

INVERSE DESIGN AND OPTIMIZATION USING CFD

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Abstract. *Inverse shape design and shape design optimization are two basic algorithmic approaches to aerodynamic shape determination. Although widely used in industry, most inverse shape design methods require significant modifications to the existing proven flow-field analysis codes. One method for the inverse shape design that requires no such modifications, can use any available flow-field analysis code, and is applicable to arbitrary configurations is the surface elastic membrane concept. Its formulation that utilizes Fourier series and analytic solutions seems to be both computationally efficient and easy to program and use.*

Since inverse shape design provides only point solutions and does not extremize any objective quantity, it is rapidly becoming popular to use aerodynamic shape optimization methods. Only those optimization methods that are robust should be used since classical gradient based optimization algorithms are excessively time consuming for larger number of design variables, they are inapplicable to non-smooth objective function spaces, and tend to terminate in the nearest available local minimum. Thus, hybrid, semi-stochastic, and stochastic optimizers are becoming popular since they can handle several objectives simultaneously, can enforce several equality constraints, and can handle a large number of design variables. Practical examples of aerodynamic shape design of a shocked transonic wing, optimized multistage axial gas turbine, optimized linear airfoil cascade, multi-objective optimized linear airfoil cascade, and optimized external magnetic field in an example of a magneto-hydrodynamic diffuser illustrate the capabilities of these design methodologies.

1. INTRODUCTION

If it is possible to describe an engineering field problem by providing governing partial differential or integral equation(s), shape(s) and size(s) of the domain(s), boundary and initial conditions, material properties of the media contained in the field, and by internal sources and external forces or inputs, then such a field problem is fully specified (completely defined) and is of an analysis (or direct) type¹. If mathematically well-posed, the analysis problems are considered solvable, that is, they are assumed to have a solution. An overwhelming amount of analysis software exists in the form of Computational Fluid Dynamics (CFD), Computational Heat Transfer (CHT), Computational Solid Mechanics (CSD), Computational Electro-Magnetics (CEM), etc. If any of this information is unknown or unavailable, the field problem becomes under-specified (incompletely defined) and is of an indirect (or inverse) type. The inverse problems are by their definition insufficiently specified, thus they cannot be solved. But, if sufficient amount and type of additional information is provided, the inverse problems can become sufficiently specified to offer the possibility of their solution if appropriate numerical algorithms are used. The inverse problems can therefore be classified as: shape determination (design) inverse problems, boundary/initial value determination inverse problems, sources and forces determination inverse problems, material properties determination inverse problems, and governing equation(s) determination inverse problems.

Thus, the word “design” as related to the engineering field problems has a very definitive meaning and should be reserved strictly for the algorithmic methods of design instead of designer’s intuitive and subjective cut-and-try traditional approach. The algorithmic methods of design could be grouped in two basic approaches: inverse design, and design optimization.

For example, the inverse design problem of determining aerodynamic sizes and shapes¹⁻⁴ can be solved if pressure is specified on the unknown boundaries in addition to the relative velocity which is known to be zero on the solid impermeable boundary in a viscous flow.

Design optimization has the objective to determine proper values for a large number of design variables that either minimize or maximize one or many global objectives while satisfying a number of user specified equality and inequality constraints⁵⁻⁷. For example, aerodynamic shape optimization has a global objective of increasing the aerodynamic efficiency of the flow-field created by the object. The shape design optimization approach is capable of achieving considerably more efficient shapes than when using the best inverse shape design algorithms since inverse methods create shapes that generate user specified (sub-optimal) surface pressure distributions. However, shape design optimization is considerably more time-consuming than the shape inverse design because it requires a large number of calls to the flow-field analysis algorithm. This was one of the main reasons why the aerodynamic shape optimization has not been widely used until the adequate computing hardware in the form of distributed parallel processors became affordable.

The objective here is to offer a brief review of research on the solution methods for aerodynamic shape inverse design and aerodynamic shape design optimization as practiced in our Multidisciplinary Analysis, Inverse Design and Optimization (MAIDO) Laboratory.

2. AERODYNAMIC SHAPE INVERSE DESIGN

During the past decade it became somewhat fashionable to work on the development of aerodynamic shape inverse design and shape design optimization using a method of adjoint system of partial differential equations or control theory approach⁸. This is an extremely complicated and model-specific formulation^{3,4} that uses an essentially sensitivity-based approach. As such, it easily terminates in a nearest available local minimum, it is unsuitable for realistic non-smooth objective function spaces, and it does not apply easily to multi-disciplinary design problems modeled by disparate systems of partial differential equations.

Consequently, industry is interested only in such shape design methods that are equally applicable to both two-dimensional and three-dimensional arbitrary configurations and that can utilize existing proven flow-field analysis codes with minimum alterations needed^{5,7}. This means that any flow-field analysis code (a panel code, an Euler code, a Navier-Stokes code, or even surface pressures obtained experimentally from a wind tunnel testing) could be used in certain aerodynamic shape inverse design methods without a need for alterations of such an analysis tool. The simplest and the least imaginative such shape design method is to use an optimization algorithm to enforce the specified surface pressures. However, there are considerably less expensive and more accurate methods for performing the aerodynamic shape inverse design⁵. In other words, it is much more cost effective to use the optimization algorithms for actual constrained optimization of the global aerodynamic and geometric parameters, instead of achieving inverse shape design by enforcing user specified surface pressure distributions.

For example, a very simple and general method of shape inverse design can be used that is based on pure heuristics. This method treats the surface of an aerodynamic body as an elastic membrane that deforms under aerodynamic loads until it achieves a desired (target) distribution of surface pressure or pressure coefficient, C_p . This simple non-physical shape evolution model (named MGM after its initiators⁹⁻¹¹) can be formulated as

$$\pm \beta_{ss} \frac{d^2 \Delta y}{ds^2} + \beta_s \frac{d \Delta y}{ds} \mp \beta_0 \Delta y = \Delta C_p, \quad (1)$$

Here, upper signs correspond to the upper body contour, lower signs correspond to the lower body contour, s is the airfoil contour-following coordinate, Δy is the local shape correction, ΔC_p is the local difference between specified and actual coefficient of surface pressure, while β_0 , β_s , and β_{ss} are the user supplied constants that control the rate of convergence of the airfoil shape. This ordinary differential equation with constant coefficients is of a simple linear forced mass-damper-spring type where the s coordinate substitutes for the time coordinate and the globally periodic location-dependent forcing function ΔC_p substitutes for the arbitrary time-varying periodic forcing function. This equation is traditionally integrated for shape corrections, Δy , by evaluating the derivatives using a finite differencing which is an

extremely slow converging process when using non-linear flow-field analysis codes. This can be eliminated with a new formulation of the elastic membrane design concept that allows a Fourier series analytical solution to the shape evolution equation¹²⁻¹⁴. The arbitrary surface distribution of ΔC_p can be represented by utilizing the Fourier series expansion as

$$\Delta C_p(s) = a_0 + \sum_{n=1}^{n_{\max}} [a_n \cos(N_n s) + b_n \sin(N_n s)] \quad (2)$$

where $N_n = \frac{2n\pi}{L}$ and L is the total length of the airfoil contour. The particular solution of Eq. (1) can be represented using Fourier series as

$$\Delta y_p = A_0 + \sum_{n=1}^{n_{\max}} [A_n \cos(N_n s) + B_n \sin(N_n s)] \quad (3)$$

Substitution of Eq. (2) and analytical derivatives of Eq. (3) into the airfoil contour evolution equation (1) yields the analytic relationship among various coefficients

$$A_n = \frac{\pm a_n (\beta_0 + N_n^2 \beta_{ss}) - b_n (\beta_s N_n)}{(\beta_0 + N_n^2 \beta_{ss})^2 + (\beta_s N_n)^2}, n = 0, 1, 2, \dots \quad (4)$$

$$B_n = \frac{\pm b_n (\beta_0 + N_n^2 \beta_{ss}) + a_n (\beta_s N_n)}{(\beta_0 + N_n^2 \beta_{ss})^2 + (\beta_s N_n)^2}, n = 1, 2, 3, \dots \quad (5)$$

The analytic solution for the correction of the airfoil contour is given by

$$\Delta y = Fe^{\pm\lambda_1 s} + Ge^{\pm\lambda_2 s} + \sum_{n=0}^{n_{\max}} [A_n \cos(N_n s) + B_n \sin(N_n s)] \quad (6)$$

where the upper signs correspond to the upper contour and the eigenvalues are

$$\lambda_{1,2} = \frac{\beta_s \pm \sqrt{\beta_s^2 + 4\beta_0 \beta_{ss}}}{2\beta_{ss}} \quad (7)$$

The unknown constants F and G can now be determined for the upper and lower airfoil contours such that zero trailing edge displacement, trailing edge closure, leading edge closure,

and smooth leading edge deformation are satisfied. Formulation of this method for inverse design of three-dimensional aerodynamic shapes is a straightforward extension and works well with smooth and discontinuous target pressures^{13,14}.

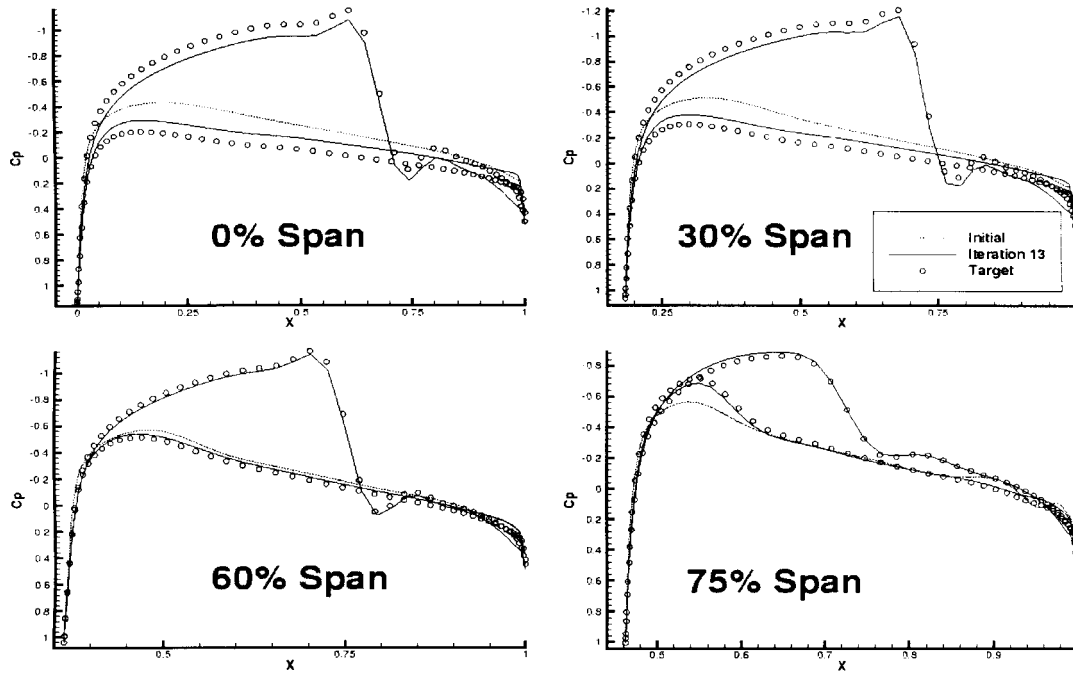


Fig. 1 Sectional C_p distributions for inverse design of a shocked twisted transonic wing using Fourier series elastic membrane method.

In the example depicted in Figure 1 the target surface pressure distribution was calculated using an Euler code from a wing at free-stream Mach number $M_\infty = 0.8$ with a root NACA 0012 airfoil at a +4.0 degree angle of attack and a tip NACA 1311 airfoil at a -2.0 degree angle of attack. The initial guess wing geometry had a NACA 0012 airfoil at zero degrees angle of attack. The wing had a taper ratio of 0.5 and no sweep at the trailing edge. The shape evolution parameters β_{tt} , β_{ss} , β_s , β_0 and α_s were set to 6.8, 1.1, 1.0, 1.5, and 0.105, respectively. Notice that this shape inverse design method requires typically 10-20 calls to any unmodified three-dimensional flow-field analysis code to match the target pressures.

This inverse shape design technique can be further improved by making the β coefficients as functions of the local surface pressure variations and by utilizing a Distributed Minimum Residual (DMR) formulation to further accelerate its convergence¹⁵. It is quite remarkable that this approach should be conceptually applicable to shape inverse design problems in other fields like elasticity, heat transfer, magnetism, electrostatics, etc.

2.1 Choosing target surface pressure distribution

Aerodynamic shape inverse design enforces desired pressure distribution on the unknown object's surface often without any direct evaluation criterion available to judge the effects of this pressure distribution on the corresponding global design objectives like lift, drag, and moment. Since the inverse shape design is based on the specified ("desired" or "target") surface pressure distribution, the common dilemma is the choice of the "best" surface target pressure. Specifically, it would be desirable to specify such aerodynamic pressure distribution on the yet unknown surface so that it maximizes the aerodynamic efficiency by minimizing all possible contributions to the entropy generation in the entire flow-field. It is well known that the separated boundary layer significantly increases flow-field vorticity and, consequently, the viscous dissipation function, entropy generation, and aerodynamic drag. To minimize these effects, the desired surface pressure distribution should first be checked for possible flow separation before it is enforced in the aerodynamic shape inverse design process. One very fast method for detecting flow separation is based on the assumption that the rate of change of flow kinetic energy reaches its minimum at the separation point¹⁶. The kinetic energy can be calculated from the surface pressure distribution by assuming that pressure does not change across a viscous boundary layer. Another method for detection of flow separation utilizes information from the computed viscous boundary layer parameters¹⁷. However, these flow separation detection methods requires knowledge of the pattern of surface streamlines which is impossible to determine on a general three-dimensional configuration in an *a priori* fashion.

Consequently, inverse shape design methods are capable of creating improved aerodynamic shapes only if an experienced aerodynamicist is to use his/her personal knowledge and intuition to specify the target surface pressure distribution in the case of a general three-dimensional configuration design.

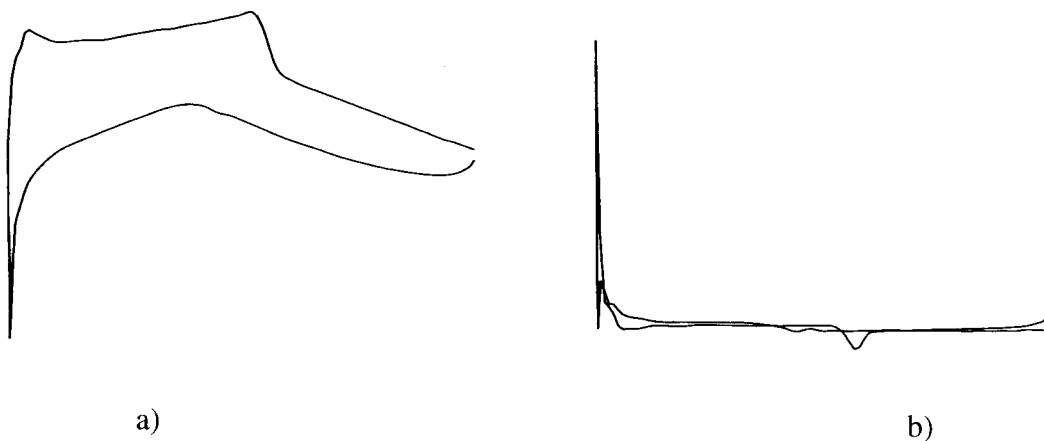


Figure 2. Detection of flow separation locations from the specified or measured surface pressure distribution: a) predicted surface Mach number distribution along a shocked RAE 2322 airfoil at Reynolds number 6.25 million, and b) corresponding computed surface variation of rate of change of kinetic energy.

3 AERODYNAMIC SHAPE DESIGN OPTIMIZATION

The main shape design objective should be minimization of entropy generation in the flow-field which is caused by viscous dissipation, heat transfer, internal heat sources, chemical reactions, and electro-magneto-hydrodynamic effects^{18,19}. In the absence of chemical reactions and electro-magnetic effects the most prominent regions of entropy generation are viscous boundary layers and shock waves. This means that any reliable Navier-Stokes flow-field analysis code could be used without a need for its alteration to calculate entropy difference from inlet to exit of the flow-field so that minimization of the entropy generation (flow losses) can be achieved by the proper reshaping of the object(s) in the flow-field.

3.1 Optimization of a multi-stage axial gas turbine

An example of such entropy minimization (efficiency maximization) design is our design system, which optimizes hub and shroud geometry and inlet and exit flow-field parameters for each blade row of a multi-stage axial flow turbine²⁰⁻²². Very fast and accurate flow calculation and performance prediction of multistage axial flow turbines at design and off-design conditions was performed using a compressible steady state inviscid through-flow code with high fidelity loss and mixing models²³. Optimization was performed using a hybrid constrained optimization code that performs automatic switching among genetic algorithm, simulated annealing, modified simplex method, sequential quadratic programming, and a gradient search algorithm⁶. By varying a relatively small number of geometric variables per each blade row it was possible to find an optimal radial distribution of flow parameters at the inlet and outlet of every blade row. The multi-stage design optimization system has been demonstrated on single-stage and two-stage transonic axial gas turbines²⁰⁻²². The optimized solution provides the maximum efficiency of the multi-stage axial turbine and is, at the same time, technically feasible. The design system has been demonstrated on examples involving well-documented sets of experimental data for a one-stage uncooled transonic axial gas turbine²⁴ and a two-stage uncooled NASA gas turbine²⁵. The comparison of computed performance of initial and optimized designs shows significant improvement in the optimized multi-stage turbine efficiency over the entire range of operating conditions. The entire design optimization process was found to be computationally quite feasible consuming less than one hour on a single processor SGI R10000 workstation. Such extraordinary speed of execution was possible mainly because of the use of a highly accurate axisymmetric through-flow analysis code instead of a complete Navier-Stokes three-dimensional rotor-stator interaction flow-field analysis code. This suggests that in order to make constrained optimization of large systems computationally feasible, one should make a judicious use of analysis tools of varying complexity and fidelity combined with a robust dynamically adaptive response surface formulation²⁶.

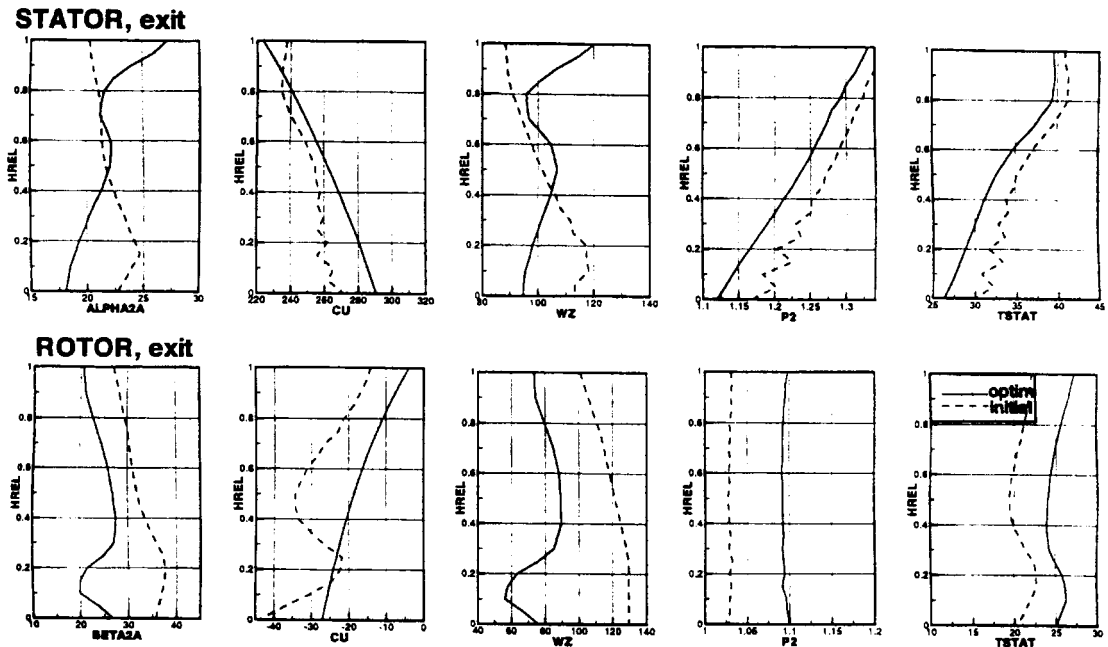


Figure 3. Initial values (dashed line) and optimized values (full line) of radial distributions of: ALPHA2 (exit flow angle, absolute flow – degrees), BETA2 (exit flow angle, relative flow – degrees), CU (tangential component of absolute velocity – m/s), WZ (axial velocity – m/s), P2 (static pressure – bar), T2 (static temperature – C). The configuration was a single stage transonic uncooled axial turbine.

3.2 Single-objective constrained optimization of a cascade of airfoil shapes

The shape design optimization algorithm was also applied in a redesign of an existing two-dimensional cascade of turbine airfoils having supersonic exit flow²⁷. The single objective was to minimize the total pressure loss across the cascade row. For minimization of the single objective function a constrained micro-genetic optimizer was used. The following equality constraints were iteratively enforced: specified aerodynamic lift force, mass flow rate, exit flow angle, and airfoil cross-section area. In addition, axial chord and the gap-to-axial chord ratio were kept fixed, while enforcing an inequality constraint that the airfoil thickness should always be greater or equal than the specified minimum allowable thickness distribution. For enforcement of those equality constraints that are easy to compute a sequential quadratic programming based optimizer was used. For the analysis of the performance of intermediate cascade shapes an unstructured grid based compressible Navier-Stokes flow-field analysis code with a k- ϵ turbulence model was used. The airfoil geometry was parameterized using nine conic section parameters and eight B-spline control points thus keeping the number of geometric design variables to a minimum while achieving a high degree of geometric flexibility and robustness.

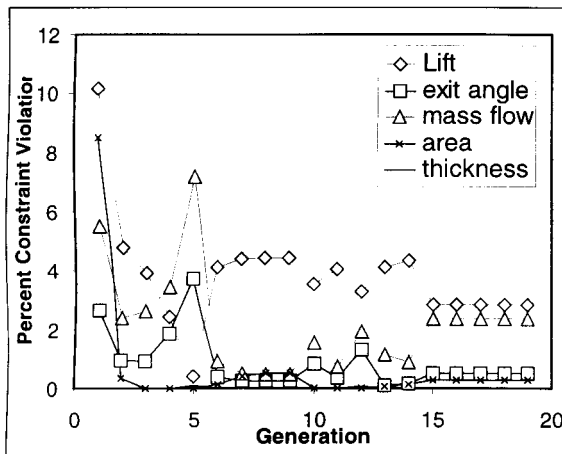


Figure 4. Violation of constraints when using penalty function with SQP, minimum thickness distribution constraint, and 9 conic sections with eight B-spline geometry perturbation points.

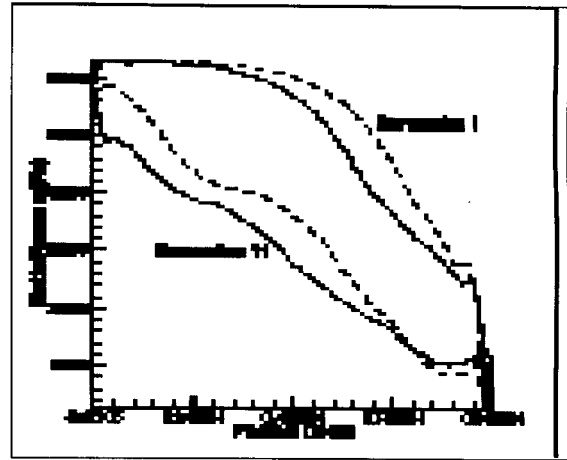


Figure 5. Static pressure distribution for best design of generation 1 and generation 11 when using penalty function with SQP, minimum thickness distribution constraint, and B-spline geometry perturbation.

The optimization code proved to be very robust since it found the narrow feasible domain and converged to a minimum that satisfied all the constraints within the tolerances specified (Fig. 4). The corresponding optimized surface pressure distribution (Fig. 5) would be practically impossible to specify in an *a priori* fashion even by the most experienced of the aerodynamics designers. This type of shape design optimization is feasible on an inexpensive single processor workstation, it requires no changes to the existing flow-field analysis code, and can be operated even by a semi-skilled designer.

3.3 Multi-objective aerodynamic shape optimization

With the increased availability of inexpensive computing resources, the attention of design engineers has been rapidly shifting from the use of inverse shape design methods that require significant personal experience and intuition towards a reliable and less educationally demanding mathematically based optimization algorithms. This trend has also exposed the substantial weakness of traditional gradient based optimization approaches that easily terminate in a local minimum, can usually produce only single-objective optimized solutions, and require that the objective function satisfies continuity and derivability conditions. These facts, together with the growing need for the multi-disciplinary and multi-objective approach to design with a large number of design variables, resulted in an increased interest in the use of various versions of hybrid⁶, semi-stochastic^{28,29}, and stochastic³⁰⁻³² optimization algorithms.

In a multi-objective optimization we strive to compute the group of the *not-dominated* solutions which is known as a Pareto front. These are the feasible solutions found during the optimization that cannot be improved for any one objective without degrading another objective. The multi-objective constrained optimization algorithm that we used is a modified version of an indirect method of optimization based upon self-organization (IOSO)²⁶ and

evolutionary simulation principles. Each iteration of IOSO consists of two steps. The first step is creation of an approximation of the objective functions. Each iteration in this step represents a decomposition of initial approximation function into a set of simple approximation functions so that the final response function is a multi-level graph. The second step is the optimization of this approximation function. This approach allows for corrective updates of the structure and the parameters of the response surface approximation. The distinctive feature of this approach is an extremely low number of trial points to initialize the algorithm (30-50 points for the optimization problems with nearly 100 design variables). In the process of each iteration of IOSO, the optimization of the response function is performed only within the current search area. This step is followed by a direct call to the mathematical analysis model for the obtained point. During the IOSO operation, the information concerning the behavior of the objective function in the vicinity of the extremum is stored, and the response function is made more accurate only for this search area. Thus, during each iteration a series of approximation functions for a particular objective of optimization is built. These functions differ from each other according to both structure and definition range. The subsequent optimization of these approximation functions allows us to determine a set of vectors of optimized variables, which are used for the computation of optimization objectives on a parallel computer.

As a practical example, we performed³³ a constrained multi-objective shape optimization of a linear cascade of gas turbine airfoils that had a finite length, thus a finite number of airfoils. The original airfoil shapes were designed at von Karman Institute of Fluid Dynamics (VKI) using a highly sophisticated inverse shape design code. Thus, this initial airfoil cascade shape was already highly efficient. This way we were able to observe if our multi-objective constrained optimization creates improved and realistic results since we were able to compare them with a realistic initial finite cascade configuration. The objectives were to simultaneously minimize the total pressure loss, maximize total aerodynamic loading (aerodynamic force component that is tangent to the airfoil cascade), and minimize the number of airfoils in the finite cascade row. The constraints were: fixed mass flow rate, fixed axial chord, fixed inlet and exit flow angles, fixed blade cross-section area, minimum allowable thickness distribution, minimum allowable lift force, and a minimum allowable trailing edge radius. This means that the entire airfoil cascade shape was optimized including its stagger angle, thickness, curvature, and solidity resulting in 18 design variables, 5 nonlinear constraints, and 3 objectives. The analysis of the performance of intermediate airfoil cascade shapes were performed using an unstructured grid based compressible Navier-Stokes flow-field analysis code with a $k-\epsilon$ turbulence model.

It is interesting to notice that although the VKI airfoil was designed by experienced aerodynamicists using sophisticated inverse shape design software, this VKI design is not a member of the final Pareto-optimal set obtained by the optimizer (Figure 6 and 7). That is, the optimizer found an entire family of feasible solutions that are better than the inversely designed VKI airfoil cascade for all three objectives³³. Specifically, cascade No.1 offers reduction of 7% in total pressure loss, needs 1 airfoil less than the VKI cascade, and generates

about 1% higher total loading. This means that it is possible to design turbomachinery blade rows that will have simultaneously lower total pressure loss, higher total loading, and fewer blades while preserving some of the same features of the original blade rows (inlet and exit flow angles, total mass flow rate, blade cross-section area, and trailing edge radius).

With such submit-and-forget automatic constrained multi-objective optimization software the role of the designer is to use a proven and robust flow-field analysis code and specify meaningful ranges of the design variables, the multiple objective functions, and the constraints. Finally, the designer ultimately must choose the best compromise solution among the optimized solutions that form the Pareto front. This multi-objective design optimization methodology can be readily applied to arbitrary three-dimensional configurations and to multi-disciplinary problems.

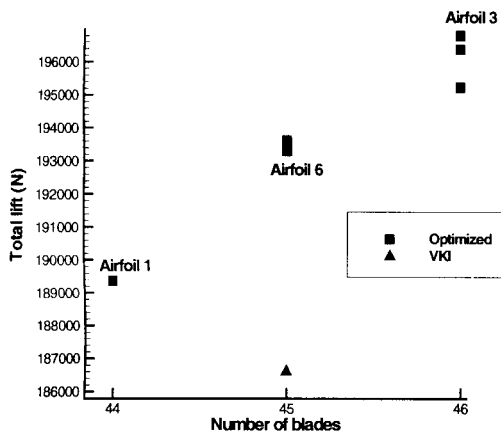


Figure 6. Comparison of total loading produced versus number of airfoils for optimized finite length cascades and the VKI airfoil cascade.

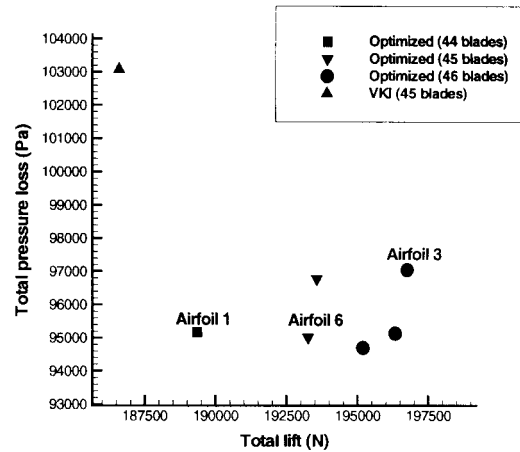


Figure 7. Comparison of total pressure loss generated versus total loading produced for optimized finite length cascades and the VKI airfoil cascade.

3.4 Multi-disciplinary design optimization applied to magneto-hydrodynamics

Most realistic design problems involve not only aerodynamics but also other interacting disciplines. One such multi-disciplinary shape design optimization example is our recent work involving magneto-hydrodynamics^{18,19}. When a viscous liquid flows from a narrow passage into a suddenly wider passage, there will be significant flow separation zones that will significantly reduce the efficiency of such flow fields. One possibility to reduce and even completely eliminate the flow separation would be to perform a straightforward wall shape optimization. But, if the shape of the passage walls is not to be altered for whatever reason, it is still possible to affect the flow-field pattern if the fluid is electrically conducting so that it can respond to externally applied magnetic or electric fields. In this situation the objective is to find the proper distribution and orientation of the externally applied magnetic field along

the passage walls so that the fluid flow separation is minimized.

Using our two-dimensional magneto-hydrodynamics analysis code³⁴ based on the least squares finite element method and our micro-genetic optimizer²⁷, we have recently shown that such optimized magnetic fields can not only create maximum static pressure rise with a minimum total pressure drop for a fixed length of a diffuser (Figure 8), but that magnetic fields can be found that entirely eliminate flow-field separation (Figure 9).

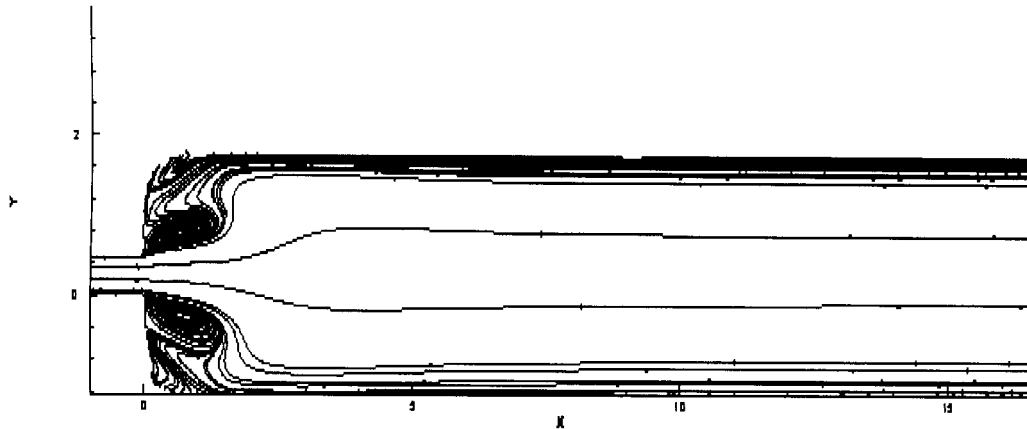


Figure 8. Streamlines for flow through a diffuser with an optimized applied magnetic field.

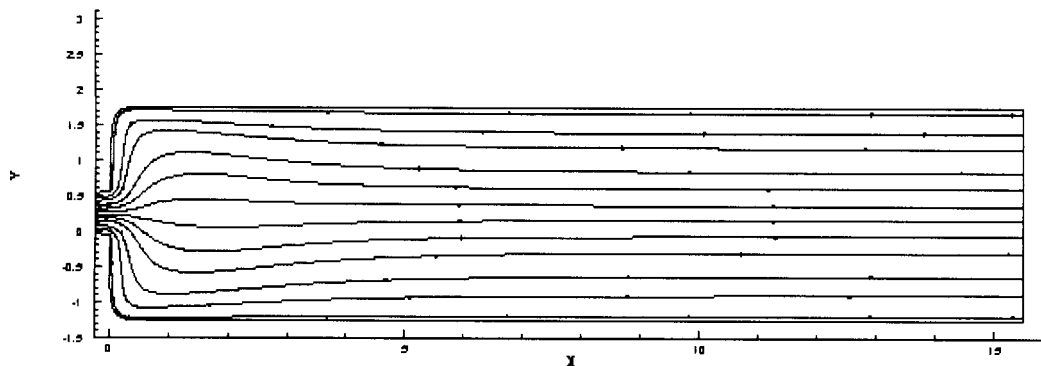


Figure 9. Streamlines for diffuser flow through an applied magnetic field designed to suppress separation.

CONCLUSIONS

Aerodynamic shape design is experiencing a general trend away from inverse shape design and gradient based optimization methods and towards multi-objective and multi-disciplinary semi-stochastic and stochastic constrained optimization. This trend is facilitated by the availability of commodity based inexpensive distributed parallel computing environments, increased need for incorporating several disciplines in the design process simultaneously, decreased need to modify existing reliable flow-field analysis codes, and especially by the decreased need for highly educated, experienced, and expensive designers.

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