2}}$ is a diagonal matrix with non-negative entries. In the Gauss-Newton method, the nonlinear least squares problem $\min_{\mathbf{a} \in \mathbb{R}^{\tilde{m}}} \left\| \Omega^{-\frac{1}{2}} f(\mathbf{a}) \right\|_2^2$ is linearized around the current iteration point $\mathbf{a}^k$ with the search direction $\mathbf{d}^k \in \mathbb{R}^{\tilde{m}}$ being computed as

$$\min_{\mathbf{d}^k} \frac{1}{2} \left\| \Omega^{-\frac{1}{2}} (f^k + \mathbf{J}^k \mathbf{d}^k) \right\|^2 \quad (3.8)$$

where $f^k = f(\mathbf{a}^k)$ and $\mathbf{J}^k = \nabla f(\mathbf{a}^k)$ is the jacobian matrix. Given the approximate solution at an iteration step k , the next iterate is

$$\mathbf{a}^{k+1} = \mathbf{a}^k + s^k \mathbf{d}^k \quad (3.9)$$

where $s^k \in \mathbb{R}$ and $\mathbf{d}^k$ are respectively the step length and the search direction at stage k .

In the presence of large weights, possibly infinite, it is appropriate to reformulate (3.8) as

$$\begin{pmatrix} \mathbf{0}^{n_c \times n_c} & \mathbf{0}^{n_c \times n_t} & \mathbf{D}_g(\mathbf{a}^k) \\ \mathbf{0}^{n_t \times n_c} & \Omega & \mathbf{D}_f(\mathbf{a}^k) \\ \mathbf{D}_g^T(\mathbf{a}^k) & \mathbf{D}_f^T(\mathbf{a}^k) & \mathbf{0}^{\tilde{m} \times \tilde{m}} \end{pmatrix} \begin{pmatrix} \mu_1^k \\ \mu_2^k \\ \mathbf{d}^k \end{pmatrix} = \begin{pmatrix} -g(\mathbf{a}^k) \\ -f(\mathbf{a}^k) \\ \mathbf{0} \end{pmatrix} \quad (3.10)$$

where $\mathbf{D}_g \in \mathbb{R}^{n_c \times \tilde{m}}$ is the Jacobian of the constraints function, $\mathbf{D}_f \in \mathbb{R}^{n_t \times \tilde{m}}$ is the Jacobian of the least-squares objective function and $(\mu_1^k, \mu_2^k)^T \in \mathbb{R}^{n_c + n_t}$ is a vector of Lagrange

multipliers at iteration stage k . The system matrix in (3.10) is nonsingular if and only if the rows in the Jacobians D_g, D_f that correspond to infinite weights are linearly independent and the Jacobians have full column rank at stage k (lemma 2.1, [453]). Hence, the Gauss-Newton method applied to constrained optimization problem (3.7) requires, at each iteration stage, solving the $(n_c + n_t + \tilde{m}) \times ((n_c + n_t + \tilde{m}))$ equation system. It should be noted that the system matrix scales with the grid size via $n_t = n_g \times n_v$. In the context of reduced-order model, it then appears impossible to solve the system matrix (3.10). Zimmermann et al. introduced a workaround solution to this hardship in [349].

Setting

$$\mathbf{R} := \begin{pmatrix} \Omega & D_f \\ D_f^T & \mathbf{0}^{\tilde{m} \times \tilde{m}} \end{pmatrix} \quad \text{and} \quad \mathbf{F} := \begin{pmatrix} \mathbf{0}^{n_t \times n_c} \\ D_g^T \end{pmatrix} \quad (3.11)$$

the system matrix (3.10) reads

$$\left(\begin{array}{c|c} \mathbf{0}^{n_c \times n_c} & \mathbf{F}^T \\ \hline \mathbf{F} & \mathbf{R} \end{array} \right) \quad (3.12)$$

and allows for a direct block-inversion ([454], p. 70), resulting in

$$\left(\begin{array}{cc} \mathbf{0} & \mathbf{F}^T \\ \mathbf{F} & \mathbf{R} \end{array} \right)^{-1} = \left(\begin{array}{c|c} \mathbf{S} & -\mathbf{S}\mathbf{F}^T\mathbf{R}^{-1} \\ \hline -\mathbf{R}^{-1}\mathbf{F}\mathbf{S} & \mathbf{R}^{-1} + \mathbf{R}^{-1}\mathbf{F}\mathbf{S}\mathbf{F}^T\mathbf{R}^{-1} \end{array} \right) \quad (3.13)$$

where $\mathbf{S} = -(\mathbf{F}^T\mathbf{R}^{-1}\mathbf{F})^{-1} \in \mathbb{R}^{n_c+n_c}$ is the so-called Schur' complement ([454], p. 68). Applying the same trick to the block matrix $\mathbf{R}$ and exploiting this in Eqn. 3.10, the following closed formula for the search direction is derived as:

$$\begin{aligned} \mathbf{d}^k &= \left(-\mathbf{T}D_g^T\mathbf{S} \left| (\mathbf{I} + \mathbf{T}D_g^T\mathbf{S}D_g)\mathbf{T}D_f^T\Omega^{-1} \right| - (\mathbf{I} + \mathbf{T}D_g^T\mathbf{S}D_g)\mathbf{T} \right) \begin{pmatrix} -\mathbf{g} \\ -\mathbf{f} \\ \mathbf{0} \end{pmatrix} \\ &= \mathbf{T}D_g^T\mathbf{S}\mathbf{g} - (\mathbf{I} + \mathbf{T}D_g^T\mathbf{S}D_g)\mathbf{T}D_f^T\Omega^{-1}\mathbf{f} \end{aligned} \quad (3.14)$$

with $\mathbf{T} = (D_f^T\Omega^{-1}D_f)^{-1}$, $\mathbf{S} = -(D_g\mathbf{T}D_g^T)^{-1}$ and $\mathbf{I} = \mathbf{I}^{\tilde{m} \times \tilde{m}}$.

To keep the computational complexity at a feasible and reasonable level, the line search for computing the optimal step size s_k is set to a constant value of $s_k = 1, \forall k$. Using a Cauchy-type stopping criterion, Convergence is achieved if there is no significant difference

between iterations $k + 1$ and k . More precisely, the algorithm stops if

$$\|\mathbf{d}^k\|_2 < \epsilon(\|\mathbf{a}^k\|_2 + \epsilon) \quad (3.15)$$

where ϵ is a user-defined threshold. Algorithm 3.1 summarizes the various steps in the above constrained Gauss-Newton optimization scheme.

Algorithm 3.1 Constrained least-squares Gauss-Newton algorithm

Input: iteration bounds k_{max} , initial vector of POD coefficients $\mathbf{a}^0$, finite difference step size $\delta > 0$, convergence threshold $\epsilon > 0$, POD data $\mathbf{U}^j, \lambda_j, j = 1, \dots, \tilde{m}$

Output: local minimizer

```

1: for  $k \leftarrow 0, \dots, k_{max}$  do
2:   take the weights into account - compute  $\tilde{\mathbf{f}}_k \leftarrow \Omega^{-\frac{1}{2}} \mathbf{f}(\mathbf{a}^k)$ 
3:   finite difference approximation of the Jacobian of residual - compute:
4:    $\mathbf{D}_{\tilde{\mathbf{f}}_k} := \mathbf{D}_{\tilde{\mathbf{f}}}(\mathbf{a}^k) \leftarrow (\partial_1 \tilde{\mathbf{f}}(\mathbf{a}^k), \dots, \partial_{\tilde{m}} \tilde{\mathbf{f}}(\mathbf{a}^k)),$ 
5:   with  $\partial_j \tilde{\mathbf{f}}(\mathbf{a}^k) \leftarrow \frac{1}{\delta \sqrt{\lambda_j}} (\tilde{\mathbf{f}}(\mathbf{a}^k + \delta \sqrt{\lambda_j} \mathbf{e}_j) - \tilde{\mathbf{f}}(\mathbf{a}^k)), j \leftarrow 1, \tilde{m}$ 
6:   finite difference approximation of the Jacobian of constraints - compute:
7:    $\mathbf{D}_{\mathbf{g}_k} := \mathbf{D}_{\mathbf{g}_k}(\mathbf{a}^k) \leftarrow (\partial_1 \mathbf{g}(\mathbf{a}^k), \dots, \partial_{\tilde{m}} \mathbf{g}(\mathbf{a}^k))$ 
8:   with  $\partial_j \mathbf{g}(\mathbf{a}^k) \leftarrow \frac{1}{\delta \sqrt{\lambda_j}} (\mathbf{g}(\mathbf{a}^k + \delta \sqrt{\lambda_j} \mathbf{e}_j) - \mathbf{g}(\mathbf{a}^k)), j \leftarrow 1, \tilde{m}$ 
9:   compute  $\mathbf{H} := \mathbf{T}^{-1} \leftarrow \mathbf{D}_{\tilde{\mathbf{f}}_k}^T \mathbf{D}_{\tilde{\mathbf{f}}_k} \in \mathbb{R}^{\tilde{m} \times \tilde{m}}$ 
10:  and  $\mathbf{h} := \mathbf{D}_{\tilde{\mathbf{f}}_k}^T \tilde{\mathbf{f}}_k \in \mathbb{R}^{\tilde{m}}$ 
11:  solve  $\mathbf{H}\mathbf{P} \leftarrow \mathbf{D}_{\mathbf{g}_k}^T, \mathbf{P} \in \mathbb{R}^{\tilde{m} \times n_c}$ 
12:  solve  $\mathbf{H}\mathbf{x} \leftarrow \mathbf{h}, \mathbf{x} \in \mathbb{R}^{\tilde{m}}$ 
13:  compute  $\mathbf{S} \leftarrow -(\mathbf{D}_{\mathbf{g}_k} \mathbf{P})^{-1} \in \mathbb{R}^{n_c \times n_c}$ 
14:  compute  $\mathbf{Q} \leftarrow \mathbf{P}\mathbf{S} \in \mathbb{R}^{\tilde{m} \times n_c}$ 
15:  compute the search direction  $\mathbf{d}^k \leftarrow \mathbf{Q}\mathbf{g}_k - (\mathbf{x} + \mathbf{Q}\mathbf{D}_{\mathbf{g}_k} \mathbf{x}) \in \mathbb{R}^{\tilde{m}}$ 
16:  if  $\|\mathbf{d}^k\|_2 < \epsilon(\|\mathbf{a}^k\|_2 + \epsilon)$  : break
17:   $\mathbf{a}^{k+1} \leftarrow \mathbf{a}^k + \mathbf{d}^k$ 
18:   $k \leftarrow k + 1$ 

```

In this thesis, Broyden's rank-one updates [454] are used to compute the Jacobian during optimization. The idea behind Broyden's method is to compute the whole Jacobian only at the first iteration and to do a rank-one update at the other iterations. A value of $\delta = 10^{-4}$ is used in the finite difference approximation in steps 3 and 4. The weighting of δ by the singular value $\sqrt{\lambda_j}$ accounts for the different orders of magnitude of the POD coefficients. A value of $\epsilon = 10^{-6}$ is specified for the stopping criterion.

3.2 The Secant Levenberg-Marquardt Method

Another iterative algorithm, that combines elements of quasi-Newton and steepest descent, for solving nonlinear least squares problems was suggested by Levenberg [329] and Mar-

quardt [330] to mitigate the drawbacks of the Gauss-Newton method previously introduced and improve both its convergence speed and robustness to initial parameter guesses. Levenberg and Marquardt each proposed damping the $\mathbf{J}^T \mathbf{J}$ matrix by a diagonal cutoff. The Levenberg-Marquardt algorithm (also known as damped Gauss-Newton method) can be considered as an interpolation between the Gauss-Newton method and the gradient descent method. Because the damping factor λ can tune as needed, the Levenberg-Marquardt algorithm is well-suited for solving nonlinear least-squares minimization problems and related numerical difficulties. The steps in the Levenberg-Marquardt algorithm are quite similar to those of the Gauss-Newton algorithm, with the Broyden method employed to update the Jacobian and reduce the computational cost (see Algorithm 3.34 in [443]). Algorithm 3.2 presents a simplified version of the steps in the Levenberg-Marquardt algorithm.

Algorithm 3.2 Simplified Levenberg-Marquardt algorithm

Input: iteration bounds k_{max} , initial vector of POD coefficients $\mathbf{a}^0$, finite difference step size $\delta > 0$, convergence threshold $\epsilon > 0$, POD data $\mathbf{U}^j, \lambda_j, j = 1, \dots, \tilde{m}$, damping factor $\mu > 0$

Output: local minimizer

- 1: $\tilde{\mathbf{f}}_k \leftarrow \Omega^{-\frac{1}{2}} \mathbf{f}(\mathbf{a}^k)$
 - 2: **for** $j \leftarrow 1, \dots, \tilde{m}$ **do**
 - 3: $\partial_j \tilde{\mathbf{f}}(\mathbf{a}^k) \leftarrow \frac{1}{\delta \sqrt{\lambda_j}} (\tilde{\mathbf{f}}(\mathbf{a}^k + \delta \sqrt{\lambda_j} \mathbf{e}_j) - \tilde{\mathbf{f}}(\mathbf{a}^k))$
 - 4: **if** $\tilde{\mathbf{f}}(\mathbf{a}^k) = 0$ **stop**
 - 5: $\mathbf{H} \leftarrow \mathbf{D}_{\tilde{\mathbf{f}}_k}^T \mathbf{D}_{\tilde{\mathbf{f}}_k}, \mathbf{h} \leftarrow \mathbf{D}_{\tilde{\mathbf{f}}_k}^T \tilde{\mathbf{f}}_k$
 - 6: compute the search direction $\mathbf{d}^k$, solving $(\mathbf{H} + \mu \mathbf{I}) \mathbf{d}^k = -\mathbf{h}, \mathbf{d}^k \in \mathbb{R}^{\tilde{m}}$
 - 7: $\mathbf{a}^{k+1} \leftarrow \mathbf{a}^k + \mathbf{d}^k, k \leftarrow k + 1$ & go to step 2:
-

Note that both algorithms are well-defined and that all iterates $\mathbf{a}^k$ belong to a feasible set.

Chapter 4

Design of experiments via surrogate modeling

Surrogate modeling has drawn an increasing interest over the years among the aerodynamic communities, in the field of real-time and many-query analyses. Despite the advances in computational fluid dynamics (CFD), numerous scenarios remain computationally expensive and intractable due to the great number of calls of the FOM algorithms. In lieu of dense computations which generally explode allocated computational budgets, mathematical-based approximations are often used starting with a generation of training points through design of experiments. The present chapter introduces the selected methodologies that are employed in this work to sample the design space (classical and modern design experiments) and to approximate the black-box functions (data-fits, projection-based and multi-fidelity models).

4.1 Classical and smart a priori sampling techniques

Quantitative and qualitative assessment of design of experiments at the exploratory phase is nowadays a topic of great interest for aircraft industrial aerodynamic engineers due to their influence on global aerodynamic optimization and their many features when scrutinizing new concepts. Furthermore, in an engineering era governed by restrained computational budgets and optimization, simulation-based experiments (sampling)[24] have appeared to be a rapid alternative to approximate expensive physical experiments and to get a better insight into problems.

Traditionally (likely due to their popularity and flexibility [356]), most aircraft aerodynamic engineers mainly use a constant but comprehensive a priori set of grid designs or latin hypercube samples (Latin Hypercube Sampling (LHS)) generated randomly or using a fusion of past experience, current knowledge and future outlooks of the systems. Moreover, though many conventional aircrafts have substantially linear aerodynamic characteristics over their flight envelopes, numerous modern civil transport aircrafts present very large flight envelopes with critical/complex aerodynamic nonlinearities at their extremes [299]; aerodynamic non-linearities whose approximate trends (via surrogate models) are not well captured using LHS or grid designs, mainly because the latter have no claim to optimality and their efficiency in high dimensional spaces still posed numerous questions mainly related to the degree of uniformity and orthogonality of the training points. Moreover, with an increasing interest towards beyond stall and buffet boundaries designs, the development and introduction of **advanced** a priori (also known as model-free or one shot or non-adaptative or offline or one-stage) sampling methods then appeared to be central, considering their effects on the surrogate models accuracy and eventually the global optimum [4, 5]. Over the years, statisticians have developed many sampling strategies to address different design space exploration demands in terms of coverage and spread [357], among which the space-filling designs [29], that tends to scatter the training points uniformly within the design space. In the context of surrogate-based optimization (especially Efficient Global Optimization (EGO)) that is influenced by a priori samplings, building the initial data set (choice of the experimental design, initial number of sample points and their locations) remain a cumbersome tasks [4, 5]. Aircraft aerodynamics engineers still have very little or no guidance on the topic due to the nature and complexity of the underlying problems [89, 90], their narrow experience on the various design of experiments and the barrier of industrial best practices. Recent papers [358, 26] addressed the issue from a global engineering design point of view, focusing on efforts to modify LHS and non-LHS based approaches by introducing several optimality and projective criteria in order to achieve minimum-bias designs in higher dimensions.

This thesis follows the industrial sampling recommendations presented in Subsubsection 1.2.2.3. A smart sampling strategy require not only a good off-line coverage of the design space, with the fewest possible number training points but also (if required) an efficient sequential sampling where required; searching for space-filling in order to simultaneously reduce the effect of noise and bias errors, and allowing considerable time-savings. Therefore, an appropriate choice of the locations of these samples in the parameter do-

main is fundamental in order to capture accurately the behavior of the physical system in the entire domain. There are numerous hands-on approaches when thinking of a smart strategy to locate the initial sampling points or snapshots and beyond, to a priori sample the parameter space for surrogate model construction or to build a ROB, among which:

- Starting with quite a good space-filling approaches at the off-line stage and smartly sequentially update the design space online,
- Taking advantage of some a priori knowledge of the problem physics to efficiently sample off-line specific areas of the design space and smartly adaptatively update the design space online,
- Starting with one or few randomly distributed training points and using greedy algorithms, stochastic optimization algorithms, simulated annealing, threshold accepting heuristic or evolutionary algorithms to optimally update the design space.

As previously mentioned, the samples location will determine the accuracy of the resulting surrogate in the entire parameter space. In the specific case of projection-based surrogate models, possible approaches:

- uniform (space-filling) designs for $d \leq 5$
- latin hypercube samplings, LCVT for high dimensional spaces
- goal-oriented greedy sampling that exploits the accuracy of the ROM-surrogate.

The following introduces the various a priori strategies used to generate samples offline in this thesis:

4.1.1 Fractional designs

Factorial designs[10, 17, 18, 20], are sets of level-combinations that enable an experimenter to study the joint effect of the design variables on the objective functions. In factorial designs, all possible combinations of the design variables levels are investigated during each complete replication of the experiment. It is assumed that the designs are completely randomized, i.e. all the design variables (level combinations in the experiment) are randomly assigned experimental units (also known as treatments). Randomization is significant in any CDoE because an experimenter cannot always be certain that all the main influences on the objective function has been considered in the experiment. A factorial design can be

either full or fractional factorial. Generally, factorial designs tend to set points at the vertex of the hypercube. with an increasing number of factors, they lead to grid designs with sample points spread evenly within the design space. However, such grid designs can also be built using simplest deterministic and symmetric modifications without having points at the boundaries nor at the vertex of the parameter space. Fig. 4.1 presents examples of 3-factors full-factorial samplings illustrating the above-mentioned cases. Fig. 4.1 and Table 4.2 respectively introduce a 2^3 full-factorial design geometric view and its design matrix.

Table 4.1: Full-factorial geometrical view[10].

Run	A	B	C	Labels	A	B	C
1	-	-	-	(1)	0	0	0
2	+	-	-	a	1	0	0
3	-	+	-	b	0	1	0
4	+	+	-	ab	1	1	0
5	-	-	+	c	0	0	1
6	+	-	+	ac	1	0	1
7	-	+	+	bc	0	1	1
8	+	+	+	abc	1	1	1

Table 4.2: 2^3 full factorial design matrix.

Figure 4.1: Examples of 3-levels full factorial sampling plan in the unit cube.

Industrial experimenters have mainly focused on factorial designs at 2-levels (2^k) or 3-levels (3^k), k being the number of factors or design variables. As an example, the 2^k full factorial design consists of all 2^k combinations of the k factors, considering two levels (2^k runs). Rarely will an experimenter go beyond 3-levels because the methodology behind the generation of such designs is very cumbersome and such designs are not the most efficient way to model the complex relationship between the factors and the experimental

responses. Full factorial designs present however numerous limitations:

- The size of the experiment is function of the number of design variables involved, restricting the use of full-factorial design to a maximum number of 4 design variables, because testing all combinations of design variables levels would be time consuming and expensive. The larger the number of dimensions (design variables), the harder the problem becomes experimentally.
- It is assumed for a 2-levels full factorial design that the response is approximately linear over the range of the design variables.

In an attempt to overcome the first drawback, fractional factorial designs were introduced by Finney [359] and consist of subsets or fractions of full factorial designs. If the experimenters assume that certain higher-order interactions are negligible, then a reasonable assessment of the influence of the design variables on the objective function and the desired interaction effects can be obtained by running only a minimum number of experimental cases, therefore a fraction of the full factorial experiment. Fractional factorial designs have been widely in industry (screening, first-order models fitting, etc) and are generally represented in the form $2^{(k-p)}$, where k is the number of design variables and $1/(2p)$ represents the fraction of the full factorial 2^k . An important question that arises is the criteria that guide the experimenter in the selection of suitable fractions. The most commonly used ones are the resolution and minimum aberration[22]. Moreover, full and fractional factorial designs have displayed some complexities while arranging the experiments in blocks (confounding), for fitting second or higher order polynomial models[10]. Extensive theoretical coverage of fractional factorials experiments is given in [32, 360, 361, 362, 363, 364, 365]. Industrial applications examples are found in [33, 366, 367, 368]. Plackett and Burman[369] proposed a special category of 2-level fractional factorial designs, where only a few specifically chosen runs are performed to investigate just the main effects (i.e. no interactions and there is a need to learn as much as possible from a smallest amount of data).

4.1.2 Uniform designs

Introduced by Fang[61] and motivated by a will of avoiding uneven designs which could yield to inaccurate surrogates that are very sparsely observed parts of experimental region, uniform experimental design represent one of the major type of space-filling designs. Let $\mathcal{X}$ be the entire design space. A design $\xi \in \mathcal{X}$ is called a uniform design under a measure of uniformity $\mathcal{M}$ if it minimizes the $\mathcal{M}$ -values of a design over ξ . Alternatively, uniform de-

signs could be simply understood as designs that scatter the sample points so as to mimic a uniform distribution. Uniform designs are pretty robust and generally flexible in term of problem dimensionality. Below are presented some well-known types of uniform designs:

1. Statistical measures-based designs

Discrepancies-based designs and entropy-based designs belong to this group of methods. Let $\mathbf{X} = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(n)}\}$ determine the spatial distribution of sample points in the γ -dimensional unit cube $\mathcal{C}_\gamma$, with $\mathbf{x}^{(i)} = (x_1^{(i)}, x_2^{(i)}, \dots, x_\gamma^{(i)})$. Let $\mathcal{U}(\mathbf{x}^{(i)})$ be the uniform cumulative distribution on $\mathcal{C}_\gamma$ and $\mathcal{U}_{\mathbf{X}}(\mathbf{x}^{(i)})$ be the empirical cumulative distribution of the design $\mathbf{X}$, i.e.

$$\mathcal{U}_{\mathbf{X}}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \mathbf{I}(x_1^{(i)} \leq x_1, \dots, x_\gamma^{(i)} \leq x_\gamma) \quad (4.1)$$

where $\mathbf{x} = x_1, x_2, \dots, x_\gamma$ and $\mathbf{I}(A) = 1$ if A occurs, or 0 otherwise.

The star L_p -discrepancy is the L_p -norm of $\|\mathcal{U}_{\mathbf{X}}(\mathbf{x}) - \mathcal{U}(\mathbf{x})\|_p$, with $p > 0$. It is a measure of the non-uniformity of a design. Special cases of L_p discrepancies include the star- L_∞ , the star- L_2 . The first has appeared to be quite complex to compute and both were found not suitable to design uniform experiments. Approaches to bypass those drawbacks lead to the development of new theories and introduction of new type of discrepancies[17, 64, 65, 370, 371]: the Modified- L_2 , the Centered- L_2 , the wrap-around, Categorical and Discrete discrepancies, etc.

Entropy-based designs find their origins in late forties when Shannon[372] introduced a criterion that measures the amount of information contained in the distribution of a set of data (experiment), namely Entropy. Let $p(\mathbf{x})$ be a probability distribution in $\mathcal{X}$. Its entropy is defined be

$$Ent(p(\mathbf{x})) = - \int_{\mathcal{X}} p(\mathbf{x}) \log(p(\mathbf{x})) d\mathbf{x} \quad (4.2)$$

Entropy has been first applied to DoE by Shewry and Wynn[373], where Maximum Entropy Sampling (Maximum Entropy Sampling (MES)) was introduced as a criterion for optimal sampling, with the aim of maximizing the gain in information about θ (the model parameters), for prediction at unsampled locations (i.e. lowering the expected posterior entropy[373]). To be able to compute point and interval estimates of parameters, prediction inference for future sample points, a clever method is to obtain the posterior distribution of the model parameters. The posterior distribution

is best understood as a weighted average between an a priori knowledge about the parameters before the experimental data are observed and the information about the parameters contained in the observed data. It represents the total knowledge about the parameters after the data have been observed. To obtain the posterior distribution of model parameters, a Bayesian approach has been adopted. The entropy criterion maximizes the difference in entropies before and after the experiment over the full joint distribution of $\mathcal{X}$ and θ , $Ent(p(\theta)) - Ent(p(\theta|x))$. Sebastiani and wynn[374] reviewed the computational issues (high dimensionality of the design space, expensive evaluations) linked with the minimization of the posterior entropy (especially for nonlinear problems) and presented the numerical approximations used to overcome that drawbacks. Shewry and wynn[373] formulated the maximum entropy problem for Gaussian process regression cases. Often, posteriors are represented by samples obtained through Gibbs sampling or Markov-Chain Monte Carlo methods.

2. Euclidean distance-based designs

Assume a Euclidean space with dimension $d \geq 2$ and a design $\mathbf{X} = \mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(n)}$. Let $\mathfrak{S} = [0, 1]^d$. The distance between two design points $\mathbf{x}^{(i)}$ and $\mathbf{x}^{(j)}$ of $\mathbf{X}$ is defined by $d_{ij} = \|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|$. Johnson et al.[66] introduced two closest neighborhood criteria, namely maximin distance and minimax distance criteria, to ensure a uniform spread of the sample points within the design space.

A Maximin[29, 66, 69, 375, 376](Mm) design maximizes the minimum inter-site distance ($\phi_{Mm}(\mathbf{X}) = \min_{i \neq j} d_{ij}$, i.e. having the smallest distance between neighboring points in $\mathbf{X}$ as large as possible. An identical design problem would be spheres packing (<http://www.packomania.com/>), with centers in $\mathfrak{S}$. A Minimax[29, 66, 377, 378, 379] (or Minimaximin, mM) design $\mathbf{X}$ attempt to minimize the maximum distance from all points in $\mathfrak{S}$ to their closest points in $\mathbf{X}$, i.e. minimizing the minimax-distance criterion

$$\phi_{mM}(\mathbf{X}) = \max_{\mathbf{x} \in \mathfrak{S}} \min_{\mathbf{x}_i} \|\mathbf{x} - \mathbf{x}_i\| \quad (4.3)$$

Morris and Mitchell[69] presented some properties of maximin and minimax optimal designs. Efficient algorithms considering both the maximin/minimax optimal designs features and the Delaunay[67, 380] or Voronoi tessellations[67, 68, 381] of points of $\mathbf{X}$ exist, for the computation of robust space-filling designs.

Fig. 4.2 displays a summary of some important features (minimum, first quartile, median, third quartile and maximum) of the respective criteria distributions in 2D, for the random latin hypercube, optimized latin hypercube, maximin latin hypercube samplings, sobol and halton sequences. Three space-filling measures (L2, C2, Maximin) are assessed, considering a number of 100 training points.

Figure 4.2: Examples of C2, L2 and Mindist criteria assessment for 100 training points in a 2D case.

4.1.3 Quasi-random designs

Ordinary random sampling techniques generate random sample points from the set of all possible solutions. The quasi variant does a different kind of sampling – not quite random but not quite regular either. Also called low discrepancy sequences generators, Quasi-random sampling approaches seek to bridge the gap between the flexibility of random sampling techniques and the advantages of grid designs. They are designed to have a high level of uniformity in a multidimensional space, but are not statistically independent. The discrepancy [382, 383] is computed by comparing the actual number of generated sample points in a given volume of a multidimensional space (unit hypercube) with the number of sample points that should be within the same volume, assuming a uniform

distribution of the sample points. Various quasi-sampling methods have been constructed in an attempt to minimize that discrepancy, in order to provide a reasonable coverage of the design space and an evenly spread of the training points. The most used in aerodynamics are Quasi-Monte Carlo designs[54, 55, 56, 384, 385], Sobol designs[54, 57, 58, 386], Faure sequences, Hammersley and Halton sampling methods[54, 59, 387] or Niederreiter sequences generators[54, 58, 61, 388]. Fig. 4.3 introduced additional examples of quasi-random designs, namely Faure and Hammersley designs for 40 sample points in a unit square.

Figure 4.3: 2D examples of Faure & Hammersley (40 design points) sampling.

4.1.4 Latin hypercubes and related sampling strategies

Numerous additional designs that do not (or only partially) fall in other groups are introduced in this section. Among them, Latin Hypercubes-LHS, symmetrical designs, top-down designs, nested designs, etc.

Latin Hypercubes are higher-dimensional generalization of Latin Square (inspired by mathematical papers by Leonhard Euler), an $N \times N$ array filled with k different symbols, each occurring exactly once in each row and exactly once in each column. They are a form of stratified random sampling and are not directly linked to any design criterion. A Latin hypercube design (Latin Hypercube Design (LHD)) with N runs and k design variables $(\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(k)})$, denoted by $\text{LHD}(N, k)$, is an $N \times k$ matrix, in which each column is a random permutation of $\{1, 2, \dots, N\}$. LHS were developed by McKay et al.[389] as an alternative approach (using a constraint Monte Carlo sampling) to address the uncertainty quantification of certain types of problems. LHS are a variant of stratified random sampling, i.e. not linked to any criterion. Under certain assumptions, LHS perform best than equally sized random sampling designs. LHS techniques remain the most applied simulation-based experiments in aerodynamics design, likely due to their popularity and

flexibility[13, 17, 69, 390, 391, 392]. One of the drawbacks with LHS is that they may not always be space-filling. Tentative remedies has been their combination with orthogonal arrays, their association with suitable space-filling criteria or the construction of secondary LHS within small regions of the design space surrounding the points of the initial LHS. A tutorial on LHS is found in Iman and Conover[393] or Burrage et al.[394]. A comparison of Latin hypercube sampling to other sampling techniques is given in Lin and Tang[395]. Fig. 4.4 depicts some variants of the LHS, namely the random LHS, the symmetric LHS and the Optimal LHS, considering 2 design variables and 40 design points. Due to the fact that at the off-line stage most DoEs perform poorly while estimating and predicting the industrial complex objective functions at untried locations, numerous hybrid DoEs have been developed as combinations of some the above-mentioned 'traditional' sampling strategies (CDoEs and MDoEs), mainly focusing on efforts to modify LHS and non-LHS based approaches by introducing several multi-space-filling criteria in their designs[29, 358]. A significant number of hybrid DoEs utilized in aerodynamics design is centered around latin hypercubes. Nearly Orthogonal Latin Hypercubes[70, 396, 397], (Orthogonal) Minimax/Maximin Latin Hypercubes[391, 398, 399, 400], Optimal(Symmetric) Latin Hypercubes[17, 401], 'Latinized' Centroidal Voronoi Tessellations[68, 402] are some examples of advanced DoEs introduced by statisticians, whose applications in aerodynamics design remain unfortunately very limited.

Figure 4.4: Examples of variants of the LHS for 40 training points in a 2D case.

4.2 Model validation and sequential sampling

As early mentioned, the choice of the surrogate model to be used within the SBO loop is still a hot topic. Globally there is no 'good' nor 'bad' surrogate model. Nonetheless, test and training error estimation methods remain, till date, the most used metrics in assessing and improving the local or global performance of the surrogates [4, 8, 358]. They stand as efficient guidance in surrogate model selection, among numerous alternatives. Moreover, they could sometimes establish whether the surrogate models are suitable to be used in aerodynamic analysis and optimization studies. It is worth reviewing the difference between a training error and a test error. Let $\tilde{f}$ denotes the surrogate of the expensive function f and $\mathbf{x} \in \mathcal{X}$ denotes the sampling plan such that

$$\mathbf{x}_i \mapsto y_i = f(\mathbf{x}^{(i)}) | i = 1, 2, \dots, n_s \text{ where } \mathbf{x} = [\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(n_s)}]^T \quad (4.4)$$

$$\mathbf{y} = [y(\mathbf{x}^1), y(\mathbf{x}^2), \dots, y(\mathbf{x}^{n_s})]^T \quad (4.5)$$

The training error, given as,

$$\text{err}_{\text{tr}} = \frac{1}{n} \sum_{i=1}^n L(y_i, \hat{f}(\mathbf{x}^{(i)})) \quad (4.6)$$

is defined to be an average loss over the trained samples, while the test error

$$\text{err}_{\text{ts}} = E_{\mathbf{x}, \mathbf{y}, \text{testset}} [L(\mathbf{y}, \hat{f}(\mathbf{x}))] \quad (4.7)$$

is the expected prediction error over an independent test sample, with L being the loss functions. Common loss functions include the **square** and **absolute errors** for continuous responses or the **0-1 loss** and the **log-likelihood** for responses that take discrete values. Training errors have shown to be very poor estimates of the test errors though the drop towards zero with increasing model complexity. Globally, the surrogate building-till-validation steps require to (randomly) split the available dataset into three sets:

- the training set, use to a build the surrogate with the model being fitted to the snapshots,
- the validation set to the prediction error during model selection,
- the test set to assess the generalized error of the final chosen model.

Deciding on the total number of snapshots (training data) or the number of snapshots to

assign to each set remain an open question; however, common practices allocate 50 – 60% to the training set, 25 – 30% to both the validation and test sets. A naïve attempt to use the full training data set may lead to overfitting and will typically generalize poorly, with the error rate estimate being lower than the true error rate. This is more pronounced with models that have a large number of parameters. The validation estimate of the test error is largely dependent on the type and amount of trained samples contained in both the training and validation sets. One of the major drawbacks is that the validation set error will generally tend to overestimate the test error of the model fit on the entire data set.

Popular prediction-error (test error) estimates found in literature[403] and mainly used to evaluate the overall performance of the surrogates include the Hold-Out method, the Split Sample method, Cross-validation (Random sub-sampling, Leave-One-Out-(Leave-One Out Cross Validation (LOOCV)), k-fold), Bootstrapping, Schwarz’s Bayesian information criterion (Schwarz’s Bayesian Information Criterion (SBIC)) or Akaike’s information criterion (Akaike’s Information Criterion (AIC)). These figures of merit present advantages and disadvantages, depending on the type of surrogate model and on an interest in global or local accuracy. Cross validation[404, 405] is often used for both assessing accuracy and surrogate selection. It is attractive because it does not depend on the statistical assumptions of a particular surrogate technique and it does not require extra expensive simulations (test points). The assumptions made for bootstrap are basically similar to those of cross-validation, i.e. stability on the algorithm on the dataset. The general procedure is to partition the data into subsets for training and testing. Training is the process of fitting a model while testing is the process of validating the fitted model through measuring the prediction error. The training and test sets are disjoint so the testing data for model evaluation are not used in model fitting. Cross validation is used across a range of areas such as parameter selection, density estimation, classification and stopping criteria in neural networks. Cross validation is not an information criterion in the sense that it does not penalize a goodness of fit measure. However, there exist asymptotic equivalences between cross-validation techniques and some information criteria. Cross-validation errors are used to measure the global accuracy of the surrogate in the whole domain. As previously mentioned, in cross-validation the training set is divided into L subsets, each of which is sequentially used as testing set for a surrogate that is built based on the other $L - 1$ subsets. If the number of subsets L is equal to the sample size p , the approach is called leave-one-out cross-validation. The prediction error can be estimated with all the L error measures obtained in this process (for example by averaging them). Cross-validation

provides an error estimation that is less biased than with the split-sample method. The disadvantage of this method is that the surrogate has to be constructed more than once. However, having multiple approximations may improve the robustness of the whole surrogate generation and validation approach, since all the data available is used with both training and testing purposes.

Numerous information criteria may give erroneous estimations and therefore could appear not to be suitable; example of cross-validation applied to Kriging that demand an excessive computational cost and may lead to erroneous model validation. The drawback with cross-validation is the highest number of times the expensive full order model need to be evaluated. B. Efron[407] shown that in certain cases, bootstrapping outperforms cross-validation approaches. Additional metrics[2, 5, 106, 408] that provide an estimate of the test errors, generally stressing on how well the training points are distributed, include: the (Root) Mean Square Error (Root) Mean Square Error (R(MSE)), the Adjusted MSE (Adjusted Mean Square Error (R(MSE))), the weighted RMSE (Weighted Root Mean Square Error (WRMSE)), the Integrated MSE (Integrated Mean Square Error (IMSE)), the Mean Absolute Error (Mean Absolute Error (MAE)), the Prediction Error Sum of Squares (Prediction Error Sum of Squares (PRESS)), the relative accuracy error (Relative Accuracy Error (RAE)) or the Pearson's correlation coefficient. Nevertheless, one of the major drawbacks with these error estimates is that they may be poor representatives of the actual error. More recently, Mehmani et al.[409] proposed a regional error measures (Regional Error Measure (REES)s) scheme that is capable of assessing both global and local error measures, but also allow to apprehend the behaviors of the surrogates in any region of interest of the parameter space. Throughout this thesis, the performance of the sequential sampling criterion used will be monitored during the infill process by means of cross validation techniques and surrogate error metrics.

The need to find a trade-off between the global accuracy of the surrogate model and its local accuracy in the region susceptible to enclose the optimum becomes central, via the use of reliable infill criterion during the adaptative sampling process (also known as sequential sampling). During the sequential sampling, new sampling points are added iteratively (possibly in parallel) to the design space by taking advantage of information gathered from the existing (earlier constructed) surrogate model and/or the newly generated surrogate model. Sequential sampling approaches make use of high-fidelities, i.e. calls of the FOM. Numerous infill sampling criteria (Infill Sampling Criteria (ISC))[4, 410, 411, 412, 413, 414] exist to guide the experimenter during the exploitation phase and include searching the

surrogate model (Searching the Surrogate Model (SSM)), minimizing the predictor (Minimizing the Prediction Error (MP)) and/or maximizing the predicted error (Maximizing the Prediction Error (ME)), the lower confidence bound (Lower Confidence Bound (LCB)), the expected improvement (Expected Improvement (EI)), the probability of improvement (Probability of Improvement (PI)), the likelihood estimation or the Kushner' criterion. Jones[415] published a taxonomy on data-fit surrogates-based global optimization methods, where he introduced seven infill criterion methods. Forrester and Keane [5], Liu et al.[416] compared methods for selecting search points in the framework of kriging-based optimization. Mackman et al.[417, 418] compared sequential sampling methods for generation of surrogate aerodynamic models. Moreover, various optimization algorithms, like meta-heuristic algorithms, have been employed for finding optimal space-filling samplings[17].

4.3 Surrogate models

A general introduction to surrogate models is given in the previous chapter, Subsection 1.2.3. The present section reviews the theory behind the surrogate modeling techniques that are further employed. An emphasis will be put on the related information criteria and errors metrics that will help improve the quality (accuracy) of the surrogate models.

4.3.1 Thin plate spline (TPS)

Thin plate spline (Thin Plate Spline (TPS))[419] is an effective tool for modeling coordinate transformations that has been applied successfully in several computer vision applications. It is a commonly used basis function for representing coordinate mappings and is a 2D generalization of the cubic spline. In TPS, the general interpolation problem is to pick a function s from $\mathbb{R}^2$ to $\mathbb{R}$ that satisfies the equations:

$$s(\mathbf{x}^{(i)}) = f_i, \quad i = 1, 2, \dots, n \quad (4.8)$$

where the interpolation points $\mathbf{x}^{(i)}$ and the responses f_i are given. All the interpolation points have to be different, and it is additionally assumed that they do not lie on a straight line; which implies $n \geq 3$, but no other restrictions is imposed on the interpolation points locations. The survey papers of Sabin[420] and Franke[421] show that several choices of s have been proposed. The method that seems to be used most in practice is piecewise

linear interpolation. Here the convex hull of the interpolation points in $\mathbb{R}^2$ is divided into triangles, such that $\{\mathbf{x}^{(i)} : i = 1, 2, \dots, n\}$ is the set of vertices of the triangles and no vertex is also the interior point of an edge of a triangle. Then s is defined on each triangle by linear interpolation to the data at the vertices. It follows that s is continuous across the edges, but discontinuities are expected to occur in the first derivatives of s . The method is excellent when these discontinuities are irrelevant.

when there is fewer than 100 interpolation points and the curvature of the underlying function is important, then usually piecewise linear interpolation is too crude. Further, for much larger values of n , the domain of the data may be so extensive that curvature is important on each typical subdomain that contains about 100 interpolation points. Therefore there is a need for interpolation algorithms that provide good smoothness when $n = 10^4$, say, without an excessive amount of computation. Consequently, an algorithm that requires $\mathcal{O}(n^2)$ operations could be useful, but $\mathcal{O}(n^3)$ complexity would probably be unacceptable. This request can be met by interpolating functions s that are composed of quadratic or cubic polynomial pieces. On the other hand, when n is such that $\mathcal{O}(n^3)$ operations are tolerable, then the use of thin plate splines is highly successful in several applications. Further, these interpolants have two strong advantages over piecewise polynomials. Specifically, there are no artificial divisions of the data into subregions for the separate pieces of s , and thin plate spline interpolants provide the solution to a very pertinent variational problem. Therefore, we are going to consider some properties of thin plate spline interpolants that may allow their coefficients to be calculated in fewer than $\mathcal{O}(n^3)$ operations.

In the variational problem, s required to have square integrable second derivatives, and the freedom in s after satisfying the interpolation equations 4.8 is taken up by minimizing the bending energy

$$I(s) = \int_{\mathbb{R}^2} \left(\frac{\partial^2 s(\mathbf{x})}{\partial x^2} \right)^2 + \left(\frac{\partial^2 s(\mathbf{x})}{\partial x \partial y} \right)^2 + \left(\frac{\partial^2 s(\mathbf{x})}{\partial y^2} \right)^2 d\mathbf{x} \quad (4.9)$$

where x and y are the components of $\mathbf{x}$. It was proven by Duchon[422] that the TPS interpolant is of the form

$$s(\mathbf{x}) = \sum_{j=1}^n w_j \left\| \mathbf{x} - \mathbf{x}^{(j)} \right\|_{L_2}^2 \log \left\| \mathbf{x} - \mathbf{x}^{(j)} \right\|_{L_2} + c_0 + c_1 x + c_2 y, \quad \mathbf{x} \in \mathbb{R}^2 \quad (4.10)$$

Further, the coefficients $\{w_j : j = 1, 2, \dots, n\}$ are constrained by the conditions:

$$\sum_{j=1}^n w_j = \sum_{j=1}^n w_j x_j = \sum_{j=1}^n w_j y_j = 0 \quad (4.11)$$

where x_j and y_j are components of $\mathbf{x}^{(j)}$ in order for $I(s)$ (Eq. 4.9) to be finite. Combining Eq. (4.8) and Eq. (4.11), we arise to a square linear system in the unknowns $\{w_j : j = 1, 2, \dots, n\}$ and $\{c_0, c_1, c_2\}$. The system can be written as

$$\left(\begin{array}{c|c} \Phi & \mathbf{P} \\ \hline \mathbf{P}^T & 0 \end{array} \right) \begin{pmatrix} \mathbf{w} \\ \mathbf{c} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{0} \end{pmatrix} \quad (4.12)$$

where Φ is a $n \times n$ whose entries are $\{\|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|_{L_2}^2 \log \|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|_{L_2} : i, j = 1, 2, \dots, n\}$, $\mathbf{P}$ is a $n \times 3$ matrix whose i^{th} row is the vector $(1 \ x_i \ y_i)$. Furthermore, the vectors $\mathbf{w}$, $\mathbf{c}$ and $\mathbf{f}$ respectively have entries $\{w_j : j = 1, 2, \dots, n\}$, $\{c_0, c_1, c_2\}$ and $\{f_i : i = 1, 2, \dots, n\}$. One can deduce from the above variational problem that the $(n+3) \times (n+3)$ matrix of the system(4.12) is nonsingular. Therefore, the data define the function (4.10) uniquely. This choice of s is the 'thin plate spline' interpolant; the aim being to solve the Equations (4.12) in fewer than $\mathcal{O}(n^3)$ operations. TPS has proven to be impractical for large scale applications. Good approximate solutions are often possible using only a small subset of interpolation points.

4.3.2 Gaussian process regression - Kriging

In this section, the essentials of spatial Gaussian processes in the context of computer experiments is reviewed. This will serve as a mathematical ground in defining the multi-fidelity kriging used in the present thesis. Gaussian processes regression (also known as Kriging or Spatial correlation models)[4, 5, 24, 113, 114, 115] are collections of random variables, any finite number of which have joint Gaussian probabilistic distribution. They are parametric interpolation methods completely specified by mean and positive definite covariance functions. Originally introduced by D.G. Krige (a South-African mining engineer) in 1951 and mathematically formulated by Matheron[423] in the sixties, Kriging was extended to surrogate modeling and optimization by the works of Sacks et al.[24], Jones et al.[410], Kleijnen et al.[424] or more recently Forrester et al.[4] that suggested modeling responses as a combination of

- a deterministic linear regression (e.g. of a polynomial) of the data with r basis functions modeling the drift of the process mean
- a realization of the stochastic process to 'stretch' the surrogate towards the observed data by quantifying the correlation of nearby points

Kriging (Figs. 4.5 & 4.6) is a weighted linear combination of the trained samples of the modeled functions. It makes use of the spatial correlation among the data samples. Closer samples are likely to have highly correlated response values (i.e. bigger weights), whereas samples taken far apart are unlikely to have highly correlated response values. In contrast to the surrogate models introduced previously, kriging was originally designed for 'deterministic' (noise-free) computer experiments[20, 113]. It has the flexibility to mimic, at reasonable computational costs, multi-modal and non-linear functions. Kriging tends to find the best linear unbiased predictor or estimator (Best Linear Unbiased Predictor or Estimator (BLUP or BLUE)), which minimizes the mean square error of the prediction subject to a constraint. Kriging and its extensions have known a continuous improvement over the years and has been popularized in the field of aircraft aerodynamics, mainly to calibrate and fuse data from different fidelities (wind-tunnel data, flight test data, CFD data or data derived from empirical aerodynamic methods for many-query analyses).

Figure 4.5: Example of kriging interpolation- Figure 4.6: Example of kriging interpolation with conf. intervals.

Several types of single Kriging interpolators have been introduced into aircraft aerodynamics literature so far. The well-known among them are Simple Kriging (SK)[24], Ordinary Kriging (OK)[114, 115], Universal Kriging (UK)[425, 426], Blind Kriging (BK)[427], Non-Stationary (covariance) Kriging [428], Taylor Kriging[429]. However, the use of hybrid interpolators such as Regression Kriging (RK)[430] or Regularized Kriging[431] remains very limited. The ordinary kriging is considered in this thesis, its robustness being guar-

anted by more enough interpolation (sample) points to construct the surrogate model; therefore the possibility to perform complex data modeling. However, we will keep the universal Kriging notation.

Consider the computer experiment to be a flow solver, whose evaluations are assumed to be expensive. It is treated as a black-box y , depending on input parameters $\mathbf{x} \in \mathbb{R}^d$. The basic objective is to approximate an unknown function (scalar response) $y : \mathbb{R}^d \rightarrow \mathbb{R}$ in a domain of interest $\mathcal{X} \subset \mathbb{R}^d$ (where $d = n_{dv}$ is the number of design variables and $\mathcal{X}$ the design space) by a surrogate model $\hat{y}(\mathbf{x})$, which can be evaluated at low computational cost. The Kriging method is a statistical method of interpolating n given data pairs $\{(\mathbf{x}^{(i)}, y(\mathbf{x}^{(i)}))\}_{i=1}^n$ of evaluations of the unknown (true) function $y(\mathbf{x})$. The Kriging models the scalar output of a deterministic computer experiment as a sum of a linear regression part and a lack-of-fit (stochastic) term

$$y(\mathbf{x}) = \sum_{j=1}^m \beta_j f_j(\mathbf{x}) + Z(\mathbf{x}) \quad (4.13)$$

where the linear model consists of known functions $f_j(\mathbf{x})$ and unknown coefficients (weights) β_j ($j = 1, 2, \dots, m$). In the case of ordinary kriging, the regression term is just a single constant β and $f \equiv 1$ ($m = 1$) and $Z(\mathbf{x})$ is assumed to be the interpolated residual or (zero-mean) stationary Gaussian stochastic process ($Z(\mathbf{x}) \sim N(0, \sigma^2)$) that satisfies

$$\mathbb{E}[Z(\mathbf{x})] = 0, \quad \text{Cov}(Z(\mathbf{x}^{(i)}), Z(\mathbf{x}^{(j)})) = \sigma^2 R(\mathbf{x}^{(i)} - \mathbf{x}^{(j)}) \quad \forall \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \in \mathcal{X}. \quad (4.14)$$

where σ^2 is the process variance and $R(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = R(\mathbf{x}^{(i)} - \mathbf{x}^{(j)})$ the spatial correlation function (Spatial Correlation Function (SCF) whose associated 'correlation' matrix is semi-definite, symmetric, with diagonals consisting of $\mathbf{1}$'s.), depending only on the distance vector of $\mathbf{x}^{(i)}$ and $\mathbf{x}^{(j)}$, not on their locations themselves.

The kriging model of the true function can be rewritten as

$$y(\mathbf{x}) = \mathbf{f}^T(\mathbf{x})\beta + Z(\mathbf{x}) = (f_0(\mathbf{x}), \dots, f_p(\mathbf{x})) \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_p \end{pmatrix} + Z(\mathbf{x}) \quad (4.15)$$

The most common choices for the regression model are constant, linear, or higher-order multivariate polynomials. The regression design matrix is

$$\mathbf{F} = \begin{pmatrix} f(\mathbf{x}^{(1)})^T \\ \vdots \\ f(\mathbf{x}^{(n)})^T \end{pmatrix} = \begin{pmatrix} f_0(\mathbf{x}^{(1)}) & f_1(\mathbf{x}^{(1)}) & \cdots & f_p(\mathbf{x}^{(1)}) \\ \vdots & \vdots & \cdots & \vdots \\ f_0(\mathbf{x}^{(n)}) & f_1(\mathbf{x}^{(n)}) & \cdots & f_p(\mathbf{x}^{(n)}) \end{pmatrix} \in \mathbb{R}^{n \times (p+1)} \quad (4.16)$$

In the context of computer experiments[23], covariances of the random errors are modeled by spatial correlation functions of the form $\text{Cov}(Z(\mathbf{x}^{(i)}), Z(\mathbf{x}^{(j)})) = \sigma^2 \rho(\theta, \mathbf{x}^{(i)}, \mathbf{x}^{(j)})$. Considering two training points $\mathbf{x}$ and $\tilde{\mathbf{x}}$ within the design space, Table 4.3 summarizes common correlation models used in Kriging regression. By convention, ρ is usually defined

Table 4.3: Common correlation models used in Kriging regression

Name	Correlation Model
Exponential	$e^{- \mathbf{x}_j - \tilde{\mathbf{x}}_j \theta_j}$
General Exponential	$e^{- \mathbf{x}_j - \tilde{\mathbf{x}}_j ^\rho_j \theta_j}, 0 < \rho_j \leq 2$
Gaussian	$e^{-(\mathbf{x}_j - \tilde{\mathbf{x}}_j)^2 \theta_j}$
Spherical	$1 - 1.5\xi_j + 0.5\xi_j^3, \xi_j = \min\{1, \theta_j \mathbf{x}_j - \tilde{\mathbf{x}}_j \}$
Linear	$\max\{0, 1 - \theta_j \mathbf{x}_j - \tilde{\mathbf{x}}_j \}$
Cubic	$1 - 3.0\xi_j + 2.0\xi_j^3, \xi_j = \min\{1, \theta_j \mathbf{x}_j - \tilde{\mathbf{x}}_j \}$

such that

$$\rho(\theta, p, q)_{p \neq q} \rightarrow \begin{cases} 0, & \text{for } \|\theta\| \rightarrow \infty \\ 1, & \text{for } \|\theta\| \rightarrow 0 \end{cases} \quad (4.17)$$

$\theta = (\theta_1, \dots, \theta_d) \in \mathbb{R}^d$ represents the vector of hyper-parameters and ρ is the correlation coefficient. The correlation matrix and the correlation vector at a location $\mathbf{x}$ are respectively defined as

$$\begin{aligned} \mathbf{R} &= \mathbf{R}(\theta) = (\rho(\theta, \mathbf{x}^{(i)}, \mathbf{x}^{(j)}))_{i,j} \in \mathbb{R}^{n \times n} \\ \mathbf{r}(\mathbf{x}) &= \mathbf{r}(\theta, \mathbf{x}) = (\rho(\theta, \mathbf{x}^{(1)}, \mathbf{x}), \dots, \rho(\theta, \mathbf{x}^{(n)}, \mathbf{x}))^T \in \mathbb{R}^n \end{aligned} \quad (4.18)$$

The kriging predictor (BLUP)

$$\hat{f}(\mathbf{x}) := w(\mathbf{x})^T \mathbf{Y} = \sum_{i=1}^n w_i(\mathbf{x}) y_i \quad (4.19)$$

is a weighted sum of the given response evaluations $\mathbf{Y} := (y(\mathbf{x}^{(1)}), \dots, y(\mathbf{x}^{(n)}))^T$ ($y_i = f(\mathbf{x}^{(i)})$ | $i = 1, 2, \dots, n$). with the weights $w(\mathbf{x})$ chosen as the solution of the optimization

problem

$$\begin{aligned} \min_{w(\mathbf{x}) \in \mathbb{R}^n} \text{MSE}[\hat{f}(\mathbf{x})] &= \mathbb{E}[(w(\mathbf{x})^T \mathbf{Y} - y(\mathbf{x}))^2] \\ \text{s.t. } \mathbb{E}[w(\mathbf{x})^T \mathbf{Y} - y(\mathbf{x})] &= 0 \end{aligned} \quad (4.20)$$

The weights in Equation (4.19) are given by the solution of the linear system (4.20)

$$\begin{bmatrix} \mathbf{R} & \mathbf{F} \\ \mathbf{F}^T & 0 \end{bmatrix} \begin{pmatrix} w(\mathbf{x}) \\ \mu(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \mathbf{r}(\mathbf{x}) \\ f(\mathbf{x}) \end{pmatrix} \in \mathbb{R}^{n+p+1} \quad (4.21)$$

where $\mu(\mathbf{x}) = (\mu_0(\mathbf{x}), \dots, \mu_p(\mathbf{x}))^T$ are the Langrange multipliers for the unbiased condition in (4.20). Combining (4.19) & (4.21), the Kriging interpolator can be rewritten as

$$\hat{f}(\mathbf{x}) := w(\mathbf{x})^T \mathbf{Y} = \begin{pmatrix} \mathbf{r}(\mathbf{x}) \\ f(\mathbf{x}) \end{pmatrix}^T \begin{bmatrix} \mathbf{R} & \mathbf{F} \\ \mathbf{F}^T & 0 \end{bmatrix}^{-1} \begin{pmatrix} \mathbf{Y} \\ 0 \end{pmatrix} \quad (4.22)$$

In numerous engineering applications, a preference for a Gaussian approach is often the case, to define the SCF with a more general form given as:

$$\mathbf{R}(\mathbf{x}, \tilde{\mathbf{x}}) = \prod_{j=1}^d e^{(-|\mathbf{x}_j - \tilde{\mathbf{x}}_j|^{\rho_j} \theta_j)} \quad (4.23)$$

The hyper-parameters $\theta^{(k)}$ are usually determined by solving a maximum likelihood problem

$$\max_{\theta, \beta, \sigma^2} (2\pi)^{\frac{n}{2}} \sigma^{-n} (\det \mathbf{R}(\theta))^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2\sigma^2} (\mathbf{Y} - \mathbf{F}\beta)^T \mathbf{R}(\theta)^{-1} (\mathbf{Y} - \mathbf{F}\beta) \right\} \quad (4.24)$$

Optimizing the profile log-likelihood, we get the following equation

$$\max_{\theta \in \mathbb{R}^d, \theta_j > 0} -n \log(\sigma^2(\theta)) - \log(\det(\mathbf{R}(\theta))) \quad (4.25)$$

where the dependency on θ is as follows

$$\begin{aligned} \beta(\theta) &= (\mathbf{F}^T \mathbf{R}(\theta)^{-1} \mathbf{F})^{-1} \mathbf{F}^T \mathbf{R}(\theta)^{-1} \mathbf{Y} \\ \sigma^2(\theta) &= \frac{1}{n} (\mathbf{Y} - \mathbf{F}\beta(\theta))^T \mathbf{R}(\theta)^{-1} (\mathbf{Y} - \mathbf{F}\beta(\theta)) \end{aligned} \quad (4.26)$$

finally reducing the problem to

$$\min_{\theta} \left\{ \sigma^2(\theta, \beta(\theta)) (\det(\mathbf{R}(\theta)))^{\frac{1}{n}} \right\} \quad (4.27)$$

4.3.3 Multi-fidelity prediction via cokriging

Multi-fidelity surrogate modeling refers to the enhanced prediction of the output of a complex system by incorporating secondary or supplementary fast-to-obtain data of lower fidelity. It offers an efficient way to generate aerodynamic data based on a set of CFD methods with varying level of fidelity and computational expense or based on a single physical model evaluated on meshes of varying refinement (cf.1.2.3.3). The goal is to reduce the number of expensive high-fidelity computations used to build the surrogate model. A low-fidelity CFD method is used to automatically compute hundreds or thousands of snapshots at points in the parameter space selected via DoE. Only a few number of points in the parameter space are computed using a high-fidelity CFD method. One of the most popular method for predicting the output of a high-fidelity computer code with assistance of the output of a lower-fidelity computer codes is cokriging. As the underlying theory of cokriging is that of two-variable or multivariable kriging, it can be regarded as a general extension of single fidelity kriging to a model that is assisted by low fidelities. Data are calibrated and fused, with low-fidelity data indicating trends and a small number of high-fidelity data; one of the key challenges being how to correct the low-fidelity model to efficiently represent more complicated correlation between low- and high-fidelity functions. In order to construct cokriging predictors, it is mandatory to estimate certain co- and cross-variances based on sampled data. Cokriging formulations for aircraft aerodynamics applications have evolved with the development of CFD codes, especially due to the possibility to incorporate information such as cheaper-to-evaluate gradients (example via adjoint methods, automatic differentiation or finite difference). The trend underlying the low-fidelity data will be mapped to the high-fidelity data through the Zimmermann et al. **Simplified Cross-Correlation** approach[282].

Suppose a d -dimensional problem. we wish to predict the trends of an expensive-to-evaluate (and unknown - high-fidelity) aerodynamic function $g^{\text{hi}} : \mathbb{R}^d \rightarrow \mathbb{R}$ with the help of a cheap-to-evaluate (low-fidelity) $g^{\text{lo}} : \mathbb{R}^d \rightarrow \mathbb{R}$. The HF and LF are obtained through variable accuracy modeling (VAM), i.e. running the same flow solver respectively with and without a relaxed convergence. Consider a spatial arrangement of the HF and LF

interpolation points to be:

$$\mathbf{x}_{\text{hi}}^{(i)} \in \mathbb{R}^d, i = 1, \dots, n_{\text{hi}} \quad \mathbf{x}_{\text{lo}}^{(j)} \in \mathbb{R}^d, j = 1, \dots, n_{\text{lo}} \quad \text{with (usually)} \quad n_{\text{hi}} \ll n_{\text{lo}} \quad (4.28)$$

and their corresponding responses

$$y^{\text{hi}} = y_i = g^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(i)}) \in \mathbb{R}, i = 1, \dots, n_{\text{hi}} \quad y^{\text{lo}} = z_j = g^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(j)}) \in \mathbb{R}, j = 1, \dots, n_{\text{lo}}. \quad (4.29)$$

A vector representation of the above responses can be written as

$$(Y^{\text{hi}}, Y^{\text{lo}})^T = (y_1, \dots, y_{n_{\text{hi}}}, z_1, \dots, z_{n_{\text{lo}}})^T \in \mathbb{R}^{n_{\text{hi}}+n_{\text{lo}}} \quad (4.30)$$

The objective is to construct a predictor based on the sample data sets, which interpolates the HF data and takes into account the information from the LF data, with the aim to approximate the HF data at untried locations. For that aim, we consider the following assumptions:

- The output of a deterministic computer experiment is treated as a realization of a stationary random function (or stochastic process)
- Both HFs and LFs sample values are treated as realizations of underlying random processes, each given by a regression model and a random error function (Gaussian) $Z(\mathbf{x}) = \varepsilon(\mathbf{x})$.

Corresponding to the outputs of high- and low-fidelity computations for the same aerodynamic characteristic, we replace y^{hi} and y^{lo} by the following random functions

$$Y^{\text{hi}}(\mathbf{x}) = f^{\text{hi}}(\mathbf{x})\beta^{\text{hi}} + \varepsilon^{\text{hi}}(\mathbf{x}) \quad Y^{\text{lo}}(\mathbf{x}) = f^{\text{lo}}(\mathbf{x})\beta^{\text{lo}} + \varepsilon^{\text{lo}}(\mathbf{x}) \quad (4.31)$$

where the row vector functions $f^{\text{hi}} : \mathbb{R}^d \rightarrow \mathbb{R}^{p+1}$ and $f^{\text{lo}} : \mathbb{R}^d \rightarrow \mathbb{R}^{q+1}$ represent the regression models, $\beta^{\text{hi}} = (\beta_0^{\text{hi}}, \dots, \beta_p^{\text{hi}})$ and $\beta^{\text{lo}} = (\beta_0^{\text{lo}}, \dots, \beta_q^{\text{lo}})$ are the corresponding regression weights. In general, the common regression choices are

$$p, q = \begin{cases} 0, \text{ const. reg. } (f(\mathbf{x})\beta = \beta \in \mathbb{R}) \\ d, \text{ lin reg. } (f(\mathbf{x})\beta = \beta_0, \dots, \beta_d x_d \in \mathbb{R}) \end{cases} \quad \text{for } f \in \{f^{\text{hi}}, f^{\text{lo}}\}, \beta \in \{\beta^{\text{hi}}, \beta^{\text{lo}}\} \quad (4.32)$$

The regression models for high- and low- fidelities need not to coincide and will be estimated from the sampled information using a Maximum Likelihood Estimate (MLE) (maximum likelihood estimate) optimization process. The regression design matrices are

defined as follow.

$$\mathbf{F}^{\text{hi}} := \begin{pmatrix} \mathbf{f}^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(1)}) \\ \vdots \\ \mathbf{f}^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(n^{\text{hi}})}) \end{pmatrix} \in \mathbb{R}^{n^{\text{hi}} \times (p+1)} \quad \mathbf{F}^{\text{lo}} := \begin{pmatrix} \mathbf{f}^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(1)}) \\ \vdots \\ \mathbf{f}^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(n^{\text{lo}})}) \end{pmatrix} \in \mathbb{R}^{n^{\text{lo}} \times (q+1)} \quad (4.33)$$

$$\mathbf{F} := \begin{pmatrix} \mathbf{F}^{\text{hi}} & \mathbf{0} \\ \mathbf{0} & \mathbf{F}^{\text{lo}} \end{pmatrix} \in \mathbb{R}^{(n^{\text{hi}}+n^{\text{lo}}) \times (p+q+2)} \quad (4.34)$$

The random errors in (4.31) ε^{hi} and ε^{lo} are assumed to be weak stationary Gaussian stochastic processes with mean 0, i.e.

$$\mathbb{E}(\varepsilon^{\text{hi}}(\mathbf{x})) = 0 = \mathbb{E}(\varepsilon^{\text{lo}}(\mathbf{x})), \forall \mathbf{x}. \quad (4.35)$$

The vectors of errors at sample locations are given as

$$\varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}) := \begin{pmatrix} \varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(1)}) \\ \vdots \\ \varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(n^{\text{hi}})}) \end{pmatrix} \quad \& \quad \varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}) := \begin{pmatrix} \varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(1)}) \\ \vdots \\ \varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(n^{\text{lo}})}) \end{pmatrix} \quad (4.36)$$

Taking advantage of Equation (4.35), the covariances matrices can be derived as

$$\begin{aligned} \mathbb{E} [\varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(i)}) \varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(j)})] &:= \text{Cov} [\varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(i)}), \varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(j)})] := \mathbf{C}^{\text{hh}}(\mathbf{x}_{\text{hi}}^{(i)}, \mathbf{x}_{\text{hi}}^{(j)}) \\ \mathbb{E} [\varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(i)}) \varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(j)})] &:= \text{Cov} [\varepsilon^{\text{hi}}(\mathbf{x}_{\text{hi}}^{(i)}), \varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(j)})] := \mathbf{C}^{\text{hl}}(\mathbf{x}_{\text{hi}}^{(i)}, \mathbf{x}_{\text{lo}}^{(j)}) = \mathbf{C}^{\text{lh}}(\mathbf{x}_{\text{lo}}^{(j)}, \mathbf{x}_{\text{hi}}^{(i)}) \\ \mathbb{E} [\varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(i)}) \varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(j)})] &:= \text{Cov} [\varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(i)}), \varepsilon^{\text{lo}}(\mathbf{x}_{\text{lo}}^{(j)})] := \mathbf{C}^{\text{ll}}(\mathbf{x}_{\text{lo}}^{(i)}, \mathbf{x}_{\text{lo}}^{(j)}) \end{aligned} \quad (4.37)$$

Summarizing, we get

$$\begin{aligned} \mathbf{C}^{\text{hh}} &:= \left\{ \mathbf{C}^{\text{hh}}(\mathbf{x}_{\text{hi}}^{(i)}, \mathbf{x}_{\text{hi}}^{(j)}) \right\}_{ij} \in \mathbb{R}^{n^{\text{hi}} \times n^{\text{hi}}} \\ \mathbf{C}^{\text{hl}} = (\mathbf{C}^{\text{lh}})^{\text{T}} &:= \left\{ \mathbf{C}^{\text{hl}}(\mathbf{x}_{\text{hi}}^{(i)}, \mathbf{x}_{\text{lo}}^{(j)}) \right\}_{ij} \in \mathbb{R}^{n^{\text{hi}} \times n^{\text{lo}}} \\ \mathbf{C}^{\text{ll}} &:= \left\{ \mathbf{C}^{\text{ll}}(\mathbf{x}_{\text{lo}}^{(i)}, \mathbf{x}_{\text{lo}}^{(j)}) \right\}_{ij} \in \mathbb{R}^{n^{\text{lo}} \times n^{\text{lo}}} \end{aligned} \quad (4.38)$$

$$\mathbf{C} := \begin{pmatrix} \mathbf{C}^{\text{hh}} & \mathbf{C}^{\text{hl}} \\ \mathbf{C}^{\text{lh}} & \mathbf{C}^{\text{ll}} \end{pmatrix} \in \mathbb{R}^{(n^{\text{hi}}+n^{\text{lo}}) \times (n^{\text{hi}}+n^{\text{lo}})} \quad (4.39)$$

By analogy with the Kriging derivations in (4.3.2) and from Santner et al.[13], the BLUP (Best Linear Unbiased Predictor) can be written as

$$\hat{f}(\mathbf{x}) := \mathbf{f}^{\text{hi}}(\mathbf{x})\beta^{\text{hi}} + \mathbf{c}^T(\mathbf{x})\mathbf{C}^{-1} \left(\begin{pmatrix} \mathbf{Y} \\ \mathbf{Z} \end{pmatrix} - \begin{pmatrix} \mathbf{F}^{\text{hi}}\beta^{\text{hi}} \\ \mathbf{F}^{\text{lo}}\beta^{\text{lo}} \end{pmatrix} \right) \quad (4.40)$$

where the i^{th} component of the vector $\mathbf{c}(\mathbf{x}) \in \mathbb{R}^{n^{\text{hi}}+n^{\text{lo}}}$ is given as

$$\mathbf{c}(\mathbf{x}^{(i)}) := \begin{pmatrix} \mathbf{C}^{\text{hh}}(\mathbf{x}_{\text{hi}}^{(i)}, \mathbf{x}), \quad i = 1, \dots, n^{\text{hi}} \\ \mathbf{C}^{\text{lh}}(\mathbf{x}_{\text{lo}}^{(i)}, \mathbf{x}), \quad i = n^{\text{hi}} + 1, \dots, n^{\text{lo}} \end{pmatrix} \quad (4.41)$$

Denoting by $\mathbf{v}$ the vector $\mathbf{v} := \begin{pmatrix} \mathbf{F}^{\text{hi}}\beta^{\text{hi}} \\ \mathbf{F}^{\text{lo}}\beta^{\text{lo}} \end{pmatrix}$ in Equation (4.40), the corresponding MSE is derived as

$$\text{MSE}[\mathbf{x}] = \sigma_{\text{hi}}^2 - \mathbf{c}^T(\mathbf{x})\mathbf{C}^{-1}\mathbf{c}(\mathbf{x}) + \frac{(\mathbf{c}^T(\mathbf{x})\mathbf{C}^{-1}\mathbf{v} - \mathbf{f}^{\text{hi}}(\mathbf{x})\beta^{\text{hi}})^2}{\mathbf{v}^T\mathbf{C}^{-1}\mathbf{v}} \quad (4.42)$$

Valid Cokriging models require the estimation of the regression weights and the covariances between sampled data. Therefore we will assumed a Gaussian distribution among the data and will consider that the errors of the responses $\varepsilon_i^{\text{hi}}, i = 1, \dots, n^{\text{hi}}$ and $\varepsilon_i^{\text{lo}}, i = 1, \dots, n^{\text{lo}}$ are correlated random variables. The corresponding jpdf (joint probability density function) is given as

$$D(\varepsilon^{\text{hi}}, \varepsilon^{\text{lo}}) = \frac{1}{2\pi\sqrt{\det\mathbf{C}}} \exp \left[\frac{1}{2} \begin{pmatrix} \varepsilon^{\text{hi}} - \mathbf{E}[\varepsilon^{\text{hi}}] \\ \varepsilon^{\text{lo}} - \mathbf{E}[\varepsilon^{\text{lo}}] \end{pmatrix}^T \mathbf{C}^{-1} \begin{pmatrix} \varepsilon^{\text{hi}} - \mathbf{E}[\varepsilon^{\text{hi}}] \\ \varepsilon^{\text{lo}} - \mathbf{E}[\varepsilon^{\text{lo}}] \end{pmatrix} \right] \quad (4.43)$$

It is worth mentioning that

$$\begin{aligned} \varepsilon^{\text{hi}} - \mathbf{E}[\varepsilon^{\text{hi}}] &= \mathbf{Y}^{\text{hi}} - \mathbf{E}[\mathbf{Y}^{\text{hi}}] \\ \varepsilon^{\text{lo}} - \mathbf{E}[\varepsilon^{\text{lo}}] &= \mathbf{Y}^{\text{lo}} - \mathbf{E}[\mathbf{Y}^{\text{lo}}] \end{aligned} \quad (4.44)$$

Estimating the MLE (from which the optimal values of the hyper-parameters are obtained) Maximizing the jpdf is equivalent to minimizing the log-likelihood:

$$\min! \bar{D}(\varepsilon^{\text{hi}}, \varepsilon^{\text{lo}}) = \ln(\det\mathbf{C}) + \begin{pmatrix} \mathbf{Y}^{\text{hi}} - \mathbf{E}[\mathbf{Y}^{\text{hi}}] \\ \mathbf{Y}^{\text{lo}} - \mathbf{E}[\mathbf{Y}^{\text{lo}}] \end{pmatrix}^T \mathbf{C}^{-1} \begin{pmatrix} \mathbf{Y}^{\text{hi}} - \mathbf{E}[\mathbf{Y}^{\text{hi}}] \\ \mathbf{Y}^{\text{lo}} - \mathbf{E}[\mathbf{Y}^{\text{lo}}] \end{pmatrix} \quad (4.45)$$

For optimization purposes we need to parametrize the covariances. For this aim, we will

utilize the correlation coefficients R and the standard deviation σ . As previously said, in the context of computer experiments, a popular class of spatial correlation models

$$R(\theta, \mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \exp \left(- \sum_k \theta_k \left\| \mathbf{x}_k^{(i)} - \mathbf{x}_k^{(j)} \right\|^p \right), \quad p = 2 \text{ for Gaussian correlation} \quad (4.46)$$

θ being a vector of distance weights. Rewriting the component of the covariance matrices, we get:

$$\begin{aligned} C^{hh} &:= \left(\sigma_{y_i} \sigma_{y_j} R(\theta^{hh}, \mathbf{x}_{hi}^{(i)}, \mathbf{x}_{hi}^{(j)}) \right), \quad i, j = 1, \dots, n^{hi} \\ C^{hl} &:= \left(\sigma_{y_i} \sigma_{z_i} R(\theta^{hl}, \mathbf{x}_{hi}^{(i)}, \mathbf{x}_{lo}^{(j)}) \right), \quad i = 1, \dots, n^{hi}, \quad j = 1, \dots, n^{lo} \\ C^{ll} &:= \left(\sigma_{z_i} \sigma_{z_j} R(\theta^{ll}, \mathbf{x}_{lo}^{(i)}, \mathbf{x}_{lo}^{(j)}) \right), \quad i, j = 1, \dots, n^{lo} \end{aligned} \quad (4.47)$$

In order to reduce the number of design parameters, it is usually assumed that the random processes are stationary, i.e.

$$\sigma_{y_i} \equiv \sigma_{hi} \forall i \in \{1, \dots, n^{hi}\} \quad \& \quad \sigma_{z_i} \equiv \sigma_{lo} \forall i \in \{1, \dots, n^{lo}\} \quad (4.48)$$

The covariance matrix can thus be rewritten as

$$C := \begin{pmatrix} \sigma_{hi}^2 R^{hh} & \sigma_{hi} \sigma_{lo} R^{hl} \\ \sigma_{hi} \sigma_{lo} R^{lh} & \sigma_{lo}^2 R^{ll} \end{pmatrix} \quad (4.49)$$

For $\Theta := (\theta^{hh}, \theta^{hl}, \theta^{ll}) \in \mathbb{R}^{3d}$ fixed, the optimal expectation values corresponding to (4.45) can be obtained analytically as followed:

$$E[Y^{hi}] = F^{hi} \beta^{hi}(\Theta) \in \mathbb{R}^{n^{hi}} \quad E[Y^{lo}] = F^{lo} \beta^{lo}(\Theta) \in \mathbb{R}^{n^{lo}} \quad (4.50)$$

with the terms F^{hi} and F^{lo} completely determined by the sample locations and thus constants. In Equation (4.45), the term $\ln(\det C)$ can be neglected in regard of optimizing expectation values because C is parameterized independently of β^{hi} and β^{lo} . Since the matrices C and C^{-1} are positive definite, the hessian of the remaining part of $\bar{D}$ is therefore positive definite so that the unique zero of the gradient of $\bar{D}$ with respect to β^{hi} and β^{lo} represents the global minimum. Henceforth for a fixed $\Theta \in \mathbb{R}^{3d}$, the associated optimal regression weight vectors $\beta^{hi}(\Theta)$ and $\beta^{lo}(\Theta)$ are determined by the following well-known

equation [13]:

$$(\mathbf{F}^T \mathbf{C}^{-1} \mathbf{F}) \begin{pmatrix} \beta^{\text{hi}} \\ \beta^{\text{lo}} \end{pmatrix} (\Theta) = \mathbf{F}^T \mathbf{C}^{-1} \begin{pmatrix} \mathbf{Y}^{\text{hi}} \\ \mathbf{Y}^{\text{lo}} \end{pmatrix} (\Theta) \quad (4.51)$$

Dealing with variable accuracy modeling, the Low Fidelities (LF) and High Fidelities (HF) data describe the same phenomenon with different levels of accuracy. Therefore, it is assumed they feature the same spatial inter-correlations. The cross-correlations will be computed based on these assumptions. we get the following:

$$\mathbb{E} [\varepsilon^{\text{hi}}(\mathbf{x}^{(i)}) \varepsilon^{\text{hi}}(\mathbf{x}^{(j)})] = \mathbb{E} [\varepsilon^{\text{lo}}(\mathbf{x}^{(i)}) \varepsilon^{\text{lo}}(\mathbf{x}^{(j)})] , \forall \mathbf{x}^{(i)}, \mathbf{x}^{(j)} \quad (4.52)$$

i.e $\sigma_{\text{hi}}^2 \mathbf{R}^{\text{hh}}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \sigma_{\text{lo}}^2 \mathbf{R}^{\text{ll}}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$. Consequently,

$$\begin{aligned} \sigma_{\text{hi}} &= \sigma_{\text{lo}} = \sigma \\ \mathbf{R}^{\text{hh}}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) &= \mathbf{R}^{\text{ll}}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \mathbf{R}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \end{aligned} \quad (4.53)$$

Using an additional parameter $\gamma \in (0, 1)$ to model the cross-correlation, we get:

$$\mathbf{R}^{\text{hl}}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \mathbf{R}^{\text{lh}}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \gamma \mathbf{R}(\theta, \mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \quad (4.54)$$

Hence, the same distance weights $\theta = (\theta_1, \dots, \theta_d)$ are used in all cases to reduce the degrees of freedom. Considering two training points $\mathbf{x}$ and $\tilde{\mathbf{x}}$ within the design space. The correlation matrix is defined as

$$\mathbf{R} = \begin{pmatrix} (\mathbf{R}(\theta, \mathbf{x}^{(i)}, \mathbf{x}^{(j)}))_{i,j=1, \dots, n^{\text{hi}}} & (\mathbf{R}(\theta, \mathbf{x}^{(i)}, \tilde{\mathbf{x}}^{(j)}))_{i=1, \dots, n^{\text{hi}}, j=1, \dots, n^{\text{lo}}} \\ (\mathbf{R}(\theta, \tilde{\mathbf{x}}^{(i)}, \mathbf{x}^{(j)}))_{i=1, \dots, n^{\text{lo}}, j=1, \dots, n^{\text{hi}}} & (\mathbf{R}(\theta, \tilde{\mathbf{x}}^{(i)}, \tilde{\mathbf{x}}^{(j)}))_{i,j=1, \dots, n^{\text{lo}}} \end{pmatrix} \quad (4.55)$$

Freezing all parameters except σ^2 , Equation (4.52) holds if and only if the global optimum of $\sigma^2 \mapsto \bar{\mathbf{D}}(\sigma^2)$ is attained for a variance of

$$\sigma^2(\theta, \gamma) = \frac{1}{n^{\text{hi}} + n^{\text{lo}}} \begin{pmatrix} \mathbf{Y}^{\text{hi}} - \mathbf{F}^{\text{hi}} \beta^{\text{hi}}(\theta, \gamma) \\ \mathbf{Y}^{\text{lo}} - \mathbf{F}^{\text{lo}} \beta^{\text{lo}}(\theta, \gamma) \end{pmatrix}^T \mathbf{R}^{-1}(\theta, \gamma) \begin{pmatrix} \mathbf{Y}^{\text{hi}} - \mathbf{F}^{\text{hi}} \beta^{\text{hi}}(\theta, \gamma) \\ \mathbf{Y}^{\text{lo}} - \mathbf{F}^{\text{lo}} \beta^{\text{lo}}(\theta, \gamma) \end{pmatrix} \quad (4.56)$$

Equation (4.51) then becomes:

$$(\mathbf{F}^T \mathbf{R}^{-1}(\theta, \gamma) \mathbf{F}) \begin{pmatrix} \beta^{\text{hi}} \\ \beta^{\text{lo}} \end{pmatrix} = \mathbf{F}^T \mathbf{R}^{-1}(\theta, \gamma) \begin{pmatrix} \mathbf{Y}^{\text{hi}} \\ \mathbf{Y}^{\text{lo}} \end{pmatrix} \quad (4.57)$$

Back substitution into Equation (4.45) gives the usual log-likelihood formula as known from Kriging literature[23].

$$\bar{D} = \bar{D}(\theta, \gamma) = (n^{\text{hi}} + n^{\text{lo}}) \ln(\sigma^2(\theta, \gamma)) \ln \det(R(\theta, \gamma)) + (n^{\text{hi}} + n^{\text{lo}}) \quad (4.58)$$

After the optimization process, the found value of γ gives a measure of how strong LF and HF are correlated. If a certain level of correlation is known beforehand or is just to be expected by intuition but not enough data is available to detect it, then a stronger connection between the variables can be enforced by imposing a lower bound on γ . In this way the influence of the LF on the HF data can be directly controlled. A deep theoretical analysis on the challenges in applying the current cokriging methodology is found in Ralf Zimmermann and Zhong-Hua Ha[282]

4.3.4 Radial basis function interpolation (RBF)

Originally developed by Hardy[432] to fit irregular topographic contours of geographical data, Radial basis function (RBF) is one of the multidimensional interpolation methods using scattered data, which has been found to be very accurate in solving high dimensional computation-intensive design problems and ideal interpolator. A RBF surrogate model is a linear combination of basis functions, whose argument is the Euclidean distance between the point $\mathbf{x}$ at which the interpolation is made and all the other interpolation points in the known data set. In other words, the interpolation at an untried location is a sum of contributions from all the known function values, the influence of which is controlled by a basis function that depends on the distance they are from the new location. In numerous aerodynamic applications, a strong preference has been given to radial basis function network (RBFN), the parametric version of RBF whose formulations are identical to that of a single layer neural network with hidden neurons that compute the radial basis function of the inputs[433]. In numerous aerodynamic applications, a strong preference has been given to RBFNN whose formulations are identical to that of a single layer neural network with hidden neurons that compute the radial basis function of the inputs[433]. Traditionally, RBFN are three-layers feed-forward network consisting in an input layer, a RBF hidden layer and an output layer. It is seen as a nonlinear surrogate model whose weights are estimated via nonlinear least squares, maximum likelihood or hybrid methods[434]. The present work is concerned only with interpolating RBF. Let $\mathbf{x} \in \mathcal{X}$ denotes the sampling

Figure 4.7: Single hidden layer RBFN.

plan such that

$$\begin{aligned} \mathbf{x}^{(i)} \mapsto y_i = f(\mathbf{x}^{(i)}) \mid i = 1, 2, \dots, n_s \text{ where } \mathbf{x} = [\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n_s)}]^T \\ \mathbf{y} = [y(\mathbf{x}^{(1)}), \dots, y(\mathbf{x}^{(n_s)})]^T \end{aligned} \quad (4.59)$$

The RBF approximation of the function f is a linear predictor of the form:

$$\hat{y}(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi} = \sum_{i=1}^{n_c} w^{(i)} \phi(\|\mathbf{x} - \mathbf{c}^{(i)}\|) \quad (4.60)$$

where $w^{(i)}$ are the weights, $\mathbf{c}^{(i)}$ the i^{th} of the n_c basis function centres and $\boldsymbol{\phi}$ the n_c -vector containing the values of the basis functions ϕ , evaluated at the Euclidean distances between the prediction $\mathbf{x}$ and the centres $\mathbf{c}^{(i)}$ of the basis functions[4]. Both the weights and the centers need to be learned or determined by fitting the data. Building an accurate RBFN model (computing the weights) requires to define a parametric or non-parametric basis function and sometimes to estimate/select additional influential parameters introduced within the basis functions to ensure certain. Typical examples are the basis functions shape parameters (ξ) or the variance σ^2 of the Gaussian basis function, that significantly affect the surrogate accuracy. Recall that an RBFN is nonlinear if there is more than one hidden layer or if the basis functions are size sensitive. Table 4.4 presents some common basis functions used in RBF regression. The value of the constant c (in Table 4.4) is

Table 4.4: Common basis functions used in RBF regression

Name	Radial Function
Linear	$\phi(r) = cr$
Cubic	$\phi(r) = (c + r)^3$
Thin Plate Spline	$\phi(r) = r^2 \ln(cr)$
Gaussian	$\phi(r) = e^{-cr^2/(2\sigma^2)}$
Hardy's Multiquadric	$\phi(r) = \sqrt{(r + c)^2 + \sigma^2}$
Hardy's inverse Multiquadric	$\phi(r) = ((r + c)^2 + \sigma^2)^{-\frac{1}{2}}$
C4 Matérn	$\phi(r) = e^{-\xi r} \times (3 + 3\xi r + (\xi r)^2)$
wendland's C6	$\phi(r) = (1 - \xi)^8 \times (32\xi^3 + 25\xi^2 + 8\xi + 1)$
Euclid's Hat	$\phi(r) = \pi(1/12\xi^3) - r^2\xi + (4/3r^3)$

approximated as the average Euclidean distance between the samples[435].

$$c = \left[\frac{\max(\mathbf{x}) - \min(\mathbf{x})}{n_s} \right]^{1/n_{dv}}. \quad (4.61)$$

The RBFN predictor being a linear combination of the basis functions weights, a necessary and sufficient condition to attain a unique solution is to have the number of bases equals to the number of sample points, i.e. $\mathbf{c}^{(i)} = \mathbf{x}^{(i)}$, $\forall i = 1, \dots, n_s$. This leads to the following matrix equation:

$$\mathbf{\Psi} \mathbf{w} = \mathbf{y} \quad (4.62)$$

where $\mathbf{\Psi}$ is the Gramian (also known as Gram matrix), a symmetric positive semi-definite matrix defined as $\Psi_{i,j} = \psi(\|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|)$, $i, j = 1, \dots, n_s$. Rendall et al.[436] introduced a different classification of basis functions, clustering them as local or compact decaying functions (Gaussian, Hardy's Inverse Multiquadric, etc) or global growing functions (Thin Plate Spline, Hardy's Multiquadratic, etc). It has been shown that under certain assumptions, decaying functions always lead to a Gramian, allowing an easy computation of $\mathbf{w}$ via the Cholesky decomposition. On the other hand, growing functions generally result in Hermitian matrices, suggesting the use of LU decomposition to derive the weights.

RBFNs have been widely used in aircraft aerodynamics[438, 439, 440] (flow control, estimation of aerodynamic coefficients, aerodynamic design, aeroelasticity, interpolation of wind tunnel data, classification problems, etc). It has shown to be quite efficient in the context of steady and unsteady flows features recovery, gappy data, data fusion or

Figure 4.8: 1D example of function approximations using RBFN.

constrained multi-objective or multi-disciplinary optimization[441, 442].

4.3.5 POD-based reduced order modeling (POD-based ROM) and some of its extensions

Numerical simulation of complex physical systems typically involve the solution of high dimensional systems of equations resulting from the discretization of partial differential equations (PDEs). The large dimensionality of these equations requires a significant amount of computational resources, leading to prohibitively intensive computations. To alleviate this computational burden, projection-based model reduction approaches reduce the dimension of the equations by projecting a high dimensional model (HDM) onto an appropriate subspace of lower dimension described by a reduced-order basis (ROB). The proper orthogonal decomposition (POD, 1.2.3.2) (also known as Karhunen Loève expansion, principle components analysis - PCA or singular value decomposition - SVD) is likely the most widely used projection-based ROMs in aerodynamics problems solving and have been very advantageous in the real-time and many-query contexts. POD is a technique that identifies the dominant spatial structures in an ensemble of experiments or numerical simulations, computing a set of orthonormal/optimal (best possible uncorrelated and data-dependent) linear basis functions (with as few basis functions as possible) representing the set of data. The resulting basis functions, called proper orthogonal (empirical, most energetic) modes, describes the dominant behavior of the dynamic system under consideration. The projection of a function of interest onto the basis functions provides a finite set of scalar coefficients that represent the mentioned function. The main advantages of POD lies in

the fact that it requires only standard matrix computations, despite of its application to nonlinear problems and for most applications, the snapshots are correlated, requiring only a small number of basis vectors to capture the largest part of the information they contain. It is therefore possible to obtain accurate approximations from a truncated basis. The construction of the ROM must be completed by the determination of the solution's coordinates in the basis, termed as coefficients of the POD, for any parameter location. Although projecting only onto linear or affine subspaces, the overall nonlinear dynamics is preserved since the surrogate model will still be nonlinear. Clearly, the choice of the initial data set plays a crucial role and relies either on engineering experience, intuition or space-filling sampling techniques. The training points used to construct the ROM determine its robustness with respect to parameter variations. It is important to note that every training point selected requires a solution of the FOAM. Common POD-based ROMs techniques encompass Galerkin and Petrov-Galerkin projections, POD/DEIM strategies, Gappy POD, interpolation-based (data-fit) methods, least-square residual-based POD and multi-fidelity based POD approaches. In this research, only the last three extensions of POD will be considered. Least-square residual methods are subject to the possibility for the FOAM (in our case the DLR TAU flow solver) to evaluate flux residuals. Subsequently, finding the POD coefficients in the subspace spanned by the reduced bases evolve into a non-linear least-square optimization problem. The construction of the ROB is done offline, through the method of snapshots (state vectors); an efficient method for computing POD for large-scale problems, introduced by Sirovich[129]. Here, the data set is chosen as time snapshots containing the spatial distribution of TAU numerical simulation at certain time instances reflecting the model dynamics.

4.3.5.1 Proper orthogonal decomposition (POD) via singular value decomposition (SVD)

In this subsection, the POD procedure is used to compress the snapshots, exploiting the optimal approximation properties of the SVD to yield a ROB offline. The method of snapshots consists of sampling the HDM at various parameter configurations and collecting snapshots, usually state vectors, from simulations computed with the DLR finite volume CFD solver TAU, which uses a cell-vertex scheme with dual control volumes. Let $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_d$ consist of independent selected parameters that specify the flow conditions at which to train the FOM and save state vector snapshots. Given a set of m steady snapshots (flow solutions) $\{\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m\} \subset \mathcal{D} \subset \mathbb{R}^d$ obtained at different flow conditions

$\mathbf{w}^i := \mathbf{w}(\boldsymbol{\mu}^i) \in \mathbb{R}^{n_t}$, where $\boldsymbol{\mu}^i = (\boldsymbol{\mu}_1^i, \boldsymbol{\mu}_2^i, \dots, \boldsymbol{\mu}_d^i)_{i=1, \dots, m} \in \mathbb{R}^d$ denotes the i^{th} combination of model parameters. The objective of POD is to represent the space spanned by the selected snapshots with mutually orthogonal basis modes ordered by information content. To compute the optimal basis, we first define the snapshot deviation matrix (also known as centered snapshot matrix)

$$\mathbf{Y} = (\hat{\mathbf{w}}^1, \dots, \hat{\mathbf{w}}^m) = (\mathbf{w}^1 - \bar{\mathbf{w}}, \dots, \mathbf{w}^m - \bar{\mathbf{w}}) \in \mathbb{R}^{n_t \times m} \quad (4.63)$$

where the ensemble mean vector is computed as (average of all snapshots) $\bar{\mathbf{w}} = \frac{1}{m} \sum_{j=1}^m \mathbf{w}^j$. Defining the snapshot matrix centered around the average has the advantage that only the deviation from the average has to be modeled. The snapshot POD is considered in the discretized L_2 space with its scalar product defined as $\langle \mathbf{w}_a, \mathbf{w}_b \rangle_{L_2} = \mathbf{w}_a^T \Omega \mathbf{w}_b$, where Ω is a diagonal scaling matrix with the volumes on the diagonal according to the collocation of the flow vectors. The goal behind the snapshot POD is to represent the space spanned by the snapshots by mutually orthonormal basis $\{\mathbf{U}^1, \dots, \mathbf{U}^{m-1}\}$ of POD eigenmodes ordered by information content, which optimally describe the snapshot matrix $\mathbf{Y}$ and satisfying the condition

$$\text{Span}\{\mathbf{U}^1, \dots, \mathbf{U}^{m-1}\} = \text{Span}\{\mathbf{w}^1 - \bar{\mathbf{w}}, \dots, \mathbf{w}^m - \bar{\mathbf{w}}\}. \quad (4.64)$$

A mathematical formulation of the modal problem above-mentioned leads to the maximization problem

$$\max_{\mathbf{U}^1, \dots, \mathbf{U}^d \in \mathbb{R}^{n_t}} \sum_{i=0}^d \sum_{j=0}^m \left| (\mathbf{w}^j, \mathbf{U}^i) \right|^2 \quad \text{s.t.} \quad (\mathbf{U}^k, \mathbf{U}^l)_{L_2} = \delta_{kl} \quad \text{for } 1 \leq k, l \leq d. \quad (4.65)$$

where $d = m - 1$ is the number of basis vectors used in the reduced order model; optimization problem that can in turn be reduced to computing the eigenvalue decomposition of the $m \times m$ dimensional correlation matrix [129]:

$$\begin{aligned} (\mathbf{Y}^T \Omega \mathbf{Y}) \mathbf{V}^j &= \lambda_j \mathbf{V}^j, \quad j = 1, \dots, m \\ &= (\mathbf{V}^1, \dots, \mathbf{V}^m) \text{diag}(\lambda_1, \dots, \lambda_m) (\mathbf{V}^1, \dots, \mathbf{V}^m)^T \end{aligned} \quad (4.66)$$

The POD basis eigenmodes can then be computed with

$$\mathbf{U}^j = (\sqrt{\lambda_j})^{-1} \mathbf{Y} \mathbf{V}^j \in \mathbb{R}^{n_t}, \quad j = 1, \dots, m \quad (4.67)$$

where the vectors $\mathbf{V}^j \in \mathbb{R}^m$ are the normalized eigenvectors of the eigenvalue problem 4.66. Since the centered snapshots are linearly dependent, a maximum of $m - 1$ POD modes is sufficient for a perfect reconstruction of the snapshots. The classification of the eigenvectors is such that the corresponding eigenvalues satisfy $\lambda_1 > \lambda_2 > \dots > \lambda_m$. Thus $\mathbf{V}^1$ and consequently $\mathbf{U}^1$ corresponds to the largest eigenvalue λ_1 and so forth. The relative information content (Relative Information Content (RIC)) or energy of the j^{th} POD mode is defined by the ratio $r_j = \frac{\lambda_j}{\sum_{i=1}^{\tilde{m}} \lambda_i}$. The space spanned by the first $\tilde{m} \leq m - 1$ POD basis eigenmodes ($\text{Span}\{\mathbf{U}^1, \dots, \mathbf{U}^{\tilde{m}}\}$, also known as **POD subspace**) is the best order- $\tilde{m}$ -representation of the initial snapshot space with respect to the underlying scalar product. The related RIC is thus given as

$$\text{RIC}(\tilde{m}) = \sum_{i=1}^{\tilde{m}} r_i \quad (4.68)$$

In practical applications, $\tilde{m}$ of the POD subspace is chosen such that $\text{RIC}(\tilde{m}) = 1 - \epsilon$, where $\epsilon \in [0, 1)$ is a user-defined threshold; i.e. such that the first $\tilde{m}$ modes contain 99.9% of the information provided by the snapshots. The vector space $\bar{\mathbf{w}} + \text{Span}\{\mathbf{U}^1, \dots, \mathbf{U}^{\tilde{m}}\}$ is called the **affine POD subspace**. The weighted snapshot matrix to the eigenvalue problem 4.66 can be factored, using a singular value decomposition (SVD), as

$$\mathbf{Y} = \mathbf{U}\Sigma\mathbf{V}^T \quad (4.69)$$

where $\mathbf{U} = (\mathbf{U}^1, \dots, \mathbf{U}^{\tilde{m}}) \in \mathbb{R}^{n_t \times m}$ and $\mathbf{V} = (\mathbf{V}^1, \dots, \mathbf{V}^{\tilde{m}}) \in \mathbb{R}^{m \times m}$ are unitary matrices, $\Sigma = \text{diag}(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_{\tilde{m}}}) \in \mathbb{R}^{m \times m}$ is a diagonal matrix. Once the POD eigenmodes have been computed, any flow solution contained in the POD subspace can be represented as a linear combination as follows

$$\mathbf{w}^i(\mathbf{a}) = \bar{\mathbf{w}} + (\mathbf{U}_1, \dots, \mathbf{U}_{\tilde{m}})\mathbf{a} = \frac{1}{m} \sum_{j=1}^m \mathbf{w}^j + \frac{1}{m} \sum_{j=1}^{\tilde{m}} \mathbf{a}_j^i \mathbf{U}_j^i \quad (4.70)$$

with uniquely determined coefficients

$$\mathbf{a}_j^i = \langle \hat{\mathbf{w}}^i, \mathbf{U}_j^i \rangle_{L_2} = (\sqrt{\lambda_j})^{-1} (\hat{\mathbf{w}}^i)^T \Omega \mathbf{Y} \mathbf{V}^j = (\sqrt{\lambda_j})^{-1} \mathbf{V}_i^j \quad (4.71)$$

An approximate flow solution in the affine POD subspace at an untried parameter combination $\mathbf{p}^*$ can be constructed based on the associated low-dimensional vector of the unknown POD coefficients $\mathbf{a}(\mathbf{p}^*) = (\mathbf{a}_*^1, \dots, \mathbf{a}_*^{\tilde{m}}) \in \mathbb{R}^{\tilde{m}}$. Two approaches to estimate the POD coefficients $\mathbf{a}$ are subsequently introduced, namely an **interpolation-based approach** and

a **residual-based approach**. A summary of the Centered POD-SVD procedure is presented in Algorithm 4.1.

Algorithm 4.1 Centered POD-based ROM construction via SVD

Input: ROB size, d
Output: ROB, reduced basis

- 1: select m training points : $\{\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_m\} \subset \mathcal{D} \subset \mathbb{R}^d$
- 2: **for** $j \leftarrow 1, \dots, m$ **do**
- 3: **for** $i \leftarrow 1, \dots, d$ **do**
- 4: compute m TAU solutions $\mathbf{w}^j(\boldsymbol{\mu}^i)$
- 5: define $\mathbf{Y} = (\mathbf{w}^1 - \bar{\mathbf{w}}, \dots, \mathbf{w}^m - \bar{\mathbf{w}}) \in \mathbb{R}^{n_t \times m}$, $\bar{\mathbf{w}} = \frac{1}{m} \sum_{j=1}^m \mathbf{w}^j$
- 6: choose a ROB dimension $m \leq \tilde{m}$ s.t. $\text{RIC}(\tilde{m}) = 1 - \epsilon$, $\epsilon \in [0, 1)$
- 7: compute POD basis via SVD, $\mathbf{Y} = \mathbf{U}\Sigma\mathbf{V}^T$, $\mathbf{U} = (\mathbf{U}^1, \dots, \mathbf{U}^{\tilde{m}}) \in \mathbb{R}^{n_t \times m}$,
- 8: $\mathbf{V} = (\mathbf{V}^1, \dots, \mathbf{V}^{\tilde{m}}) \in \mathbb{R}^{m \times m}$, $\Sigma = \text{diag}(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_{\tilde{m}}}) \in \mathbb{R}^{m \times m}$
- 9: compute POD positive eigenvalues $\lambda_1, \dots, \lambda_{\tilde{m}}$
- 10: compute POD eigenmodes $\mathbf{U}^1, \dots, \mathbf{U}^{\tilde{m}} \in \mathbb{R}^{n_t}$
- 11: define $\mathbf{U} = (\mathbf{U}^1, \dots, \mathbf{U}^{\tilde{m}})$

4.3.5.2 Interpolation-based proper orthogonal decomposition (POD+I)

POD approximations of any snapshot belonging to the initial training set used to generate the POD basis can be obtained through Eqn. 3.6. In order to estimate the model at untried locations, within or outside the range of the ensemble of a priori used samples, there is a need to establish a functional relationship between the a^i coefficients, that represent the projection of a generic CFD field onto the set of POD basis vectors, with reference to some design parameters. Every coefficient associated with each and every POD eigenmode is interpolated or extrapolated solely via a data-fitting method such as RBR, Kriging or TPS. In this article, the choice has been made to use RBF as data-fitting model, due to their ability to deal with large design spaces. The main advantage of data-fitting approaches lies in their non-intrusiveness (purely algebraic features), it applies generally to black-box simulation models and combines computational modeling outputs with real system data. This ROM procedure uses POD to perform the dimensional reduction, while generic data-fitting models are used for the low-dimensional manifold reconstruction. Moreover, interpolation methods have been used to enhance the robustness of the POD-ROM subject to parameter change. Mainly referred as POD + Interpolation (POD+I), the present methodology falls in the class of non physics-based ROMs and has been widely used in both linear and nonlinear aerodynamics. Apart from the a priori known drawbacks linked with the expensive off-line computational cost, POD+I surrogates optimally represent the most energetic modes contained in the set of state solutions and therefore generally result in good

objectives predictions with regards to the intrapolation of the POD coefficients; which is not the case when considering extrapolation, because the resulting ROM hardly queries the underlying FOM away from the training configurations. Algorithm 4.2, based on [164] summarized the various steps in the POD+I projection-based surrogate procedure.

Algorithm 4.2 POD+I surrogate procedure

- 1: collect m flow snapshots, $\mathbf{w}^j(\boldsymbol{\mu}^i)_{i=1,\dots,d;j=1,\dots,m}$, corresponding to the parameters set $\boldsymbol{\mu}^i$
- 2: perform POD procedure in Algorithm 4.1.
- 3: derive the orthonormal POD basis $\mathbf{U} = (\mathbf{U}^1, \dots, \mathbf{U}^{\tilde{m}})$
- 4: snapshot reconstruction:

$$\mathbf{w}^i = \sum_{k=1}^{\tilde{m}} a_k^i \mathbf{U}^k + A \quad \hat{\mathbf{w}}(\boldsymbol{\mu}^i) = \mathbf{w}(\boldsymbol{\mu}^i) - A, \quad \hat{\mathbf{w}}(\boldsymbol{\mu}^i) = \mathbf{w}(\boldsymbol{\mu}^i) - \frac{1}{\tilde{m}} \sum_{k=1}^{\tilde{m}} \mathbf{w}(\boldsymbol{\mu}^k)$$

- 5: define POD coefficients $a_k^i = \langle \hat{\mathbf{w}}^i, \mathbf{U}^k \rangle$
 - 6: **if** a is a smooth function of $\boldsymbol{\mu}$ **then**
 - 7: use interpolation to determine POD coefficients a^*
 - 8: $a^* = a_1^*, \dots, a_{\tilde{m}}^*$ for intermediate values $\boldsymbol{\mu}^*$ not in the original training set.
 - 9: prediction of $\mathbf{w}^i$ at any intermediate value of $\boldsymbol{\mu}^*$
 - 10: coefficients a^* are found via RBF, TPS or Kriging interpolation.
-

4.3.5.3 Residual-based proper orthogonal decomposition (RPOD)

To predict the flow solution in the POD affine subspace at untried parameter combinations, it is sufficient to compute the associated low-dimensional vector of POD coefficients $\mathbf{x} \in \mathbb{R}^{\tilde{m}}$. LeGresley and Alonso[170] proposed an alternative physics-based method for computing the POD coefficients by minimizing the associated CFD flux residuals, evaluated using a full-order CFD solver (in our case TAU).

$$\min_{a_1, \dots, a_{\tilde{m}}} \left\| \Omega^{-1} \text{res}(\mathbf{w}(\mathbf{a})) \right\|_{L_2}^2 = \sum_{k=1}^{n_v} \sum_{i=1}^{n_g} \frac{1}{\text{vol}_i} (\text{res}_{k,i}(\mathbf{w}(\mathbf{a})))^2 \quad (4.72)$$

Since, in general, the POD subspace does not contain steady-state flow solutions that feature a zero residual, solutions to Eqn. 4.72 are the best possible approximations to converged CFD flow solutions inside the POD subspace in a least-squares average sense. Therefore, the order- n_t equation system 2.8 is replaced by the (unconstrained) non-linear least squares optimization problem. Note that the residual res_{ki} is minimized for all the control volumes $1 \leq i \leq n_v$ and for all primitive variables $1 \leq k \leq n_g$.

In this thesis, Eqn. 4.72 will be solved using nonlinear equality algorithms(cf. 3). The Jacobian of the flux residual with respect to the POD coefficients will be required and obtained through finite difference approximation and rank-one Broyden updates to alleviate

the problem posed by the Jacobian calculation [443]. The flux residual is optimized with respect to the primitive mean-flow variables for two-dimensional cases and with respect to the energy for dimensional cases. The evaluation of the flux residual requires complete flow vectors $\mathbf{w} \in \mathbb{R}^{n_t}$ containing values for the considered primitive variables at all grid points as an input. Therefore, it is required that the POD basis modes account for the considered primitive variables simultaneously. Optimization with respect to all or selected flow variables is presented in [444]. In order to allow for the same impact of all residual variables on the optimization problem 4.72 regardless of their scales for each flow variable, the residuals are normalized by the corresponding mean value of the residuals of the initial solution. The normalization is based on the residual values of the starting solution used to initialize optimization problem. More precisely, if $\text{res}(\rho)^0 = (\text{res}(\rho)_1^0, \dots, \text{res}(\rho)_{n_g}^0)$ is the starting vector of the density residuals in all grid points, then the normalized vector is given as

$$\bar{\text{res}}(\rho)^0 = \frac{1}{\|\text{res}(\rho)^0\|} \text{res}(\rho)^0 \quad (4.73)$$

This normalization is performed in an analogous way for all residual variables. In contrast to POD-based interpolation, the sampled POD-coefficients of the snapshots are not used in determining the optimized coefficients. Thus, the least-squares ROM approach is per se better suited for extrapolation. All POD-based methods boil down to estimating POD coefficients rather than solution vector entries. The approximate solution is constructed based entirely on the information contained in the initial snapshots set. Note that the solution to the optimization problem 4.72 is constructed relying entirely on the information contained in the initial snapshot set. Therefore, model order reduction and error estimates (assessment of the regions of validity of the ROM) are respectively introduced by both POD mode reduction and (snapshot) a priori-based sampling of the parameter space. Moreover, the optimization problem 4.72 requires a starting point. Numerous ways of initializing the optimization procedure exist [197]. Starting from interpolated solutions per 4.3.5.2 is the strategy that will be adopted in this work, if required, since they have shown to be good initial guesses [197]. Solving the Residual Based Proper Orthogonal Decomposition (RPOD) with the least squares methods boils down to follow Algorithm 4.1 & Algorithm 3.2

4.3.5.4 Greedy proper orthogonal decomposition (GRPOD)

The following introduces a classical greedy POD approach. As presented in [144, 459, 460, 461], Greedy Proper Orthogonal Decomposition (GRPOD) is a procedure that sequentially and approximately update the ROB, constructed by proper orthogonal decomposition, at each step of the greedy iteration, starting from an initial sample. The GRPOD relies on the inexpensive computation of an a posteriori error indicator, in this thesis the norm of the residual, associated with a ROM solution. In other words, we are progressively building a ROM and increasing its dimension by considering additional samples and their corresponding snapshots at locations of the parameter space where the current ROM is inaccurate. The classical GRPOD presented in this thesis arose from the procedure defined in [459].

Algorithm 4.3 Classical Greedy POD procedure

Input: parameter domain $\mathcal{D}$, maximum error indicator tolerance $\mathcal{I}^{max}$, maximum number of 'reduced' optimization iterations N_{iter}^{max} , maximum number of candidates N_c

Output: global ROB $\mathbf{V} \in \mathbb{R}^{d \times k}$

- 1: Randomly select a first sample $\boldsymbol{\mu}^1 \in \mathcal{X}$
- 2: Compute the FOM $\mathbf{w}(\boldsymbol{\mu}^1)$ associated with the sampled parameter $\boldsymbol{\mu}^1$, $\mathbf{f}(\mathbf{w}(\boldsymbol{\mu}^1); \boldsymbol{\mu}^1) = 0$
- 3: Build a corresponding ROB $\mathbf{V}_1$ by POD using the FOM $\mathbf{w}(\boldsymbol{\mu}^1)$
- 4: Randomly select a large discrete set of N_c parameters $\mathcal{C} = \{\boldsymbol{\mu}^{(1)}, \dots, \boldsymbol{\mu}^{(N_c^{max})}\} \subset \mathcal{D}$
- 5: **for** $N_{iter} \leftarrow 2, \dots, N_{iter}^{max}$ **do**
- 6: **for** $j \leftarrow 1, \dots, N_c$ **do**
- 7: Compute the ROM solution $\mathbf{q}(\boldsymbol{\mu}^j)$ for $\boldsymbol{\mu}^j$: ROB $\mathbf{V}_{N_{iter}-1}$, $\mathbf{f}(\mathbf{w}(\boldsymbol{\mu}^j); \boldsymbol{\mu}^j) = 0$
- 8: Compute the associated a posteriori norm of residual $\mathcal{I}(\boldsymbol{\mu}^j)$
- 9: Find $\boldsymbol{\mu}_{N_{iter}} = \underset{\boldsymbol{\mu} \in \mathcal{C}}{\operatorname{argmax}} \mathcal{I}(\boldsymbol{\mu})$
- 10: **if** $\mathcal{I}(\boldsymbol{\mu}_{N_{iter}}) < \mathcal{I}^{max}$ **then**
- 11: Set $\mathbf{V} = \mathbf{V}_{N_{iter}-1}$
- 12: **Break**
- 13: Compute the FOM $\mathbf{w}(\boldsymbol{\mu}_{N_{iter}})$ associated with $\boldsymbol{\mu}_{N_{iter}}$
- 14: Construct a ROB $\mathbf{V}_{N_{iter}}$ by POD using the solutions $\{\mathbf{w}(\boldsymbol{\mu}^i)\}_{i=1}^{N_{iter}}$
- 15: **if** $N_{iter} = N_{iter}^{max}$ **then**
- 16: Set $\mathbf{V} = \mathbf{V}_{N_{iter}}$

At each iteration N_{iter} , the GRPOD proceeds by selecting the value of the parameter $\boldsymbol{\mu}_{N_{iter}}$ that maximizes the norm of the error between the full order solution and the associated ROM solution. As previously mentioned, in this thesis, error indicators involve computing the norm of the residual vector, constructed by offline/online decomposition. To avoid bottlenecks with the decomposition, i.e. the case where its complexity does not scale with the dimension of the full order model, it is assumed that the parameter dependence is affine. Therefore, the number of potential ROM simulations is constrained and a posteriori

error estimations is in general constrained from the order of 10^5 to 10^2 [461]. The test cases presented in this thesis deal with less than 5 design variables; therefore the drawbacks associated with the algorithm of Haasdonk and M. Ohlberger [459] should not posed any burden. Furthermore, the training phase terminates if the norm of residual is smaller than a specified error tolerance. Algorithm 4.3 summarizes the steps to be taken.

4.3.5.5 Multi-Fidelity Proper Orthogonal Decomposition (MF POD)

Below are implemented two multi-fidelity POD algorithms:

- a novel Multi-Fidelity Proper Orthogonal Decomposition + Interpolation (MF POD+I) approach that partly follows the trends of the POD+I algorithm (4.2), never implemented before to the best of the author's knowledge,
- and a naive extension to multi-fidelity of the single-fidelity non-linear least squares POD-Based ROM introduced by Zimmermann et al. [169, 188, 444]

Both algorithms can be used to reconstruct the flowfield and approximate global aerodynamic functions over the entire parameter space. The HF arise from the full order model and LF are obtained through variable accuracy modeling (VAM), i.e. relaxing the convergence and limiting the number of iterations. Consider a spatial arrangement of the HF and LF interpolation points to be:

$$\mathcal{X}^{\text{hi}} = \{\boldsymbol{\mu}_{\text{hi}}^1, \dots, \boldsymbol{\mu}_{\text{hi}}^m\} \subset \mathbb{R}^d \quad \& \quad \mathcal{X}^{\text{lo}} = \{\boldsymbol{\mu}_{\text{lo}}^1, \dots, \boldsymbol{\mu}_{\text{lo}}^n\} \subset \mathbb{R}^d, \quad \text{with } n_{\text{hi}} \ll n_{\text{lo}} \quad (4.74)$$

1. The MF POD+I algorithm

In this algorithm, we stress on the reduced basis obtained from the POD decomposition of the output on the HF level. The multi-fidelity surrogate is applied to the projection coefficients on the above-mentioned basis. The steps to be taken are described in Algorithm 4.4 below:

Fig.4.9 presents the framework encompassing the various procedures.

2. The multi-fidelity non-linear least squares POD-Based ROM

The current approach does not involve any adaptative sampling and is based on a naive generation of a multi-fidelity surrogate model based on an extended snapshot matrix within which are stored the low- and high-fidelity steady-state surface fields (Fig.4.10). It is simply an extension of the single-fidelity RPOD (4.3.5.3) to multi-fidelity problems.

Algorithm 4.4 MF POD+I procedure

Input: parameter domain $\mathcal{D}$, high fidelity spatial arrangement $\mathcal{X}^{\text{hi}}$,
low fidelity spatial arrangement $\mathcal{X}^{\text{lo}}$

Output: reconstructed snapshots

- 1: select m training points : $\{\boldsymbol{\mu}_{\text{hi}}^1, \dots, \boldsymbol{\mu}_{\text{hi}}^m\} \subset \mathcal{X}^{\text{hi}} \subset \mathbb{R}^d$
- 2: select n training points : $\{\boldsymbol{\mu}_{\text{lo}}^1, \dots, \boldsymbol{\mu}_{\text{lo}}^n\} \subset \mathcal{X}^{\text{lo}} \subset \mathbb{R}^d$
- 3: Compute the truncated HF centered POD basis (POD eigenmodes) :
 $\mathbf{U}_{\text{hi}} = (\mathbf{U}_{\text{hi}}^1, \dots, \mathbf{U}_{\text{hi}}^{\tilde{m}})$ as in Algorithm 4.1
- 4: Compute the HF level projection coefficients α_k^i by projecting the HF level outputs ($\mathbf{w}(\boldsymbol{\mu}_{\text{hi}})$) on the truncated HF POD basis : $\alpha_k^i = \langle \hat{\mathbf{w}}_{\text{hi}}^i, \mathbf{U}_{\text{hi}}^k \rangle$
- 5: Compute the LF level projection coefficients β_k^i by projecting the LF level outputs ($\mathbf{w}(\boldsymbol{\mu}_{\text{lo}})$) on the truncated HF POD basis : $\beta_k^i = \langle \hat{\mathbf{w}}_{\text{lo}}^i, \mathbf{U}_{\text{hi}}^k \rangle$
- 6: **for** $k \leftarrow 1, \dots, \tilde{m}$ **do**
- 7: Construct a co-kriging model $\tilde{\alpha}_k^i$, considering the coefficients α_k^i as HF sampled data & the coefficients β_k^i as LF sampled data
- 8: The surrogate model output (centered POD snapshot reconstruction) at untried location $\boldsymbol{\mu}^*$:
 $\hat{\mathbf{w}}(\boldsymbol{\mu}^i) = \mathbf{w}(\boldsymbol{\mu}^i) - \mathbf{A}$, $\hat{\mathbf{w}}(\boldsymbol{\mu}^i) = \mathbf{w}(\boldsymbol{\mu}^i) - \frac{1}{\tilde{m}} \sum_{k=1}^{\tilde{m}} \mathbf{w}(\boldsymbol{\mu}^k)$

$$\hat{\mathbf{w}}(\boldsymbol{\mu}^i) = \sum_{k=1}^{\tilde{m}} \tilde{\alpha}_k^i \mathbf{U}_{\text{hi}}^k - \frac{1}{\tilde{m}} \sum_{k=1}^{\tilde{m}} \mathbf{w}(\boldsymbol{\mu}^k)$$

Figure 4.9: The MF POD+I ROM framework.

Recall the spatial arrangement of the HF and LF interpolation points to be

$$\mathcal{X}^{\text{hi}} = \{\boldsymbol{\mu}_{\text{hi}}^1, \dots, \boldsymbol{\mu}_{\text{hi}}^m\} \subset \mathbb{R}^d \quad \& \quad \mathcal{X}^{\text{lo}} = \{\boldsymbol{\mu}_{\text{lo}}^1, \dots, \boldsymbol{\mu}_{\text{lo}}^n\} \subset \mathbb{R}^d, \quad \text{with } n_{\text{hi}} \ll n_{\text{lo}}$$

and their corresponding responses. Algorithm 4.5 summarizes the procedures to mimic the full order model.

Figure 4.10: The multi-fidelity non-linear LSQ POD-Based ROM framework.

Algorithm 4.5 Multi-fidelity LSQ POD-Based ROM

Input: parameter domain $\mathcal{D}$, high fidelity spatial arrangement $\mathcal{X}^{\text{hi}}$,
low fidelity spatial arrangement $\mathcal{X}^{\text{lo}}$

Output: reconstructed snapshots

- 1: Select a 'smart' a priori high & low fidelity sampling sets:
 $\mathcal{X}^{\text{hi}} = \{\mu_{\text{hi}}^1, \dots, \mu_{\text{hi}}^m\} \subset \mathbb{R}^d$ & $\mathcal{X}^{\text{lo}} = \{\mu_{\text{lo}}^1, \dots, \mu_{\text{lo}}^n\} \subset \mathbb{R}^d$, with $m \lll n$
- 2: Compute the LF & HF offline solutions
 $\mathbf{Y}^{\text{hi}} = (\mathbf{w}(\mu_{\text{hi}}^1), \dots, \mathbf{w}(\mu_{\text{hi}}^m)) \in \mathbb{R}^{d \times m}$ & $\mathbf{Y}^{\text{lo}} = (\mathbf{w}(\mu_{\text{lo}}^1), \dots, \mathbf{w}(\mu_{\text{lo}}^n)) \in \mathbb{R}^{d \times n}$
- 3: Build the extended snapshots matrix
 $\mathbf{E} = [\mathbf{w}(\mu_{\text{hi}}^1), \dots, \mathbf{w}(\mu_{\text{hi}}^m), \mathbf{w}(\mu_{\text{lo}}^1), \dots, \mathbf{w}(\mu_{\text{lo}}^n)]$, $\mathbf{E} \in \mathbb{R}^{d \times (m+n)}$
- 4: Build the Multi-Fidelity POD basis via SVD & proceed as described in 4.3.5.3
- 5: Snapshot reconstruction (centered POD):

$$\hat{\mathbf{w}}(\mu^i) = \mathbf{w}(\mu^i) - \mathbf{A}, \quad \hat{\mathbf{w}}(\mu^i) = \mathbf{w}(\mu^i) - \frac{1}{\tilde{m}} \sum_{k=1}^{\tilde{m}} \mathbf{w}(\mu^k)$$

Chapter 5

Test cases, results and discussions

In the following, the single fidelity LSQ-POD ROM, the GRPOD, the MPOD+I and the naive multi-fidelity LSQ-POD ROM algorithms described in the previous chapters are used to perform a flowfield reconstruction and to compute the aerodynamic characteristics of two different test cases, namely the NACA64A010 airfoil and the wing-body NASA common research model. Global and/or local aerodynamics coefficients comparisons are achieved to assess the performance and efficiency of the various reduced order models. All the snapshots (reference flow solutions) are obtained running the DLR TAU Solver. All the flows considered in different test cases are in the steady transonic regime and are modeled with the RANS equations, using the Spalart-Allmaras one-equation turbulence model and the Menter-SST, respectively for the NACA airfoil and the Common research model, to accurately capture the flow physics. The computations were performed partly within the Airbus HPC environment, the UPM school of aeronautics clusters, both operating under Linux/Unix and an Intel(R) Core(TM) i5-4200M windows-based laptop. The CFD calculations were run in serial or in parallel, using 8 or 12 cores whenever possible. The use of these various environments made it impractical to compare computational times and calculation of the speedups. However, whenever possible, the duration of the computation is given in wall clock time or in CPU time.

5.1 The NACA 64A010 Airfoil

Two independent design parameters are investigated in this case, namely the angle of attack (AoA) and the Mach number (Ma), with $(Ma, \alpha) \in [0.72, 0.84] \times [0^\circ, 10^\circ]$. The computational grid size is 21.454 points. The NACA64A010 airfoil has better tran-

sonic performance than numerous airfoils and was designed to have a high drag rise Mach number. Figs.5.1 & 5.2 introduce the airfoil and the associated grid. The aerodynamic characteristics are approximated at four locations selected randomly, two intrapolation samples ($Ma = 0.725$, $AoA = 6.0$), ($Ma = 0.8$, $AoA = 4.5$) and two extrapolation samples ($Ma = 0.78$, $AoA = 11.0$), ($Ma = 0.85$, $AoA = 5.9$). All the computations are performed with a fixed Reynolds number of 8.25 mio subject to a single constraint of a random lift coefficient value, equivalent to 0.7. Full order computations are performed in parallel on a HPC cluster in parallel, distributed on 12 domains, with the minimum residual being set to 1e-11.

Figure 5.1: NACA64A010 airfoil.

Figure 5.2: NACA64A010 grid.

To generate POD bases, the following procedures are considered for the four algorithms mentioned above:

- In the case of the single fidelity LSQ-POD ROM, a Halton Quasi-Random sampling of 30HF training points to generate the high-fidelity snapshots (Fig. 5.3a)
- a one-iteration-based error estimate error indicator in the case of the GRPOD
- an optimized LHS for HF training point locations combined with Halton Quasi-Random sampling for LF training point locations (8HF + 60LF), in the case of both multi-fidelity approaches. Prior to these computations, a couple of tests and analyses were run and the simplified cross-correlation approach [282] was applied to detect the level of correlation between low and high fidelities.

Having in mind our low fidelity models are partially converged ones (VAM), and considering we wish to attain a certain(acceptable) level of correlation, a lower bound on γ , $\gamma \geq 0.85$ was imposed in order to enforce a strong connection between the design parameters. it was then sufficient to foresee when to relax the convergence or stop the computations after a certain number of iterations to have low fidelities influencing the high fidelities per the set level of correlation. This approach was preferred to the LOOCV that appeared to be computationally expensive to select appropriate low fidelities when combined to the simplified cross correlation co-kriging and considering the γ lower bound.

(a) 30HF Halton.

(b) 8HF OLHS + 60LF Halton.

Note that all the training points locations are determined a priori/offline, using the above-mentioned sampling methods. The variables considered are the density, both x,z velocity components, the pressure, the SA and the eddy viscosities. Therefore, a global POD-SVD of the set of snapshots with respect to the discrete L_2 inner product induce an orthogonal representation that extracts dominant structures (POD modes), represented by vectors whose dimension is $6 \times 21.454 = 128.724$. This projection on the subspace to be used

to model the NACA64A010 system (choice of the dimension) is quite delicate when the relative information content is measured with respect to the L2 inner product. The POD is the most efficient in the sense that for a given number of modes, the projection on the manifold $\mathcal{V}_d$ of low dimension d_s will on average contain the most energy possible. Moreover, the (Ma, AoA) snapshots turn up to be numerically almost linearly dependent, because the nonlinearities are essentially confined to a narrow neighborhood in the vicinity of the airfoil [305]. When varying the Mach number and the angle of attack, the most essential nonlinear changes in the flow field are expected to occur close to the surface due to the moving shocks. The goal is to choose d_s small enough while the RIC of the basis for $\mathcal{V}_d$, defined in 4.3.5.1, is close to 1; i.e. if the manifold $\mathcal{V}_d$ should contain a percentage p of the information, then one should choose d such that $d = \operatorname{argmin} \{I(d) : I(d) \geq \frac{p}{100}\}$. Often, the basis of POD modes is truncated to exclude contributions to the flow from low-energy modes. Furthermore, the complexity of flow descriptions resulting from truncated POD bases can be greatly mitigated by severe basis truncations of important higher-order modes (4.3.5.1). For both the single- and multi-fidelity modelings, a rapid decrease in magnitude of the RIC was noticed respectively after approximately 3-4 basis functions, indicating that the first few basis functions account for most of the variation in the snapshot ensembles (more than 99.9% of the RIC). An approximate number of 21 and 45 POD modes respectively were necessary to capture the complete RIC, with only little gain of additional information being possible from there on. However, it is also important to mention that an order $\mathcal{O}(10)$ POD modes are sufficient and that the computational costs linked with the pressure predictions with 21 or 45 basis functions do not differ significantly as if we would have considered respectively 29 and 67 eigenfunctions (the maximum number of modes corresponding to non-zero eigenvalues). Thus, a total of $6 \times 29 = 174$ and $6 \times 67 = 402$ mode vectors of size 128.724 are respectively required reducing the both problems to an order-29 and an order-67 optimization problems. It is worth mentioning that only the primitive mean-flow variables are considered while optimizing the residuals. To perform the classical POD-Greedy algorithm, the maximum number of candidates N_c is set to 100; candidates spread uniformly in the parameter space. As seen from the classical POD Greedy algorithm (4.3), the error indicator is the norm of the residual. Therefore, specifying a maximum a posteriori error indicator tolerance $\mathcal{I}^{max}$ that correspond to a desired exact error tolerance should rely on trial and error [465]. Since in classical POD-greedy algorithms, the a posteriori error bound $\Delta^k(\mu)$ can be computed at lower costs, it is therefore possible for a certain number of iterations to estimate the error between the

FOM and the Greedy-POD ROM at step k of the procedure, on the discrete set $\mathcal{C} \in \mathcal{D}$ of the parameter space. At step k of the procedure, the FOM is evaluated at the parameter value $\boldsymbol{\mu}_k^{\max} = \max_{\boldsymbol{\mu} \in \mathcal{C}} \Delta^k(\boldsymbol{\mu})$. The ROM is sequentially updated with new information and the procedure is going on until it reaches a certain tolerance. Few tests allowed to randomly assign a tolerance value of 10^{-4} to $\mathcal{I}^{\max}$ after monitoring the trends of the maximum relative error and the average relative error plots in log scale versus the number of iterations N_{iter} (Fig. 5.4). From both error plots, it can be notice that they are far away to reach asymptotic errors at approximately $N_{\text{iter}} = 20$ iterations; however, this served as guidance in the choice of the maximum number of 'reduced' iterations $N_{\text{iter}}^{\max}$ that was fixed at 40, allowing for 40 greedy iterations to be performed. Unfortunately, the computations continuously presented an error above the threshold value and therefore it was not possible to foresee a constant variation of the error around the set maximum number of 'reduced' iterations; which indicates that the maximum error indicator could be decrease further than the 40 iterations. To summarize, we were not able to provide a rigorous upper bound for the error approximation; and keeping in mind the dimensionality of the subspace is critical in the design of accurate predictions, we knew from this stage that we will not obtained optimal ROMs. Note that the POD-Greedy algorithm performs an expensive greedy-search over the whole training set ($\mathcal{C}$) in every iteration during the extension algorithm that render the construction of the POD basis very time consuming; this indeed makes it one of the most expensive algorithm considered in this research work. It is worth mentioning that computations of the ROB are based on the open source library `libMesh` (<http://libmesh.github.io/>) that interfaces to `PETSc` and `LASPack` for the solutions of linear systems and to `SLEPc` for eigenproblem routines.

Figs. 5.5 to 5.8 present the predicted and TAU CFD pressure contours at the intrapolation and extrapolation locations for all the algorithms above-discussed. The TPS-RBF approximations at the mentioned locations, not represented on the plots for the sake of good visualization, are used as a starting point for both the single-fidelity and multi-fidelity LSQ POD-ROM optimizations. A straight observation that can be made is that the prediction seem to be more sensitive to Mach number than angle of attack, which consolidate our idea of considering more eigenfunctions when building the POD bases for better predictions accuracy.

The corresponding surface C_p distributions are displayed in Figs. 5.9 to 5.12. The single-fidelity models and the multi-fidelity models are separately compared to the TAU CFD reference results. In the intrapolation case ($Ma = 0.725$, $AoA = 6.0$), both the greedy

Figure 5.4: Maximum and average relative errors - Classical Greedy POD algorithm.

and the single-fidelity least-squares POD-based models display a quasi good match with TAU reference results, especially on the pressure side of the airfoil. However, upstream and approximately from 40% downstream of the chord on the suction side, some disparities (that can be seen from the C_p distributions and the C_p plots below) occur not only between both surrogate models but also when compared to the TAU reference results. Similarly to the high-fidelity models, the multi-fidelity models depict a virtual agreement with the TAU reference results on the lower surface. However, the differences between the C_p trends are found all over the upper surface and are more pronounced. In the interpolation case ($Ma = 0.8$, $AoA = 4.5$), almost similar observations to the case of ($Ma = 0.725$, $AoA = 6.0$) can be made, with the differences that both least-squares based approaches are in nearly good accordance with the TAU reference results. Nonetheless, the greedy and MF POD+I ROMs exhibit considerable deviations from the TAU reference plot, notably on the upper surface. Two different extrapolation samples were selected, ($Ma = 0.78$, $AoA = 11.0$) and ($Ma = 0.85$, $AoA = 5.9$) with the AoA and Mach number being respectively out of range. In the case ($Ma = 0.78$, $AoA = 11.0$), both the contours of the single-fidelity and multi-fidelity LSQ POD pressure contours almost accurately predict the TAU reference steady-state pressure fields over a range of parameter values; which is not the case for the two other approaches. In the case of ($Ma = 0.85$, $AoA = 5.9$), though it cannot be

Figure 5.5: NACA64A010 pressure contours at $Ma = 0.725$, $AoA = 6.0$

clearly see from Fig. 5.12, there exist some disparities between the single fidelity LSQ POD-ROM predicted pressure contours and the TAU CFD pressure contours. The other methods pressure contours appear to be dissimilar from the TAU CFD reference contours, especially downstream on the lower surface.

Numerous reasons can explain the failure of the trained surrogate models. Though the

Figure 5.6: NACA64A010 pressure contours at $Ma = 0.80$, $AoA = 4.5$

single-fidelity LSQ-POD ROM has given very satisfactory results, the partial inaccuracy of the predictions arising from the other reduced-order models posed the problem of the generation and truncation of the full POD basis. The offline construction of the global POD basis is based on the information contained in the snapshots ensemble. It therefore becomes apparent that an optimal location of the snapshots combined to a dynamic a posteriori

Figure 5.7: NACA64A010 pressure contours at $Ma = 0.78$, $AoA = 11.0$

monitoring of the POD errors estimates or the bounds of POD errors and, whenever required, correction of the reduced-order models, would have improved the quality of the predictions. Moreover, the size of the multi-fidelity training set, the choice of the number of high and low fidelities can also be one of the reasons explaining the poor prediction of the MF POD+I surrogate model. On the other hand, various drawbacks could be at the

Figure 5.8: NACA64A010 pressure contours at $Ma = 0.85$, $AoA = 5.9$

origin of the bad performance of the greedy POD model; among those, the choice of the size of the set N_c or the inappropriate choice of the maximum a posteriori error indicator tolerance $\mathcal{I}^{max}$. Moreover, a suitable procedure to estimate, at each iteration N_{iter} , the parameter $\mu_{N_{iter}}$ maximizing the a posteriori error indicator $\mathcal{I}(\mu)$ over the set $\mathcal{D}$. It is worth mentioning the fact that the problem at hand is of low dimension have ease the

computation of a norm of residual-based error indicator; in general these computations scale with the dimension of the FOM.

Figure 5.9: NACA64A010 C_p distributions at $Ma = 0.725$, $AoA = 6.0$

Figure 5.10: NACA64A010 C_p distributions at $Ma = 0.80$, $AoA = 4.5$

The offline computations of all the TAU snapshots took approximately 45 min and on average, The CPU time for the single fidelity and the multi-fidelity LSQ ROMs took about 70s and 120s respectively at one sample location. Moreover, the total wall clock time of MF POD+I computations was approximately 12 min on 8 cores. The construction of the POD-Greedy basis, that includes the offline and online stages, took about half an hour. This time is high due to the fact that not only it incorporates the offline generation of the candidates, the extraction of the reduced basis, the estimation of the ROB coefficients but also the adaptative generation of new snapshots.

Figure 5.11: NACA64A010 C_p distributions at $Ma = 0.78$, $AoA = 11.0$ Figure 5.12: NACA64A010 C_p distributions at $Ma = 0.85$, $AoA = 5.9$

5.2 Generic civil transport aircraft configuration

The present section introduces reduced-order models of compressible (steady-state) Reynolds-Averaged Navier-Stokes equations for flows around a generic civil transport aircraft configuration, namely the NASA Common Research Model (CRM). The present aircraft served as backbone for providing wind tunnel data for code validation and verification. Similarly to the NACA64A010, unstructured computational grids are used to generate the snapshots through computations performed with the TAU flow solver. To account for the transport of the turbulent shear stress, the Menter-SST turbulence model was chosen. The predicted and TAU CFD pressure contours are compared for two aircraft flight conditions, within the range of validity of the global POD bases. The model employed is the MF POD+I. Only one independent parameter, the AoA , is investigated. Full order computations are carried

out in parallel on a HPC cluster in parallel, distributed on 8 domains, with the minimum residual set to $1e-16$. The partially converged solutions used in lieu of low-fidelity models are obtained relaxing the convergence and stopping the simulations after a certain number of iterations. Deciding on the later was done with the help of the convergence history of few TAU runs, expecting a certain level of correlation between the high and low fidelities. The NASA Common Research Model (CRM) is an open geometry, generic transport model developed by NASA that consists of a supercritical transonic wing and a fuselage, representing a widebody commercial transport aircraft. The CRM is designed for a cruise Mach number of $Ma = 0.85$ and a corresponding design lift coefficient of $C_L = 0.5$ that was set as a constraint. The computational grid size is approximately 4.075 mio grid points. Fig.5.13 displays the CRM aircraft grid.

Figure 5.13: NASA Common Research Model grid.

To create the POD basis, a total of 11 snapshots are computed at a constant cruise Mach number of 0.85 and a Reynolds number of $5e6$. High fidelities are computed at 4 different AoA, $0^\circ, 3^\circ, 4^\circ, 6^\circ$. Similarly to the high fidelities, the computation of the low-fidelities are based on the RANS but exploit a relaxed convergence criteria that we expect guaranty a certain level of correlation with full order model snapshots. Low fidelities are generated at 8 different AoA, $1^\circ, 1.5^\circ, 2.5^\circ, 3.5^\circ, 4.5^\circ, 5.0^\circ, 6.5^\circ$. The flow features are predicted at two locations, ($Ma = 0.85$, $AoA = 2.0$) and ($Ma = 0.85$, $AoA = 7.0$). To generate the low fidelities, the minimum residual was set to $1e-8$ and the maximal time step number to 4000 (based on Fig. 5.14) in order to stop the solver when the number of iterations is equal the prescribed value.

A maximum number of $\tilde{m} = 11 - 1 = 10$ POD modes is retained in the construction of the truncated POD basis. Following Algorithm 4.4, the obtained pressure contours for

Figure 5.14: Sample convergence history for the NASA Common Research Model

Figure 5.15: NASA Common Research Model C_p contour plots at $Ma = 0.85$, $AoA = 2.0$.

both flight conditions are displayed in Figs. 5.15 and 5.16. Though the MF POD+I model turned up to fairly emulate the trends of the pressure contours at $AoA = 2^\circ$, it failed to give satisfactory outcomes at $AoA = 7^\circ$. The latter was more or less expected since the AoA falls out of the range of values used to build the global POD basis and POD+I interpolation models traditionally offer no guarantee in terms of ROM quality or accuracy out of the initial training set.

To corroborate these results, a close view of the pressure distribution plots of the prediction against the TAU CFD reference is done at three locations spanwise, $\eta = 0.15$, $\eta = 0.40$ and $\eta = 0.75$ (Fig. 5.17). Figs. 5.18 & 5.19 illustrate the above-mentioned discrepancies. Though the pressure contour lines (derived from the MF POD+I model) in the

Figure 5.16: NASA Common Research Model C_p contour plots at $Ma = 0.85$, $AoA = 7.0$.

inboard section of the wing, on the fuselage and the tail-plane are in a quasi-accord with their TAU solver reference counterparts, they seem not to rightly represent the large shock motions as we move towards the outboard sections of the wing. While the computations of the converged TAU CFD lasted nearly 6.5h on 12 cores, the total wall-clock time of the MF POD+I ROM computations was approximately 8 min.

Figure 5.17: Slices locations spanwise

Table 5.1 summarizes the global aerodynamic coefficients predictions at $AoA 2^\circ$ and 7° .

Figure 5.18: Pressure distribution comparisons at 3 spanwise locations, $Re = 5.0e6$, $Ma = 0.85$, $AoA = 2^\circ$

		C_l	C_d	C_{m_y}
$Ma = 0.85$, $AoA = 2^\circ$	TAU CFD	0.49988	0.02769	-0.03540
	MF POD+I	0.48931 (-2.11%)	0.02758 (-0.39%)	-0.03102 (-12.37%)
$Ma = 0.85$, $AoA = 7^\circ$	TAU CFD	0.50997	0.02828	-0.03835
	MF POD+I	0.52136 (+2.23%)	0.02843 (+0.50%)	-0.02087 (+45.58%)

Table 5.1: Global aerodynamic coefficients predictions at $AoA 2^\circ$ and 7°

Figure 5.19: Pressure distribution comparisons at 3 spanwise locations, $Re = 5.0 \times 10^6$, $Ma = 0.85$, $AoA = 7^\circ$

Chapter 6

Conclusion

The present chapter summarizes the tasks conducted throughout this thesis, in the design of novel reduced-order single- and multi-fidelity models capable of spanning the main features (physics and dynamics) of the full order models. Furthermore, it provides leads for future investigations. One of the major challenges addressed has been the generation of partially converged sufficiently well-correlated low fidelity models . A summary of the assignments performed to meet our research objectives is given in the section below, followed by an indication on possible areas for future research.

6.1 Summary

The primary objective of this research is to build hybrid surrogate model frameworks, combining multi-fidelity and projection-based surrogates, that would be efficient when applied to equality constrained full order aerodynamic models. This thesis is organized as follows: **Chapter 2** briefly reviews the fundamentals of aerodynamic design, steady and transonic aerodynamics. The steady formulation of the governing equations are presented, as well as the SMARTy toolbox and the DLR TAU flow solver. The latter is used to generate the various high- and low- fidelities (snapshots) required in the cokriging model and to build the POD basis for example. Challenges linked with the reduced-order basis are enlightened. **Chapter 4** familiarizes oneself with the various sampling methodologies implemented in this thesis. Moreover, the chapter introduces the theoretical background on all the surrogate modeling techniques employed (cokriging, POD, etc). **Chapter 3** accustoms the reader to methods for nonlinear least squares problems and discusses the parallel between them and the optimization of steady-state aerodynamic problems solutions. An

emphasis is put on algorithms for equality constrained nonlinear least squares problems and the major issues related to their application in large scale problems. **Chapter 5** introduces and discusses results from two aircraft steady aerodynamics applications. Those test cases encompass the prediction, in transonic regime, of local/global aerodynamic coefficients (intrappolation within and extrapolation out of the a priori training set) for the 2D NACA64A010 airfoil using two independent parameters (Ma , AoA) and the NASA Common Research Model (wing-body DPW4 A/C) for a single parameter. Furthermore, comparisons of the reconstructed pressure fields (pressure contours) to their counterparts obtained using the FOM (full TAU simulations) will be performed. Additionally, pressure coefficient plots comparisons are presented at 4 different (Ma , AoA) locations for the 2D airfoil and at 3 spanwise locations for the model aircraft case.

As above-mentioned, this thesis introduces two novel multi-fidelity approaches, namely a naive nonlinear multi-fidelity LSQ POD-Based ROM and a multi-fidelity interpolation-based procedure. In order to assess the characteristics (quality, accuracy, speed, etc) of both predictions, their performances are compared with those of the TAU solver, the single-fidelity LSQ POD-based ROM and the classical Greedy POD-based ROM. To build the latter, the norm of residuals is chosen as an error indicator and the maximum a posteriori error indicator tolerance specified relying on a trial and error method. In order to generate the partially converged low-fidelity models in the process of building the multi-fidelity models, two approaches were implemented:

- the cross-correlation simplified co-kriging using a parameter measuring the level of correlation between the low-fidelity models and the full order model (for the NACA64A010 airfoil),
- and a relaxed convergence approach, relying on the trends of the convergence plots and considering a low minimum residual value (for the NASA CRM).

The single-fidelity and the multi-fidelity models results are respectively compared against the TAU solver reference results. However, only the multi-fidelity POD+I was compared to the FOM in the case of the NASA CRM. In the case of the NACA64A010 airfoil, the pressure contours and the C_p plots indicate that there is a quite good agreement with TAU computations, especially for lower mach numbers within our range of Mach number values. Moreover, a straight observation that can be made is that the predictions seem to be more sensitive with increasing Mach number than angle of attack, making it more difficult for our surrogate (reduced-order) models to capture the nonlinearities (shocks,

etc), mainly in the vicinity of leading edge and the suction side of the airfoil. For high Mach numbers, similar observations are made; additionally, on the pressure side of the airfoil, the surrogates fail to mimic the trends of the pressure distribution downstream of the airfoil. These discontinuities and gaps from the full order model could be explained by the lack of robustness of the classical greedy algorithm, considering the various parameters that were approximately defined a priori. In the case of both multi-fidelity models, one cause of failure can be the generation of the POD basis, the spread of the training points within the parameter space and the everlasting issue concerning the trade-off to be made when deciding on the number of high- and low fidelities. Nonetheless, outside of the initial training set used to generate the POD basis, it is common that global ROB and interpolation-based algorithms are unable to reconstruct the flow features.

Talking about the NASA Common Research Model, though the pressure contour lines (derived from the MF POD+I model) in the inboard section of the wing, on the fuselage and the tail-plane are in a quasi-accord with their TAU solver reference counterparts, they seem not to rightly represent the large shock motions happening in the outboard section of the wing. Likewise the NACA64A010, major improvements could be achieved while building the global POD basis featuring the very explanations. However in both cases, raising the number of snapshots may not necessarily be a guarantee to capture more information; one the drawbacks being the rise of the computational time.

6.2 Perspectives for future work

The present section aimed at addressing some shortcomings concerned with the developed/presented algorithms, examining possible developments and extending the latter to more challenging high-dimensional industrial cases (uncertainty quantification, multifidelity optimization, multidisciplinary optimization, etc). Although the presented reduced-order models have globally shown to provide satisfactory results, numerous paths of improvement are possible. The goal of ROMs being to provide fast and accurate predictions by reducing the dimensionality of the solution space, one of the main lines of enhancement include the generation and truncation of the POD basis. Our research has shown the hardship of training a static global ROB, that is expected to perform well throughout the parameter space and beyond. This was due to the fact that the a priori sampling approach is a model free procedure, that leads to a fast construction of the ROB, but that tends to include unneeded samples. This suggests the use of an adaptive procedure that merges the

offline and online phases, and that rely on repeated evaluations of the errors of the model (or some error indicators) to assess the accuracy of the model; which explain the reason why we studied alongside the performance of a classical greedy POD algorithm. Albeit the approximations were not as expected, online basis enrichment procedures with a flexible control on the prediction error remain a favorite procedure. Additionally, to make the ROMs more robust to changes in parameters and also to try to avoid the violation of the residual error indicator (or the prediction error tolerance, a posteriori error bounds) when performing simulations for parameters outside of the training set, an hypothesis could be the introduction of sensitivities (via adjoint methods or automatic differentiation) in the construction of the ROB, that is, exploiting the gradient. This implies the use of Hermite or Taylor basis to build an optimal ROB (keeping in mind the sensitivities of the ROM shall minimize the distance to the corresponding FOM sensitivities).

Another approach in the construction of an optimal ROB could be the use of local ROBs, associated to the subspaces that arise from the partition of the parameter domain; this approach poses the challenges of interpolating on the Grassmann manifold and updating the local ROBs when switching between solution subspaces. However, ROB and related methods have mainly found successful applications in problems which can well be approximated using linear approximation spaces. Therefore, the need to use nonlinear projection-based models, with an increased interest in the Gauss-Newton with approximated tensors method (GNAT). The latter, a nonlinear manifold learning scheme, is nowadays very popular among computational mathematicians when solving fluid dynamics problems. GNAT decreases the FOM dimension by a least-squares Petrov-Galerkin projection and reduces by orders of magnitude the computational complexity while preserving accuracy by approximating the residual and Jacobian using Gappy POD. It is worth to remind that Gappy POD has proven to be an effective multi-fidelity method to reconstruct both steady and unsteady flowfield data from limited surface pressure measurements. Another line of improvement could be the development of a novel approach in the generation of well correlated low-fidelity models, with a possibility to introduce an automated detection of the correlation between the high and low fidelities combine with a trust region management that helps define exactly the locations where full order computations are required.

Acronyms

AIC Akaike's Information Criterion.

ANN Artificial Neural Networks.

ANOVA Analysis of Variance.

APR A Priori Model Reduction.

BLUP or BLUE Best Linear Unbiased Predictor or Estimator.

BPOD Balanced Proper Orthogonal Decomposition.

CDoE Classical Design of Experiments.

CFD Computational Fluid Dynamics.

CNLE Constrained Nonlinear Least Squares Equality.

CVT Centroidal Voronoi Tessellation.

DACE Design and Analysis of Computer Experiments.

DEIM Direct Empirical Interpolation Method.

DFM Data-Fit Model.

DLR Deutsche Luft und Raumfahrt - German Aerospace Center.

DNS Direct Numerical Simulations.

DoE Design of Experiments.

EDK External Drift Kriging.

EGO Efficient Global Optimization.

EI Expected Improvement.

FAIPA Feasible Arc Interior Point.

FOAM Full Order Aerodynamic Model.

FOM Full Order Model.

FT Flight Testing.

GNAT Gauss Newton with Approximated Tensors.

GRPOD Greedy Proper Orthogonal Decomposition.

HDAM High Dimensional Aerodynamic Model.

HDM High Dimension Model.

HF High Fidelities.

IMSE Integrated Mean Square Error.

ISC Infill Sampling Criteria.

LCB Lower Confidence Bound.

LCVT Latinized Centroidal Voronoi Tessellation.

LES Large Eddies Simulations.

LF Low Fidelities.

LHD Latin Hypercube Design.

LHS Latin Hypercube Sampling.

LOOCV Leave-One Out Cross Validation.

LSQ Least Square.

MAE Mean Absolute Error.

MDoE Modern Design of Experiments.

ME Maximizing the Prediction Error.

MES Maximum Entropy Sampling.

MF POD+I Multi-Fidelity Proper Orthogonal Decomposition + Interpolation.

MFIS Multi-Fidelity Importance Sampling.

MFm Multi-Fidelity Model.

MLE Maximum Likelihood Estimate.

MOR Model Order Reduction.

MP Minimizing the Prediction Error.

MPE Missing Point Estimation.

- MPI** Message Passing Interface.
- ODE** Ordinary Differential Equation.
- OFAT or OVAT** One Factor/Variable at a Time.
- PCA** Principal Component Analysis.
- PI** Probability of Improvement.
- POD** Proper Orthogonal Decomposition.
- PRESS** Prediction Error Sum of Squares.
- R(MSE)** Adjusted Mean Square Error.
- R(MSE)** (Root) Mean Square Error.
- RAE** Relative Accuracy Error.
- RANS** Reynolds Averaged Navier-Stokes Equations.
- RBF** Radial Basis Functions.
- REES** Regional Error Measure.
- RIC** Relative Information Content.
- ROB** Reduced Order Basis.
- ROM** Reduced-Order Model.
- RPOD** Residual Based Proper Orthogonal Decomposition.
- RSM** Response Surface Model.
- SBIC** Schwarz's Bayesian Information Criterion.
- SBO** Surrogate-Based Optimization.
- SCF** Spatial Correlation Function.
- SMARTy** Surrogate Modeling for AeRo-data Toolbox.
- SQP** Sequential Quadratic Programming.
- SSA** Stochastic Spectral Approximations.
- SSM** Searching the Surrogate Model.
- SUMO** Surrogate Model.
- SVD** Singular Value Decomposition.
- TAU** DLR Flow Solver.

TPS Thin Plate Spline.

TPWL Trajectory Piecewise Linear Approximation.

VAM Variable Accuracy Model.

VCM Variable Complexity Model.

VCM Variable Resolution Model.

VFM Variable Fidelity Model.

WRMSE Weighted Root Mean Square Error.

WTT Wind Tunnel Testing.

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