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Global optimization of benchmark aerodynamic cases using physics-based surrogate models

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ABSTRACT

The paper proposes the combination of physics-based surrogate models, adaptive sampling of the design space and evolutionary optimization towards the solution of aerodynamic design problems. The Proper Orthogonal Decomposition is used to extract the main features of the flow field and Radial Basis Function networks allow the surrogate model to predict the target response over the entire design space. In order to train accurate and usable surrogates, *ad hoc* in-fill criteria are provided which smartly rank and select new samples to enrich the model database. The solution of two aerodynamic benchmark problems is proposed within the framework of the AIAA Aerodynamic Design Optimization Discussion Group. The two benchmark problems consist respectively in the drag minimization of the RAE 2822 airfoil in transonic viscous flow and of the NACA 0012 airfoil in transonic inviscid flow. The shape parameterization approach is based on the Class-Shape Transformation (CST) method with a sufficient degree of Bernstein polynomials to cover a wide range of shapes. Mesh convergence is demonstrated on single-block C-grid structured meshes. The in-house ZEN flow solver is used for Euler/RANS aerodynamic solution. Results show that, thanks to the combined usage of surrogate models and adaptive training in an evolutionary optimization framework, optimal candidates may be located even with limited computational resources with respect to plain evolutionary approaches and similar standard methodologies.

1. Background and introduction

The solution of aerodynamic shape optimization problems by high-fidelity Navier–Stokes models requires a huge amount of computational resources even on modern state-of-art computing platforms. Indeed, not only a single evaluation can be time-demanding, but often hundreds or thousands of CFD analyses have to be performed to find an optimal solution. In order to speed up the optimization process while keeping a high level of fidelity, the scientific community is increasingly focusing on surrogate methodologies like meta-models, multi-fidelity models or reduced order models, which can provide a compact, accurate and computationally efficient representation of the aircraft design performance. Nevertheless, the usage of such models is not straightforward as the amount and quality of information the user has to provide in the learning phase is not known a priori; furthermore, the efficient exploitation of learning data may be hampered by the inherent complexity of the design problem, e.g. non-linearities in the physical model, constraints handling, curse of dimensionality, multi-modal fitness landscape, accuracy *vs* computational effort trade-off. Hence, no general rule exists on the optimal choice of the type of surrogate model, the training and validation strategy, the combination of surrogate model and optimization algorithm. Finding the set of parameters which best fit the model to the available data is known as the training phase. The training dataset is usually obtained by sampling the design space (Design of Experiments, DOE) and performing expensive high-fidelity computations on the selected points. Depending on the adopted surrogate technique, design objectives and constraints or vector/scalar fields of interest are used to feed the surrogate model. The strategy to properly and optimally choose the DACE sampling data set is of paramount importance to achieve a satisfactory accuracy of the surrogate model. Unfortunately, classical sampling methods, like Latin Hypercube sampling, are very sensible to the nature of the problem at hand and they may deceive the surrogate-based optimization by hiding or masking the optima locations. This is especially true in aerodynamic shape design problems where both the aerodynamic model non-linearities and the large dimension of the search space combine to emphasize this issue: classical DACE techniques would lead to intensively sample the search space, thus vanishing the actual advantage of surrogate-based optimization.

Jones et al. [1], among the first, proposed a response surface methodology based on modelling the objective and constraint

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functions with stochastic processes (Kriging). The DACE stochastic process model was built as a sum of regression terms and normally distributed error terms. The main conceptual assumption was that the lack of fit due only to the regression terms can be considered as entirely due to modelling error, not measurement error or noise, because the training data are derived from a deterministic simulation. Hence, by assuming that the errors at different points in the design space are not independent and the correlation between them is related to the distance between the computed points, the authors came up with an interpolating surrogate model able to provide not only the prediction of objectives/constraints at a desired sample point, but also an estimation of the approximation error. After the construction of such a surrogate model, this last powerful property is exploited to build an Efficient Global Optimization (EGO), which can be considered as the progenitor of a long and still in development chain of surrogate-based optimization (SBO) methods. Indeed, they found a proper balancing between the need to exploit the approximation surface (by sampling where it is minimized) with the need to improve the approximation (by sampling where prediction error may be high). This was done by introducing the Expected Improvement (EI) concept, already proposed by Schonlau et al. [2], that is an auxiliary function to be maximized instead of the original objective. Sampling at a point where this auxiliary function is maximized improves both the local (exploitation) and global (exploration) search.

The right choice of the number of points which the initial sampling plan would comprise and the ratio between initial/in-fill points has been the focus of several recent studies. However, it must be underlined that no universal rules exist, as each choice should be carefully evaluated according to the design problem (e.g., number of variables, computational budget, type of surrogate). Forrester and Keane [3] assumed that there is a maximum budget of function evaluations, so as to define the number of points as a fraction of this budget. They identified three main cases according to the aim of the surrogate construction: pure visualization and design space comprehension, model exploitation and balanced exploration/exploitation. In the first case, the sampling plan should contain all of budgeted points as no further refinement of the model is foreseen. In the exploitation case, the surrogate can be used as the basis for an in-fill criterion, that means some computational budget must be saved for adding points to improve the model. They also proposed to reserve less than one half points to the exploitation phase as a small amount of surrogate enhancement is possible during the in-fill process. In the third case, that is two-stage balanced exploitation/exploration in-fill criterion, as also shown by Sóbester [4], they suggested to employ one third of the points in the initial sample while saving the remaining for the in-fill stage. Indeed, such balanced methods rely less on the initial prediction and so fewer points are required. Concerning the choice of the surrogate, the authors observed that it should depend on the problem size, i.e. the dimensionality of the design space, the expected complexity, the cost of the true analyses and the in-fill strategy to be adopted. However, for a given problem, there is not a general rule. The proper choice could come up past various model selection and validation criteria. The accuracy of a number of surrogates could be compared by assessing their ability to predict a validation data set. Therefore, part of the true computed data should be used for validation purposes only and not for model training. This approach can be infeasible when the true evaluations is computationally expensive.

Forrester also underlined that some in-fill criteria and certain surrogate models are somewhat intimately connected. For a surrogate model to be considered suitable for a given in-fill criterion, the mathematical foundation of the surrogate should exhibit the capability to adapt to unexpected, local non-linear behaviour of the true function to be mimicked. From this point of view, polynomials can be immediately excluded since a very high order would be required to match this capability, implying a high number of sampling points. In general, a global search would require a surrogate model able to provide an estimate of the error it commits when predicting. To this aim, the authors recognized the work of Gutmann et al. [5] who employed various radial basis functions in a one-stage goal seeking approach. However, they suggested to use Gaussian process methods (e.g., Kriging) as surrogate model in a global optimization context. Finally, some interesting suitable convergence criterion to stop the surrogate in-fill process were proposed. In an exploitation case, i.e. when minimizing the surrogate prediction, one can rather obviously choose to stop when no further significant improvement is detected. On the other hand, when an exploration method is employed, one is interested in obtaining a satisfying prediction everywhere, so that he can decide to stop the in-filling when some generalization error metrics, e.g. cross-validation, falls below a certain threshold. When using the probability or expectation of improvement, a natural choice is to consider the algorithm converged when the probability is very low or the expected improvement drops below a percentage of the range of observed objective function values. However, the authors also observed that discussing on convergence criterion may be interesting and fruitful, but “in many real engineering problems we actually stop when we run out of available time or resources, dictated by design cycle scheduling or costs”. This is what typically happens in aerodynamic design, where the high dimensionality of the design space and expensive computer simulations often do not allow to reach the global optimum of the design problem but suggest to consider even a premature, sub-optimal solution as a converged point.

In this framework, the paper proposes a surrogate-based evolutionary optimization approach which includes the training and exploitation of physics-based surrogate models by means of *ad hoc* in-fill criteria. A three-stage optimization process is envisaged, where each phase reflects a different need in design space exploration (namely surrogate initialization, “smart” exploration and meta-model optimization). The next section will introduce the single components of the optimization process, giving details both on the surrogate model and on the adaptive training method. The final section will be devoted to the critical analysis and comparison of the optimization results obtained on the benchmark problems.

2. Surrogate-based optimization approach

The surrogate-assisted optimization method consists of a procedure embedding several software modules for design space sampling, surrogate models training and testing, in-fill criteria evaluation and evolutionary-based optimization. The core of the computational approach is represented by the surrogate model and its training process: a Proper Orthogonal Decomposition (POD) model is used to extract the main features from a set of computed flow fields, supplemented with Radial Basis Function (RBF) networks to fit the POD coefficients and provide the surrogate model with global prediction [6]. The POD model is fed both with the mesh points and the flow field main variables in order to capture the correlation between the physical domain deformation, due to shape changing, and the most significant flow features. Details about the surrogate model are given in section 2.1. The first stage of the surrogate-based optimization approach foresees a space-filling (e.g. Latin Hypercube, Centroidal Voronoi Tessellation,...) design space sampling to initialize the surrogate model. As a result, a predefined number of samples are placed to cover the whole design space and aerodynamic analyses are performed to compute the objective target function value. This preliminary phase is known as *a priori* sampling. Once initialized the surrogate, the choice of the training points is of paramount importance