JOURNAL OF AIRCRAFT
Vol. 33, No. 5, September–October 1996

# Stochastic Approach to Optimal Aerodynamic Shape Design

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**The purpose of this study was to show that stochastic methods can be applied effectively to optimal aerodynamic shape design problems, and that optimal solutions within relatively complex design spaces can be located in a reasonable amount of computation time. The design methodology presented is based on a modified simulated annealing algorithm and is global in nature, i.e., relative large complex design spaces can be automatically investigated. Current approaches that typically employ gradient-based optimization schemes tend to get caught in the numerous real and false local minima common in the design spaces of practical aerodynamics shape design problems. Within the context of the optimal shape design of a minimum drag axisymmetric forebody problem, a comparison was made between the proposed stochastic methodology and a gradient-based optimization approach. The results obtained clearly demonstrated the ability of this methodology to locate optimal designs in relatively complex design spaces where gradient-based optimization approaches experience difficulties. Further, the computation time required by the stochastic approach compared favorably to that of the gradient-based method.**

## Nomenclature

$A$ = cross-sectional area of forebody, m$^2$
$C_d$ = coefficient of drag
$F_d$ = force of drag, N
$m$ = length of Markov chain
$n$ = number of cross sections
$P$ = Metropolis criterion
$R$ = random number uniformly distributed over the range [0, 1]
$R_p$ = baseline parabolic shape
$r_i$ = radius at the $i$th cross section, ft
$T$ = control parameter
$U_\infty$ = freestream air velocity, m/s
$z$ = distance from the nose of the forebody measured along the $z$ axis, ft
$z_{\max}$ = length of forebody, ft
$\alpha$ = nose angle, deg
$\beta$ = control parameter reduction coefficient
$\Delta E$ = change in objective function value
$\rho$ = freestream air density, kg/m$^3$

## Introduction

COMPUTATIONAL FLUID DYNAMICS (CFD) has begun to play an increasingly important role in the aircraft industry because of its ability to produce detailed insights into complex flow phenomena and its ease of parameterization, which can help identify the cause of weak aerodynamic performance. Some of the earlier uses of CFD in the design process were based on the cut-and-try approach. Here the designer iteratively modifies and evaluates a design.[1] While considerable gains in aerodynamic performance can be achieved by this approach, continued improvement is much more difficult to attain. Because of the complexity of fluid flow and shape, it is unlikely that repeated interactive trials in a design procedure can lead to a truly optimum design. Therefore, automatic design techniques are needed to fully realize potential improvements in aerodynamic efficiency.[2]

The use of constrained numeric optimizers has recently become increasingly attractive. In one approach, often referred to as shape perturbation methods, a CFD analysis code is coupled with a numeric optimizer. The optimizer, usually gradient-based, determines the values for a set of user-generated design parameters that define an optimal geometry with desirable characteristics while satisfying some design constraints. This approach was used by Hager et al.[3] for the two-point design of a transonic airfoil for improved off-design performance. Cheung et al.[4] utilized the methodology for the design of a theoretical minimum-drag body. Other demonstrations of the use of shape perturbation methods include the design of a high-speed civil transport (HSCT) wing,[5] the shape optimization of an airfoil under inviscid flow,[6] and the evaluation of an aircraft's performance using unstructured grids.[7]

The predominant use of gradient-based optimizers, however, limits the success that can be achieved through shape perturbation. Gradient-based optimizers typically use finite difference techniques to estimate gradients. This approach consumes the bulk of the computational effort and can often yield inaccurate gradients.[8] In addition, there is a rapid rise in the number of function evaluations required as the number of design variables increases. Finally, this approach can be impractical in domains with a large number of local minima.[9] The success of the optimization process for these domains, which are common in shape optimization problems, will depend on the location of the initial guess within the design space. To circumvent these difficulties, researchers often start the optimization process from relatively good initial designs and use a linear combination of base analytical body shapes to define their final configuration. This formulation ensures that the design optimization procedure will yield a reasonable or physically acceptable shape for the optimal solution.

Other design approaches, collectively referred to as inverse design methods, directly determine airfoil geometry by finding a shape that generates specified surface conditions.[10–12] An intrinsic problem with these methods, however, is that the quality of the optimized shape depends on the surface distribution, usually pressure or velocity, that it is required to match. Therefore, an inverse design approach depends on the knowledge of the designer to establish a desirable optimum.[13] Further, they do not lend themselves to the imposition of constraints.[4]

For shape perturbation approaches to be effectively applied to aerodynamic design, they must be able to arrive at an op-

Received Nov. 25, 1995; revision received April 23, 1996; accepted for publication April 23, 1996. 

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timal solution within a reasonable amount of computation time. This goal can be realized by 1) minimizing the computation time required for each flowsolve, and 2) reducing the total number of flowsolves. Reducing the computation time necessary for each flowsolve can be achieved in several ways. The most common and simplest is through the use of coarser grids and incomplete convergence. Care must be taken, however, to ensure that the validity of the objective function is not compromised. This approach introduces numerical errors that add a roughness to the objective function surface, creating problems for gradient-based optimizers. The roughness may cause the calculation of inaccurate gradients and could be mistaken for local extrema by the optimization algorithm.[14]

Several researchers have employed response surface methodologies to overcome the problems presented by noisy objective functions surfaces.[15] Response surfaces are smooth functions that define the relationship between the independent and dependent variables. These smooth functions are selected so that the prominent features of the objective function are retained while false local minima may be avoided. However, response surfaces, which are typically polynomial approximations, may not accurately represent the actual objective function surface that may not be polynomial in nature. Further, the creation of the response surface demands a high computational cost because of the large number of design points, upon which the response surface is based, that must be evaluated.

The purpose of this investigation is to demonstrate the practicality of using a stochastic approach for optimal aerodynamic shape design. Specifically, this study seeks to 1) demonstrate how stochastic methods can overcome some of the previously enumerated difficulties experienced by gradient-based optimizers, and 2) arrive at optimal or near-optimal solutions without requiring an excessive amount of computation time. These issues are explored and discussed within the context of the optimal shape design of a minimum drag axisymmetric forebody problem. The next section will discuss previous efforts in stochastic shape optimization. This will be followed by a description of the numerical optimizers used in this study to solve the forebody problem along with the Euler formulation used. Next is the problem description followed by the results from the gradient-based and stochastic approaches. Finally, a comparison of the two approaches is presented and discussed.

## Background on Stochastic Aerodynamic Shape Optimization

Several researchers have recognized the limitations of gradient-based approaches to CFD shape design and have initiated investigations into the use of stochastic methods. As an alternative to gradient-based optimization for the preliminary design of wings, Gage and Kroo[8] employed genetic algorithms (GA). GAs occupy a gap in the range of optimization techniques between gradient-based methods and random search techniques. The objective function in their study was the minimization of induced drag with fixed lift. They found that a standard GA was able to locate optimal designs, but it was sensitive to constraint-handling schemes and required significantly more computation time than a gradient-based method. Despite modifications made to the algorithm to improve the handling of constraints, the GA still remained more computationally intensive than gradient-based methods. However, their work was successful in demonstrating that a noncalculus based approach can be applied to problems that cannot possibly be solved by gradient-based methods.

Other researchers who have employed GA for aerodynamic shape design acknowledge the large number of function evaluations (each function evaluation corresponds to a flowsolve) required to converge to an optimal solution.[10,13] They suggest that coupling a GA with a gradient-based optimizer may reduce computation time. Genetic algorithms are applied to an inverse design optimization method in Obayashi and Takanashi.[16] Once target pressure distributions are obtained, corresponding airfoil or wing geometries are computed by an inverse design code coupled with a Navier–Stokes solver. In this study, the authors conclude that to reduce computation time further, enhancement of the GA and parallel computing techniques need to be investigated.

The results from the limited studies conducted in stochastic optimal aerodynamic shape design demonstrate the ability of stochastic methods to overcome the difficulties experienced by gradient-based approaches. These studies, however, also illustrate that the excessive computation time required still serves as an obstacle to their broader use. The aim of this investigation, therefore, is to develop a practical stochastic approach to aerodynamic shape design, which overcomes the limitations of gradient-based approaches, while maintaining a computational effort comparable to those of current gradient-based approaches. This investigation employs a stochastic approach to the optimal aerodynamic shape design of an axisymmetric forebody. A comparative study was conducted between the stochastic approach (SAWI) and a gradient-based optimizer (NPSOL).

## Numeric Optimizers

### Simulated Annealing with Iterative Improvement

Simulated annealing (SA) was first introduced by Kirkpatrick et al.[17] and is analogous to the physical process of annealing solids. The algorithm, based on Monte Carlo techniques, consists of the following steps:

1) Select an initial configuration and calculate the objective function value $E$.

2) Randomly generate a new system configuration and measure $\Delta E$.

3) If $\Delta E \leq 0$, accept the new configuration, i.e., the new configuration becomes the current configuration, or, if $\Delta E > 0$ and $P = e^{-\Delta E/T} \geq R$, accept the new configuration.

4) Repeat steps 2 and 3 $m$ times to complete a Markov chain.

5) Lower the value of $T$ and repeat steps 2–5 until convergence.

The number of new configurations generated at a particular $T$ constitutes a Markov chain. They are generated by randomly assigning different values to the design variables. As $T$ is lowered, the probability that an inferior configuration is accepted approaches zero. The rate of convergence, and the corresponding quality of the final solution is determined by a cooling schedule, which establishes the rate at which $T$ is lowered. If $T$ is lowered too fast, quenching, or the convergence of the optimization process to high-lying local minima can occur. Numerous methods for implementing a cooling schedule have been proposed in other publications.[18] For this study the method proposed by Kirkpatrick et al.[17] is used. After every Markov chain, $T$ is reduced by a factor $\beta T$, where $\beta$ is predefined and typically lies between 0.05–0.30.

By accepting configurations that yield inferior solutions in a controlled fashion, SA is able to jump out of local minima and potentially find a more promising downhill path. The acceptance of uphill moves is carefully controlled by $T$. Although the global optimal solution is not guaranteed, SA has been found to consistently provide solutions close to it. Because of its probabilistic nature, SA is independent of its initial starting design.

A typical annealing process can be divided into high, intermediate, and low-control parameter regions (refer to Fig. 1). Within the low-control parameter region, SA is relatively inefficient since a large number of function evaluations are required to produce a relatively small improvement in the objective function.[19] To reduce the number of function evaluations required in this region, and therefore increase the overall efficiency of SA, a modified simulated annealing algorithm, simulated annealing with iterative improvement (SAWI), was developed by the authors and is used in this study.[20] By pre-

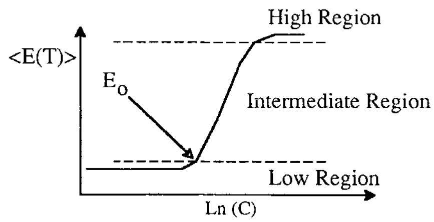


**Fig. 1 Typical annealing curve showing high, intermediate, and low regions.**

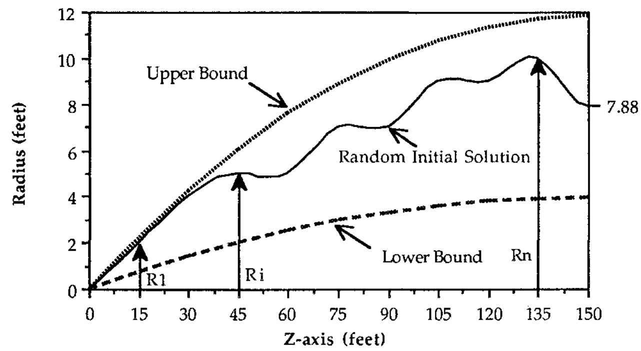


**Fig. 2 Geometric definition of forebody profile. Radii defined at *n* cross sections equally spaced along the *Z* axis.**

maturely terminating SA at the end of the intermediate region (identified by $E_0$ in Fig. 1) and employing a random search iterative improvement method to conduct a local search for the optimal solution within the low-control parameter region, the overall number of function evaluations required can be significantly reduced. The point of premature termination of the SA run that signifies the end of the intermediate region is not known a priori, and must therefore be predicted. For this purpose a transition parameter is used that monitors the number of inferior solutions that the algorithm has accepted vs the total number of inferior solutions during each Markov chain.[21] The authors found from experimentation that when this ratio lies between 0.10–0.30, the transition point has been reached. For several test problems in mechanical design, SAWI was found to require 30–40% less computation time than pure SA.[20]

To further reduce computation time requirements and maintain the number of flowsolves required on the order of hundreds, two strategies were employed. First, employing a relatively fast cooling schedule, i.e., decreasing the control parameter relatively rapidly, results in the acceptance of fewer inferior solutions and faster convergence. However, care must be taken in specifying a cooling schedule because rates that are too fast will result in quenching, or convergence to nearby high-lying local minima. For this study a $\beta$ of 0.30 was found to yield good solutions. Second, each design variable was allowed to take on a finite number of equally spaced discrete values within its upper and lower bounds. The number of discrete values ranged from 30–50 points equally spaced over the range of each design variable. Discretization results in a more uniform search of the design space when compared to a continuous design space with an infinite number of points. A uniform search increases the probability of convergence to optimal regions in the design space, and once an optimal region is located, a local search can be conducted to find the optimal solution.

### NPSOL

The gradient-based optimizer utilized in this study was NPSOL.[22] NPSOL is a collection of Fortran subroutines designed to solve nonlinear programming problems subject to both linear and nonlinear constraints. The optimizer employs a sequential quadratic programming algorithm to search for the objective function minimum. At each iteration, the search direction is found from the solution of a quadratic programming problem. In using the NPSOL optimizer, care must be taken in specifying the difference interval used in the finite difference approximation of the gradient. Incorrect specification of the interval may lead to erroneous results.[23] Consequently, prior to the design optimization runs, several difference intervals were tested to establish a value that consistently yielded the best solutions. Based on these studies a difference interval of 0.0075 was used in all of the examples presented in this article.

## Problem Description

The design goal of the present study is to determine the geometry of an axisymmetric forebody that minimizes the aerodynamic drag. Typically, for these kinds of problems, a linear combination of a relatively small number of base analytical functions is used to define the body shape. In this investigation, however, to expand the design space, a more general body shape definition is used. Referring to Fig. 2, $n$ equally spaced cross sections are defined between the nose and the end of the forebody. At each of these cross sections a radius $r_i$ is specified. By fitting cubic splines between the radii and enforcing an equal slope constraint between successive splines, the profile of the forebody is defined. A full rotation of the profile creates the three-dimensional shape of the forebody. Each radius can take on any value within its upper and lower bounds, providing an infinite number of possible solutions.

The design optimization problem can therefore be formulated as

$$\begin{aligned} &\min\ C_d(r) = F_d/0.5\rho U_\infty^2 A \\ &\text{subject to:}\quad 0.5R_p(z) \le r_i(z) \le 1.5R_p(z) \qquad i = 1, \ldots, n \end{aligned} \tag{1}$$

where $R_p(z)$ is a baseline parabolic shape defined as

$$R_p(z) = 0.5z_{\max} \tan\alpha[1 - (1 - z/150)^2] \tag{2}$$

The flight conditions are supersonic (Mach 2.4) with zero angle of attack and zero lift. The nose angle is fixed at 6 deg. The length of the forebody is 150 ft, with the cross-sectional radius at the end fixed at $\frac{1}{2}z_{\max}\tan\alpha$ and the slope maintained at 0 deg.

The problem was solved for $n = 4$ and 9. The use of four cross sections serves to provide a comparison within a relatively simple design space, while the nine cross-sectional problem illustrates the relative merits of each approach in a relatively complex design space.

## Euler Formulation

A very efficient hybrid finite volume implicit Euler marching method that has been in use for several years[24–26] was employed in this study. The numerical formulation of this method is based on the node-centered scheme developed originally by Jameson (i.e., FLO67, FLO97). The three-dimensional unsteady Euler equations are transformed to a spherical coordinate system. A central-difference, physical space, finite volume scheme is then applied to the crossflow terms and upwind finite differences are employed in the marching direction. Runge–Kutta time integration is then used, along with local time stepping and residual smoothing, to accelerate convergence to a steady state at each crossflow plane using the flow solution at the previous plane as an initial guess.

The implicit formulation for the streamwise terms removes any stability constraints on the marching step-size other than those dictated by geometric accuracy. This results in a very fast method to compute supersonic flows with complete configurations being computed with as little as 100 steps in the streamwise direction. Simple wings and wing–body configurations can be computed in a few minutes on a Cray supercomputer. The code is also cast in a multiblock context with nonmatching grid interfaces. This allows for flexibility in treating complex geometries including multiple lifting surfaces and discontinuities such as inlets and engine nacelles. The primary restriction to this method is that the flow must remain supersonic. The method is also easily extended to include viscous terms in a parabolized Navier–Stokes fashion.

The aerodynamic calculations were carried out on a relatively coarse mesh consisting of 39 circumferential and 40 radial crossflow mesh points of the first conical mesh at 50 streamwise stations. This mesh was selected because it provided accurate results while neither requiring excessive amounts of memory nor computation time. Flowsolves were terminated when the final tolerance on the residual reached 0.001. Increasing the convergence tolerance by two orders of magnitude more than doubled the amount of computation time needed for one function evaluation. This combination of parameters is within a range that would allow several hundred function evaluations to be practical on current supercomputers.

## Results

### Four Cross Sections

For this problem, the body radii, $r = \{r_1, r_2, r_3, \text{and } r_4\}$ constitute the design variables. With $n = 4$, the cross sections are spaced 30 ft apart along the forebody axis of symmetry. NPSOL was able to find an optimal solution of $C_d = 0.0098$ in 101 function evaluations, with $r = \{2.3189, 4.0886, 5.7020, \text{and } 6.9950 \text{ ft}\}$. Note that each function evaluation corresponds to a flowsolve and for these types of problems the total number of flowsolves provides a good measure of computation time.

During the stochastic optimizations trials, the specified range for each radius $r_i$ in the design variable set $r$ was discretized into 50 points, equally spaced between their upper and lower bounds. Initiated from the same point in the design space as NPSOL, SAWI was able to find an optimal solution of $C_d = 0.0110$ in 112 function evaluations, with $r = \{2.0999, 3.8342, 5.2973, \text{and } 6.8108 \text{ ft}\}$. Comparison with the NPSOL solution shows that both designs lie in the same region of the design space. The profile for both solutions is illustrated in Fig. 3. This example has shown that for a relatively simple design space and a small number of design variables the stochastic approach performs almost as well as the gradient-based approach, yielding comparable results with similar computational requirements.

### Nine Cross Sections

For this problem, the body radii $r = \{r_1, \ldots, r_9\}$ constitute the design variables. With $n = 9$, the cross sections are now spaced 15 ft apart along the forebody axis of symmetry. Design runs were initiated from two distinct points in the design space. From the first location, identified as Initial Design I in Fig. 4, NPSOL converged to a solution of $C_d = 0.0120$ in 262 function evaluations [identified as Local Minimum (a) in Fig. 4]. Since the four cross-sectional design space is a subset of the nine, the best solution in the four cross-sectional problem must exist in the nine. However, Local Minimum (a) is significantly higher than the four cross-sectional problem optimal solution, and is therefore classified as a high-lying local minimum. From the second initial solution, identified as Initial Design II in Fig. 4, NPSOL converged to another high-lying local minimum, identified as Local Minimum (b) in Fig. 4, with $C_d = 0.01781$ in 266 function evaluations.

For the stochastic optimizations trials, the specified range for each radius $r_i$ in the design variable set $r$ was discretized into 30 points equally spaced between their upper and lower bounds. From Initial Design I, SAWI converged to a solution with $C_d = 0.0110$ in 198 function evaluations. This solution represents an 8.3% improvement over NPSOLs with a 24% reduction in computation time. Because of the discretized nature of the design space, this approach can only locate optimal regions in the design space. A local search employing continuous variables must then be initiated to find the optimal solution in this region. Since gradient-based methods are superior to stochastic approaches for local searches, NPSOL was used for this task. It required an additional 31 function evaluations (for a total of 229), converging to a solution with $C_d = 0.00956$, identified as Local Minimum (c) in Fig. 5. The design variable set for this solution is $r = \{1.4850, 2.6254, 3.6353, 4.4298, 5.0886, 5.7350, 6.3127, \text{and } 6.8766 \text{ ft}\}$. This represents a 2.5% improvement over the best solution found in the four cross-sectional problem, and a 20.3% improvement over that found by NPSOL alone. NPSOL's solution, which got stuck at a high-lying local minimum previously identified as Local Minimum (a), is included in Fig. 5 for comparison.

When initiated from Initial Design II, SAWI converged to a solution with $C_d = 0.01232$ in 217 function evaluations. This region in the design space contains Local Minimum (a) found by NPSOL when initiated from Initial Design I. A subsequent local search conducted with NPSOL yielded a solution with $C_d = 0.01108$, requiring an additional 98 function evaluations for a total of 315. This solution, identified as Local Minimum (d) in Fig. 6, represents less than a 1% deterioration when

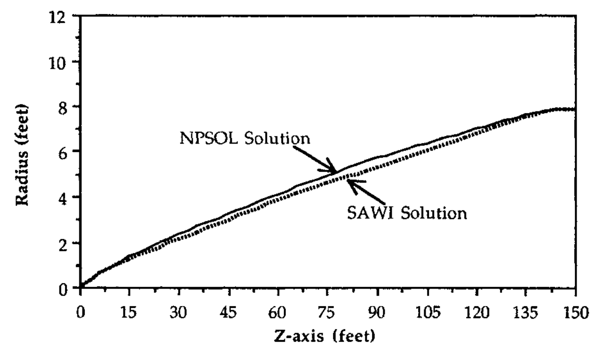


**Fig. 3 Forebody shape profiles of best solutions for four cross-sectional problem. Design process initiated from Initial Design I.**

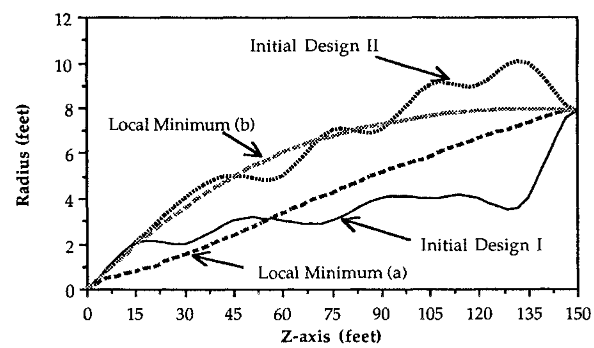


**Fig. 4 Forebody shape profiles of gradient-based solutions for nine cross-sectional problem.**

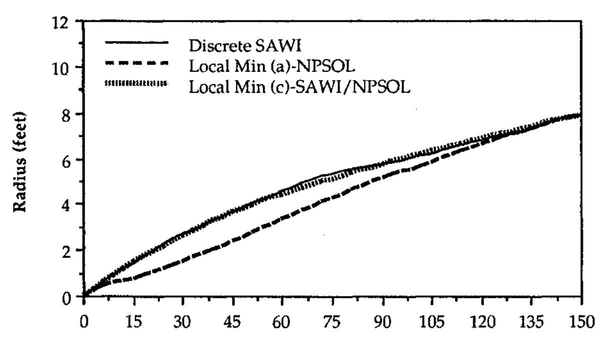


**Fig. 5 Forebody shape profiles of solutions for nine cross-sectional problem. Design process initiated from Initial Design I.**

**Table 1 Summary of local minima found in Figs. 4–6**

| Shape profile | Method | Initial design | Coefficient of drag | No. of function evaluations |
|---|---|---|---|---|
| Local minimum (a) | NPSOL | I | 0.01201 | 262 |
| Local minimum (b) | NPSOL | II | 0.01781 | 266 |
| Local minimum (c) | Discrete SAWI/NPSOL | I | 0.00956 | 229 |
| Local minimum (d) | Discrete SAWI/NPSOL | II | 0.01108 | 317 |

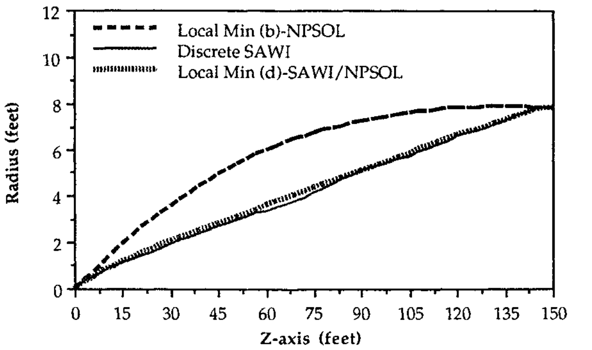


**Fig. 6 Forebody shape profiles of solutions for nine cross-sectional problem. Design process initiated from Initial Design II.**

compared to the best four cross-sectional solution. On the other hand, it represents a 37.7% reduction over the solution found by NPSOL alone, identified as Local Minimum (b) in Fig. 6. For comparative purposes, Table 1 summarizes the results from the four local minima whose profiles are illustrated in Figs. 4–6. These minimum drag results agree extremely well with the minimum drag shape derived by Parker using linearized supersonic theory.[27] Such agreement is noteworthy because of the constraints of zero slope at the base and the inclusion of nonisentropic effects that are not present in linearized supersonic theory.

## Concluding Remarks

The optimization approach adopted in this study has shown that stochastic methods can effectively be applied to aerodynamic shape optimization. For relatively complex design spaces, the approach is able to overcome the main difficulty experienced by gradient-based optimizers, i.e., convergence to high-lying local minima. Unlike previous investigations, the computation time required by this formulation compares favorably with the computational requirements of gradient-based approaches. This was achieved by using a discrete design space and employing relatively fast cooling schedules to the modified simulated annealing algorithm. In this manner optimal regions in the design space were located relatively inexpensively. Within this region, local gradient-based searches were conducted to identify the optimal solutions.

For simple well-behaved design spaces, represented by the four cross-sectional problem, the stochastic approach yielded comparable solutions with similar computational requirements. However, as the level of complexity of the design space was increased as represented by the nine cross-sectional problem, the combination of the stochastic approach to locate optimal regions and the gradient-based optimizer to identify optimal solutions within those regions, yielded far superior solutions than the gradient-based approach alone. Further, the computation time required for the combined effort of both optimizers was comparable to the runs by the gradient-based optimizer alone. This study has therefore demonstrated that stochastic methods do have a practical role to play in CFD shape design.

## Acknowledgments

Financial support was provided by NASA Langley Research Center Grant NAG-1-1559. Their financial support is gratefully acknowledged. The computer codes used in this investigation were run on the Cray Y-MP at NCSA at the University of Illinois and the Cray C90 at the Pittsburgh Supercomputing Center. We would also like to acknowledge the contribution of Mike Siclari of the Northrop Grumman Corporation for formulating the CFD design problem and for supplying the flowsolver.

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