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Régis Duvigneau, Michel Visonneau. A Hybrid Shape Optimization Approach for Complex Applications in Computational Fluid Dynamics. Ship Technology Research, 2003, 50 (4), pp.157-164. 10.1179/str.2003.50.4.003 . hal-01731292

HAL Id: hal-01731292
https://inria.hal.science/hal-01731292

Submitted on 24 Jan 2022

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A Hybrid Shape Optimization Approach for Complex Applications in Computational Fluid Dynamics

Régis Duvigneau, Michel Visonneau, Ecole Centrale de Nantes[1]

1 Introduction

Computational Fluid Dynamics (CFD) flow solvers have been integrated in fully automated design optimization procedures. In hydrodynamics and ship building industries, potential flow solvers were first included in the design loop for the sake of robustness and low computational effort, *Maisonneuve et al. (1996), Rosetti et al. (1999), Yasukawa (2000), Hendrix et al. (2001), Peri et al. (2000,2001).* The reduction of the wave resistance is usually aimed at. However, a more accurate prediction of the flow may be required, for instance for drag minimization or when precise characteristics of the flow are considered as optimization objective. Therefore viscous flow solvers were included in hull shape optimization procedures, *Jansson and Larsson (1996), Hino (1999), Chen and Huang (2002), Duvigneau and Visonneau (2003).* The implementation of such complex flow solvers in a shape optimization procedure introduce some additional difficulties.

The physical and geometrical configurations encountered in industrial applications often require viscous flow solvers with sophisticated turbulence models capable of dealing with realistic geometries. The naive use of a standardized toolbox optimization software connected to a flow solver and an automated grid generator is not a sensible strategy. Instead the peculiarities of the flow solver should be taken into account. E.g. the constraints on the grid ($y^+ = O(1)$ near the wall) linked to the use of near-wall turbulence models will have serious consequences on the mesh update procedure. If a particular strategy taking into account the high stretching of the volumes near the wall is not included, the mesh update will fail. Another reason is related to the mandatory use of parallelization strategies, such as domain decomposition, as soon as 3-d problems are considered. The mesh update, as well as the parameterization of the shape, should be adapted to this multi-block partition to work within each block independently and to send information for updating the overall domain. Otherwise, the parallelization becomes useless. The high computational costs implied by 3-d calculations, as well as the possible occurrence of numerical noises of various origins during the evaluations, should be taken into account for the choice of an optimization strategy. Finally, if different connected programs are employed in the design loop, some practical difficulties may arise, when distant computers are involved in the optimization process. All these remarks motivated the development of an optimization procedure, in which all numerical tools are adapted to the flow solver and integrated into a single code.

2 The ISIS flow solver

The flow solver ISIS (developed in our laboratory) is included in the design procedure. It solves the incompressible Reynolds-Averaged Navier-Stokes Equations (RANSE) on unstructured grids, with a strongly conservative formulation:

$$\frac{\partial}{\partial t}\int_V \rho \, dV + \int_S \rho(\vec{U} - \vec{U}_d)\cdot\vec{n}\, dS = 0 \tag{1}$$

$$\frac{\partial}{\partial t}\int_V \rho U_i \, dV + \int_S \rho U_i(\vec{U} - \vec{U}_d)\cdot\vec{n}\, dS = \int_S (\tau_{ij} I_j - p I_i)\cdot\vec{n}\, dS + \int_V \rho g_i \, dV \quad i = 1,2,3 \tag{2}$$

V is the domain of interest, or control volume, bounded by the closed surface S moving at the velocity $\vec{U}_d$ with a unit normal vector $\vec{n}$ directed outward. $\vec{U}$ is the velocity, p the pressure. τ_{ij} and g_i are the

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components of the viscous stress tensor and the gravity, I_j a vector with components zero except for the component j which is 1.

The discretization scheme uses a finite-volume method, generalized to unstructured meshes composed of arbitrary volume shapes. Thus, calculations involving complex grids may be taken into account. The flow variables are stored at the center of the control volumes, surface and volume integrals being evaluated using second-order accurate approximations. The pressure-velocity coupling is performed by a SIMPLE-like algorithm. Several near-wall low Reynolds number turbulence models, ranging from one-equation Spalart-Allmaras model, *Spalart and Allmaras (1991)*, two-equation k-ω models, *Menter (1993)*, to a full Reynolds stress transport R_{ij}-ω model, *Deng and Visonneau (2000)*, are implemented in the flow solver.

3 Optimization strategies

Several strategies may be considered to lead the search of the optimal shape. In order to reduce the computational costs, one may propose to use gradient-based methods, characterized by a super-linear convergence and a weak dependency on the number of design parameters. However, the implementation of this strategy in a complex numerical framework is particularly tedious. Indeed, the evaluation of the derivatives of the objective function with respect to the design parameters relies on the differentiation of the flow solver, through the resolution of an adjoint equation, *Anderson and Venkatakrishnan (1999), Jameson et al. (1998)*. Thus, this approach is still limited to mildly complex problems, involving typically inviscid flows. Some viscous flow solvers were linearized with success, but with some limitations, as pointed out in *Hino (1999)*. Two alternative approaches may be considered to evaluate the derivatives: automatic differentiation software, *Hovland et al. (1997)* and an incomplete evaluation of the gradient, *Mohammadi (1999)*, *Mohammadi et al. (2000)*, neglecting the modifications of the flow. These methods are still limited (by the complexity of flow solver in the first case and the range of application in the second case) and gradient-based methods have several drawbacks: they can only consider one optimization criterion and are particularly sensitive to the numerical noise arising from the use of complex numerical methods and generating spurious local optima. Considering all these remarks, the use of gradient-based strategies may not be so wise in such a context. However, the choice to reject gradient-based methods has crucial consequences, since all other approaches are submitted to the "curse of dimensionality", the number of evaluations required growing more than linearly with the dimension of the problem. Thus, the parameterization of the shapes should involve as few design variables as possible.

Derivative-free deterministic algorithms, such as the simplex method, *Nelder and Mead (1965)*, based only on function values comparisons, may be easily implemented in the design procedure, since the flow solver is considered as a "black box", yielding both flexibility and robustness to solve complex optimization problems, *Duvigneau and Visonneau (2001a)*, while being less sensitive to the noisy errors. Nevertheless, they are still limited to local optimizations including one criterion.

Stochastic methods, such as Genetic Algorithms (GAs), *Goldberg (1989)*, are particularly appealing, as they allow global optimizations and concept exploration in multi-objective problems. Their robustness and capability to solve multi-modal problems have been demonstrated often, *Kitamura et al. (2000), Yasukawa (2000), Maisonneuve et al. (2002)*. As derivative-free methods, they allow easy implementation of complex CFD applications, *Duvigneau and Visonneau (2001b)*. However, GAs are particularly expensive, since the number of evaluations is about ten times higher than the number required by deterministic methods. These costs make GAs often unrealistic for 3-d CFD problems.

One may combine the advantages of the different strategies and use approximation methods to reduce the computational time. GAs have two main drawbacks: the number of evaluations and the low local convergence rate. To reduce the number of evaluations through the flow solver, one may use the knowledge already collected on the problem to build local approximations replacing some expensive evaluations, *Giotis and Giannakoglou (1999,2000)*. More precisely, all exact evaluations by

the flow solver during the optimization procedure are stored in a database, used to train Artificial Neural Networks (ANNs). They are employed to perform approximate pre-evaluations of the shapes at each generation. Only the most promising shapes are then exactly evaluated by the flow solver. This reduces the number of expensive evaluations significantly, without losing the interesting capabilities of genetic algorithms. A hybridization technique is proposed to improve the low local convergence rate of GAs in the vicinity of the solution: the GAs determine the overall characteristics of the optimal shape and the final precise local search is performed by a deterministic algorithm.

This strategy, based on hybrid genetic algorithms and neural networks, has been successfully applied to the optimization of the shape of a 3-d wing at 8° incidence with respect to the lift, *Duvigneau and Visonneau (2002)*. Recently, a new optimization exercise was performed with the same configuration. The goal of this exercise was the reduction of the intensity of the longitudinal vortex generated at a salmon. The vorticity modulus is used as objective function. For this case, an unstructured mesh of about 800,000 cells was used, for a Reynolds number $R_n = 2 \cdot 10^6$, employing the near-wall low Reynolds number SST k-ω model. The shape modifications, located in the vicinity of the salmon, are described by 6 design parameters. Fig.1 illustrates the strategy. For some generations, all evaluations are performed exactly by the flow solver to build a coarse database. Then, the approximate pre-evaluations procedure is activated, reducing strongly the number of expensive evaluations. Finally, when the best solution found by GAs seem to be close to the optimal shape, a deterministic approach is used to reach quickly the solution. A reduction of 12% of the vorticity modulus is observed. The use of the deterministic method alone leads to a poor improvement, Fig.1.

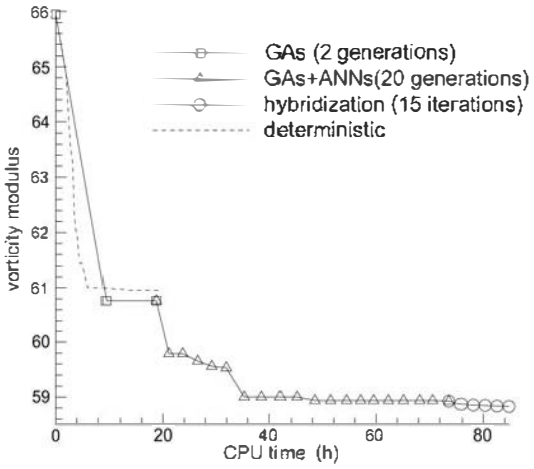


Fig.1: Evolution of the objective function

Thus, very complex problems may be solved using this strategy. Even if the costs remain high (although calculations were performed on 60 processors), the CPU time has been reduced more than five times with respect to a simple genetic algorithm. Although this approach still has some limitations, such as the number of design variables involved, it seems to be a realistic and promising way.

4 Shape parameterization

When 3-d unstructured meshes are employed, the parameterization of the shape required by the design process is difficult. A curvilinear representation of the shape is not available. Thus, the use of B-spline net representations is tedious. The nodes coordinates on the shape and connectivities are the only knowledge which could be used. Therefore, a Free Form Deformation (FFD) technique, *Sederberg and Parry (1986)* is proposed to control the shape perturbations during the design process. It consists in first embedding the object to be deformed in a box, and then in modifying the metrics of the space in the box and the object inside, by deforming the box, rather than in modifying the object itself.

Thus, the shape of the object can be modified without even identifying its nature. Actually, a local coordinate system is attached on a parallel-epipedic volume including the object to be deformed. The coordinates of any point P in this reference system are :

$$P = \xi \vec{e}_1 + \eta \vec{e}_2 + \zeta \vec{e}_3 \tag{3}$$

$\vec{e}_1$, $\vec{e}_2$ and $\vec{e}_3$ are vectors of unit length, parallel to the leading directions of the parallel-epipedic volume. A mapping function is then applied to the space inside the volume, by the use of a trivariate B-spline product. The new position P_{FFD} of the previous point P is provided by the algebraic relation:

$$P_{FFD} = \sum_{i,j,k} N_i(\xi) N_j(\eta) N_k(\zeta) P_{BS}^{ijk} \tag{4}$$

N_i, N_j and N_k are the B-spline basis functions and P_{BS}^{ijk} are the Cartesian coordinates of the control points. By moving some of these control points, the metrics of the space in the parallel-epipedic volume are modified, yielding a smooth deformation of the shape inside. This approach provides an easy-to-use solution, requiring only a few control points to control the deformation of the shape. However, this general technique may be inadequate to deal with a particular and specialized problem.

5 Mesh update

The automated mesh update is problematic, when unstructured grids using a near-wall turbulence modeling formulation are employed, since the grid volumes are highly stretched near the wall to fulfill the condition $y^+ \leq 1$. Therefore, a classical spring analogy based on linear springs will fail, *Anderson and Venkatakrishnan (1999)*. We used a powerful method based on both linear and torsional spring analogy, *Farhat et al. (1998)*, with success for 2-d two-dimensional shape optimization problems, *Duvigneau and Visonneau (2001a)*. But this more complicated approach may hardly be employed for 3-d problems. Therefore, one may recommend to smoothly deform the shape and the mesh by the FFD method at the same time, since the FFD approach relies on a spatial deformation. This strategy may be carried out for 2-d as well as 3-d grids and is obviously adequate for multi-block calculations. However, the quality of the resulting grid is not ensured. Figs.2 to 4 show an example of deformation of a hybrid grid around the NACA 0012 airfoil. The FFD method provides a smoother deformation, but the orthogonality of the grid near the wall is not maintained, contrary to the spring analogy. Nevertheless, the FFD method gives satisfactory results, when reasonable perturbations are taken into account.

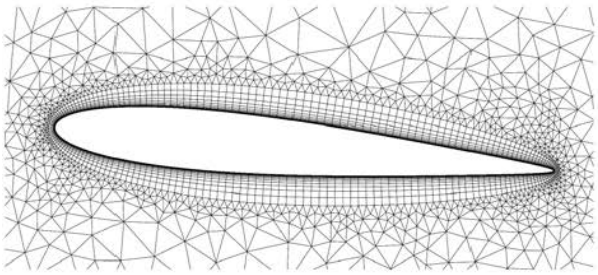


Fig.2: Initial mesh

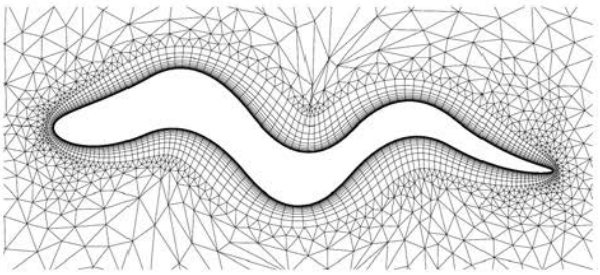


Fig.3: Spring analogy

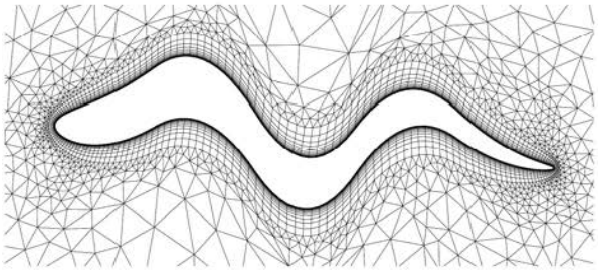


Fig.4: Free form deformation

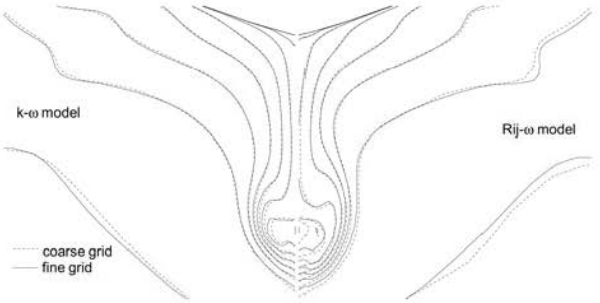


Fig.5: Isowakes at full scale for two grids and two turbulence models

6 Influence of turbulence modeling

Several quantities influence the predicted flow and thus on the search for an optimum: grid size, stopping criteria, discretization schemes, turbulence modeling, etc. generate noisy errors during the evaluations, *Grossman et al. (2002), Madsen (2000). Duvigneau et al. (2002)* studied in depth the role played by turbulence models for hull shape optimization.

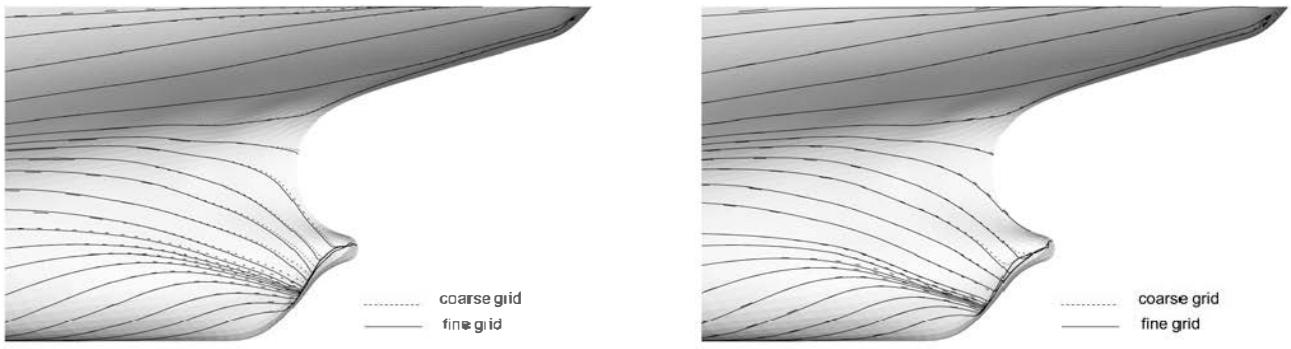


Fig.6: Streamlines for the SST k-ω (left) and R_{ij}-ω (right) models

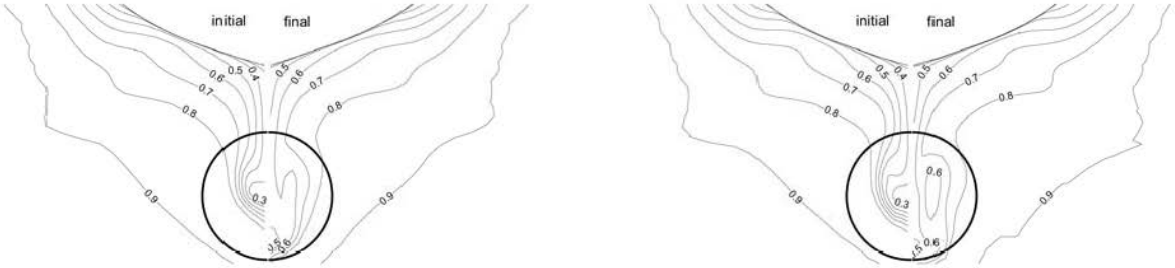


Fig.7: Isowakes for the SST k-ω (left) and R_{ij}-ω (right) models

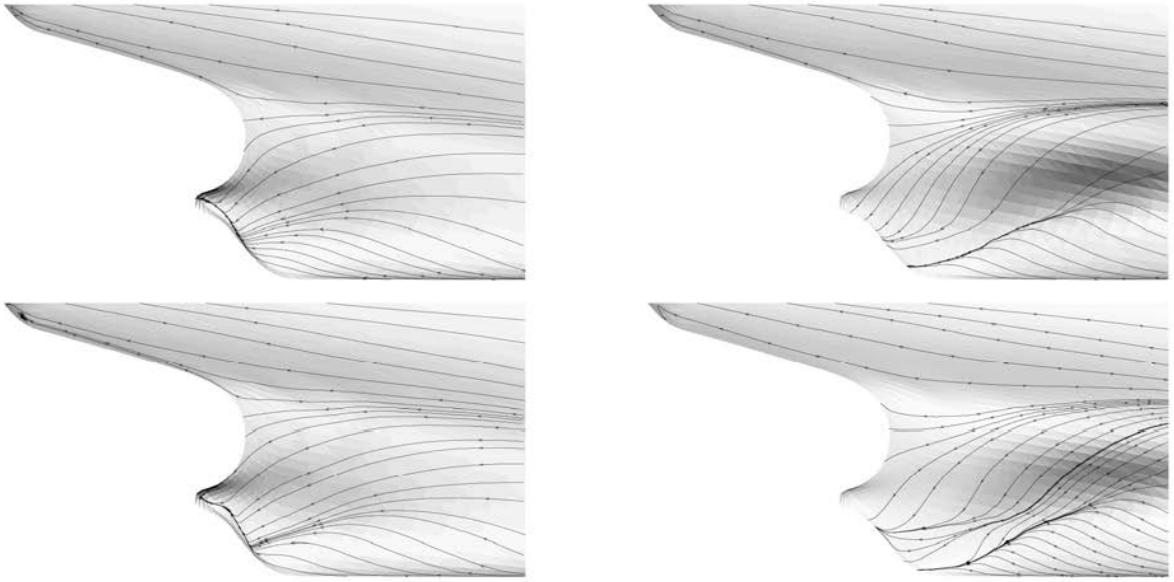


Fig.8: Streamlines for the SST k-ω (top) and R_{ij}-ω (bottom) models

To illustrate the influence of turbulence modeling during the design process, a realistic hull shape optimization problem is considered. The flow around the KVLCC2 tanker of length l is computed at full scale ($R_n = 10^9$), using a structured mesh of about 400,000 control volumes. Two turbulence models are tested: the eddy-viscosity SST k-ω model of Menter and a second-order closure R_{ij}-ω model. The two models give different predictions of the wake, *Deng and Visonneau (2000)*, the longitudinal vortex generated being intensified by the second-order closure. However, these differences are less important at full scale than at model scale. To validate the full-scale results, computations are performed with a finer grid of about one million nodes, Figs.5 and 6. Grid convergence is almost reached for both turbulence models and differences between considered turbulence models are far more important than numerical errors. For the sake of pragmatism, shape optimization computations are performed with the coarser grid.

The goal of the optimization is to homogenize the longitudinal velocity field at the location of the propeller, modifying the stern of the ship described by 6 design variables. This exercise consists in reducing the mean deviation of the longitudinal component of the velocity, computed in the propeller disk. One intends to quantify the influence of the turbulence modeling during the optimization process. Since preliminary tests show that the topology of the objective function is quite simple, a deterministic optimization algorithm based on linear or quadratic interpolations is used, *Marazzi and Nocedal (2002)*.

Fig.7 shows the isowakes for the initial and final shapes. The optimal shapes are characterized by a far more intense longitudinal vortex homogenizing the flow. This evolution during the design process enforces the influence of the turbulence modeling. Fig.8 represents the streamlines close to the wall. The topology of the flow has changed and is finally similar to model scale flows. Thus, some differences between the models appear even at full scale. Looking at the optimized shapes, Fig.9, at $x = 0.94l$, similar trends are obtained. Differences are due to the fact that the use of second-order closure leads to a flow characterized by a stronger longitudinal vorticity in the near wake. Therefore, lower modifications of the shape may generate a more intense vortex. The final shapes give U-shaped sections. The evolution of the objective function, Fig.10, shows a reduction of about 70% of the velocity mean deviation at the propeller location. The reduction is smaller for the second-order closure. This phenomenon is maybe due to the presence of more complex turbulence structures in the wake, not described by the linear eddy-viscosity model.

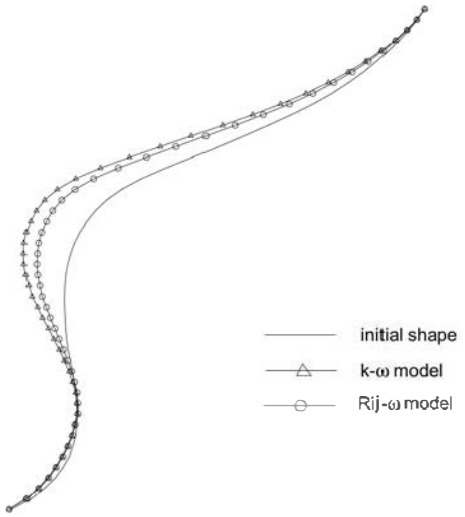


Fig.9: Initial and final shapes at $x = 0.94l$

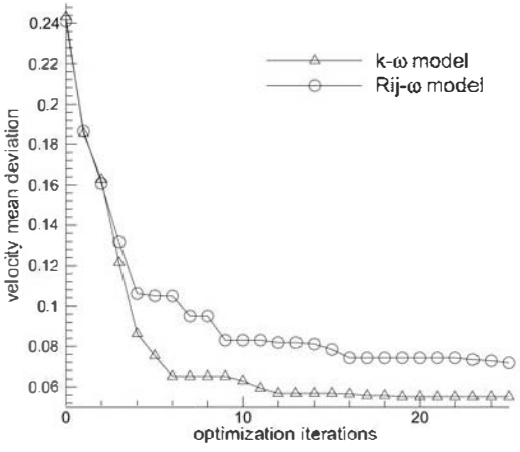


Fig.10: Evolution of the objective function

This example underlines the influence of turbulence modeling in the framework of hull shape optimization. Although less important at full scale, the turbulence model still has a crucial influence, when local characteristics of the flow in critical regions are considered during the optimization.

7 Conclusion

This study explored different strategies to solve shape optimization problems involving complex flow solvers. The choice of the optimizer has crucial consequences. Genetic algorithms have several advantages over deterministic approaches. Their use is now realistic, providing that acceleration techniques are employed, such as hybridization and inexact pre-evaluations through artificial neural networks. Some practical difficulties still exist, e.g. the mesh update for 3-d problems. However, the main limitation may be the influence of turbulence modeling on the design process for some problems, since this modeling error cannot be reduced, contrary to other numerical parameters, such as grid size or partial convergence.

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