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On the use of orthogonal functions in fluid-dynamic gradient-based optimization

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SUMMARY

This paper proposes a method to derive a set of symmetrical and antisymmetric orthogonal shape functions, which can be efficiently used in fluid-dynamic design optimization. The inverse design of an airfoil in inviscid transonic flow conditions is proposed to demonstrate that a gradient-based optimization using orthogonal profiles is 6–10 times faster than the same procedure using non-orthogonal interpolation functions. Copyright © 2008 John Wiley & Sons, Ltd.

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KEY WORDS: orthogonal profiles; optimization; efficiency

1. INTRODUCTION

In the last years, automatic design employing computational fluid dynamics has significantly grown in importance due to the rapid advances in numerical methods for the solution of Navier–Stokes equations. Besides the fundamental designer's work devoted to the development of optimization methodologies, a crucial point is encountered when using a gradient-based approach, which can influence both the optimizer performance and the product definition, namely the choice of the design parameters. Great efforts have been recently made by several authors in order to select an appropriate set of design parameters, which could reduce the design cost and, at the same time, could be effective in finding improved designs. The best choice in terms of flexibility consists of keeping the ordinates of the mesh points on the profile surface as design parameters [1], with the drawback that a very high number of parameters is needed. Moreover, since a perturbation of a

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design parameter would produce only a local perturbation of the flow solution (thus deteriorating the convergence of the optimization problem), a smoothing of the blade profile is required. A very common approach, close to the direct use of coordinates and thus very flexible, is the representation of all or part of the airfoil surface by spline curves or Bezier–Bernstein polynomials [2] using some points of the blade or control points as design parameters, respectively. Another widely employed parametrization consists of combining a number of existing profiles (shape functions), using the corresponding weights as design parameters, see, e.g. Reference [3], where a limited number of base functions are used. Other representations apply modifying functions, such as the widely used Hicks–Henne functions [4], to an existing base airfoil or blade.

It should be noticed that none of the above parameterizations form an orthogonal basis and in some cases there could even be the risk of a non-unique mapping between parameter values and geometry [5]. On the contrary, orthogonal profiles have been chosen by several authors with the aim of representing wing sections with a number of parameters as smaller as possible [6, 7]. Apart from this undoubtable advantage, none of them has analyzed how a gradient-based optimization procedure can take advantage of choosing an orthogonal basis rather than a non-orthogonal one.

The aim of this paper is two-fold: (i) to propose a method to derive a set of orthogonal shape functions by modifying an airfoil-like Bézier–Bernstein polynomial; the method is able to provide a set of symmetrical and antisymmetrical shape functions that will be combined according to the values of the design parameters to define the profile to be optimized; and (ii) to demonstrate that the efficiency of a gradient-based optimization method is significantly improved when using such orthogonal profiles, rather than a non-orthogonal basis.

2. ADVANTAGES OF USING AN ORTHOGONAL BASIS

A simple optimization problem is proposed to motivate why an orthogonal basis should be preferred to a non-orthogonal one, when applying a gradient-based optimization procedure: find the design parameters ξ_1 and ξ_2 that minimize the L_2-norm of a two-dimensional vector $\mathbf{f}$, obtained by a linear combination of the vectors $\mathbf{f}_1=(1,0)$ and $\mathbf{f}_2=(\alpha,1)$ (α is a free parameter), namely as

$$\mathbf{f}=\xi_1\mathbf{f}_1+\xi_2\mathbf{f}_2=(\xi_1+\alpha\xi_2,\xi_2) \tag{1}$$

Clearly, $\mathbf{f}_1$ and $\mathbf{f}_2$ represent an orthogonal basis only for $\alpha=0$ and the absolute minimum of the objective function

$$I=(\xi_1+\alpha\xi_2)^2+\xi_2^2=\xi_1^2+2\alpha\xi_1\xi_2+(1+\alpha^2)\xi_2^2 \tag{2}$$

is obtained for $\xi_1=\xi_2=0$. Suppose to start a gradient-based optimization procedure from the point $(\xi_1,\xi_2)=(1,1)$, where the following sensitivity derivatives can be analytically retrieved:

$$\begin{aligned} \left.\frac{\partial I}{\partial \xi_1}\right|_{(1,1)} &= 2(1+\alpha) \\ \left.\frac{\partial I}{\partial \xi_2}\right|_{(1,1)} &= 2(1+\alpha+\alpha^2) \end{aligned} \tag{3}$$

Equation (3) shows that when an orthogonal basis is employed (i.e. when $\alpha=0$), the two partial derivatives are equal and the search direction $-\nabla I$ points exactly towards the solution $(\xi_1,\xi_2)=$

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$(0,0)$ of the optimization problem. On the other hand, as $|\alpha|$ increases, the objective function gradient is shifted more and more aside from the *exact* search direction. As a consequence, the convergence rate of the optimization procedure would become slower. In the limit case of linearly dependent vectors ($|\alpha| \to \infty$), the solution $(0,0)$ cannot be achieved.

3. GENERATION OF ORTHOGONAL PROFILES

This section proposes the application of the Gram–Schmidt procedure to derive a set of orthogonal profiles, whose combination can be effectively used to define a single-element airfoil.

A set of airfoil-like profiles p_ℓ, $\ell = 1, \ldots, n_p$, is generated by using the Bézier–Bernstein polynomials

$$\mathbf{b}^n(q) = \sum_{j=0}^{n} \mathbf{b}_j \frac{n!}{j!(n-j)!} q^j (1-q)^{n-j}, \quad q \in [0,1] \tag{4}$$

where $\mathbf{b}_j$, $j = 0, \ldots, n$ contains the coordinates of the jth Bézier–Bernstein control point. The first ($\mathbf{b}_0$) and the last ($\mathbf{b}_n$) control points coincide, so as to obtain a wedged trailing edge. The Bézier–Bernstein polynomials are here scaled so as to fix the leading edge at $(0,0)$ and the trailing edge at $(1,0)$. Thus, the number of independent profiles, p_ℓ, reduces to $n_p = n-2$.

The first curve, p_1, is obtained by fixing the $(n+1)$ Bézier–Bernstein control points $\mathbf{b}_j$ so as to draw a reasonable aerodynamic profile. Additional (n_p-1) aerodynamic profiles p_ℓ can be generated by shifting the control points along y, $\mathbf{b}_0$ and $\mathbf{b}_n$ remaining unchanged. Then, the set of orthogonal shape functions f_ℓ, $\ell = 1, \ldots, n_p$, is finally obtained as follows: the first curve remains unchanged, namely $f_1 = p_1$; the other curves f_ℓ, $\ell = 2, \ldots, n_p$, are obtained from the curve p_ℓ and from the orthogonal shape functions f_j, $1 \leqslant j < \ell$, previously computed, according to the Gram–Schmidt orthogonalization process:

$$f_\ell = p_\ell - \sum_{j=1}^{\ell-1} \frac{\oint p_\ell f_j \, \mathrm{d}x}{\oint f_j^2 \, \mathrm{d}x} f_j \tag{5}$$

Finally, the shape functions f_ℓ, $\ell = 2, \ldots, n_p$, are empirically scaled so that the maximum of f_ℓ is equal to the maximum of f_1.

During the optimization process, each current geometry is defined by a linear combination of N_ξ shape functions f_ℓ:

$$f = \sum_{\ell=1}^{N_\xi} \xi_\ell f_\ell \tag{6}$$

where the weights ξ_ℓ are the N_ξ design parameters, with $N_\xi \leqslant n_p$ (n_p being the number of generated profiles, N_ξ being the number of actually employed profiles).

An example with $n = 12$ is proposed, where the above strategy is slightly modified so as to recover a set of symmetric and antisymmetric profiles. Figure 1 shows the location of the control points, which provides the first curve p_1. The second curve p_2 is obtained by shifting downwards the ordinate y_6 of the leading-edge control point while keeping the other control points fixed. The resulting base function f_2, derived from the application of Equations (5) to the Bézier–Bernstein polynomials p_1 and p_2, is antisymmetric: $y_{\text{lower}} = y_{\text{upper}}$, $\forall x \in [0,1]$. The third curve p_3 is the

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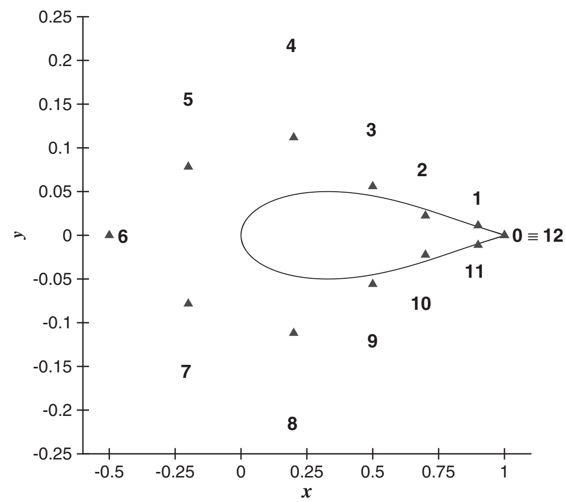

Figure 1. Control points and first profile generated.

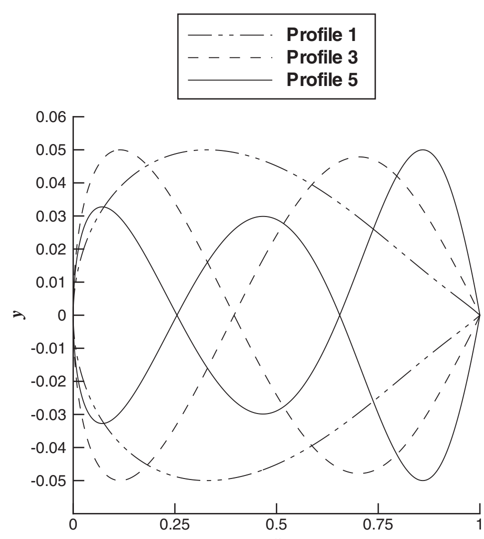

Figure 2. Symmetrical orthogonal functions 1, 3 and 5.

Bézier–Bernstein polynomial obtained by an upward shifting of y_5 and a downward shifting of y_7 with the same (small) amplitude. The resulting curve f_3 is symmetrical: $y_{\text{lower}} = -y_{\text{upper}}$, $\forall x \in [0,1]$. The fourth curve p_4 is obtained by assigning a downward shifting to ordinates y_5 and y_7. The resulting base function f_4, derived from the application of Equations (5) to the Bézier–Bernstein polynomials p_ℓ ($\ell = 1, \ldots, 4$), is antisymmetric. Other symmetric and antisymmetric

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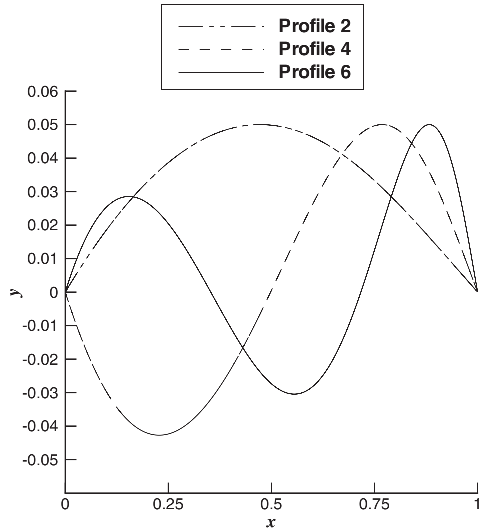

Figure 3. Antisymmetric orthogonal functions 2, 4 and 6.

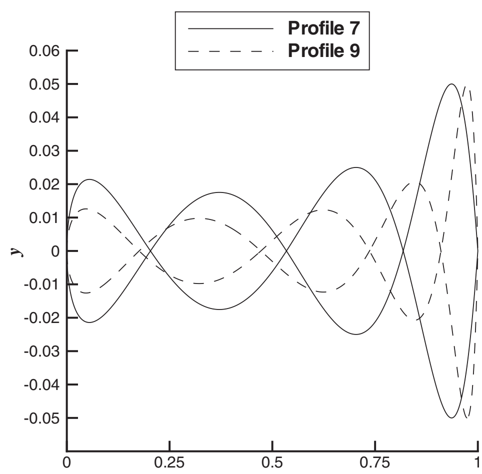

Figure 4. Symmetrical orthogonal functions 7 and 9.

curves with higher frequency are obtained by shifting the other control points along y. In particular, the symmetrical base functions f_5, f_7 and f_9 are obtained by means of a symmetric divergent shifting of y_4 and y_8, of y_3 and y_9, and of y_2 and of y_{10}, respectively; the antisymmetric base functions are obtained by means of a downward shifting of y_4 and y_8, of y_3 and y_9 and of y_2 and y_{10}, respectively. Figures 2–5 show the resulting orthogonal profiles, after scaling. Thanks to the generality of the Gram–Schmidt method, the above procedure can be straightforwardly

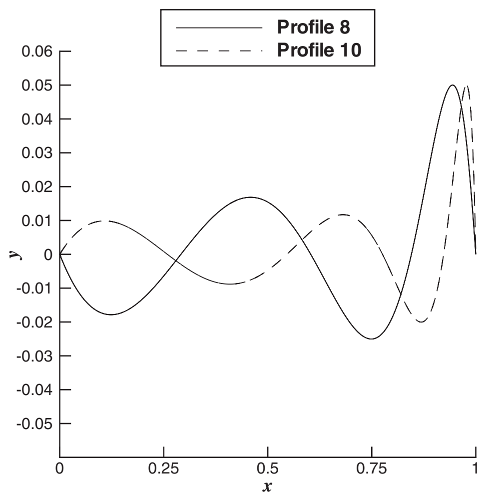

Figure 5. Antisymmetric orthogonal functions 8 and 10.

applied to other aerodynamic or general-purpose single-element shapes, even using interpolation functions different from the Bézier–Bernstein polynomials. In case of multi-element geometries, the procedure should be preferably applied to each component.

4. MULTIGRID-AIDED FINITE-DIFFERENCE PROGRESSIVE OPTIMIZATION

The gradient-based progressive optimization strategy firstly proposed in Reference [8] is here employed in combination with the multigrid-aided finite-difference (MAFD) gradient evaluation procedure of References [9, 10]. The upwind second-order-accurate flow solver for unstructured grids described in References [11, 12] is used to compute the flow field.

5. PERFORMANCE COMPARISON

The inverse design of a transonic (inviscid) airfoil is proposed in this section to analyze the different performance of a gradient-based optimization when changing the design parameter choice from a linear combination of orthogonal profiles to a linear combination of the original Bézier–Bernstein polynomials. The objective function is defined as follows:

$$I(\xi)=\frac{1}{2N_b}\sum_{i=1}^{N_b}[p(i)-\hat{p}(i)]^2 \tag{7}$$

where p is the current pressure and $\hat{p}$ is the target pressure on the airfoil surface, discretized by N_b intervals. Since a low number of orthogonal functions are sufficient to define existing airfoils [6, 7], the number of design parameters has been here fixed as $N_\xi = 4$. When using the orthogonal shape functions, the initial profile is derived from Equation (6) by setting $\xi_1 = 3.0$ and $\xi_\ell = 0.0$ for $\ell > 1$, whereas the target pressure distribution has been obtained by computing the inviscid transonic flow ($M_\infty = 0.7$) past the airfoil corresponding to $\xi_1 = 1.2$, $\xi_2 = 0.5$, $\xi_3 = 0.1$, $\xi_4 = 0.1$. In order to recover the initial and the target profiles with both representations, the initial set of control points $\mathbf{b}_j = (x_j^0, y_j^0)$, $j = 0, \ldots, n$, is modified as follows:

1. Determine the profile thickness by amplifying the ordinate of each control point:

$$\hat{y}_j = \xi_1 y_j^0, \quad j = 0, \ldots, n \tag{8}$$

2. Modify the profile shape by moving the leading-edge control points:

$$\begin{aligned} y_k &= \hat{y}_k k = 0, \ldots, 4 \quad \text{and} \quad k = n-5, \ldots, n, \quad y_6 = \hat{y}_6 + \xi_2 \\ y_5 &= \hat{y}_5 + \xi_3 + \xi_4, \quad y_7 = \hat{y}_7 - \xi_3 + \xi_4 \end{aligned} \tag{9}$$

The first performance comparison employs a steepest-descent search direction and a step size computed by simply multiplying the objective function gradient times the negative constant coefficient which empirically minimizes the computational time required by each application. Figures 6 and 7 provide the convergence histories of the flow residual, of the objective function and of the magnitude of the objective function gradient, obtained by using orthogonal and non-orthogonal profiles, respectively. One work unit is defined as one (converged) MG computation of the target flow. As clearly visible, the same (almost standard) gradient-based procedure is about six times faster when employing an orthogonal basis. Then, the strategy proposed in Reference [8] for modifying the search direction and the step size according to the sign of each sensitivity and to the convergence level of the optimization procedure is employed for a further comparison between orthogonal and non-orthogonal bases. Figures 8 and 9 provide the corresponding convergence histories: the use of an adaptive search strategy allows a further, significant reduction of the required computational time in the case of the orthogonal profiles, whereas a negligible improvement

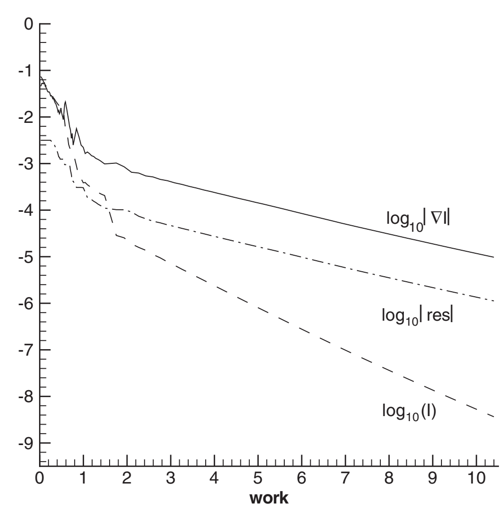

Figure 6. Steepest-descent constant-coefficient MAFD progressive optimization using orthogonal profiles.

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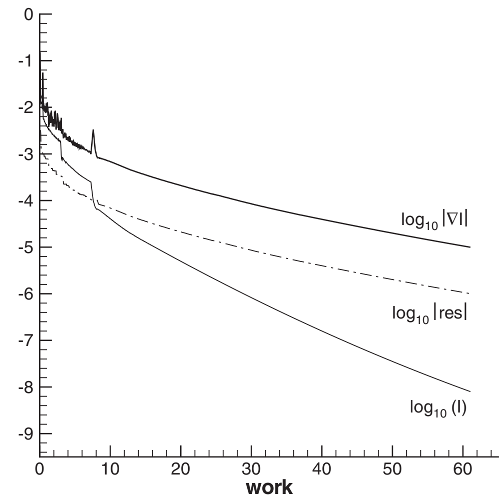

Figure 7. Steepest-descent constant-coefficient MAFD progressive optimization using the Bézier–Bernstein representation.

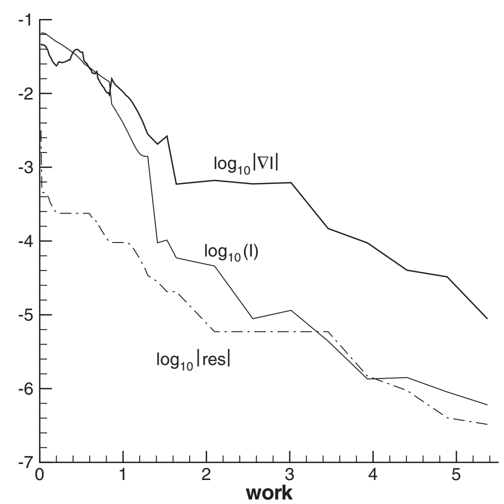

Figure 8. MAFD progressive optimization of References [9, 10] using orthogonal profiles.

is obtained when using the original Bézier–Bernstein representation: the strong oscillations in the convergence history (different choices of the coefficients produce less oscillations but slower convergence) clearly evidentiate that the Bézier–Bernstein polynomials suffer from this adaptive search strategy. Using the orthogonal profiles makes the adaptive MAFD progressive optimization ten times faster than the same procedure using the original Bézier–Bernstein representation.

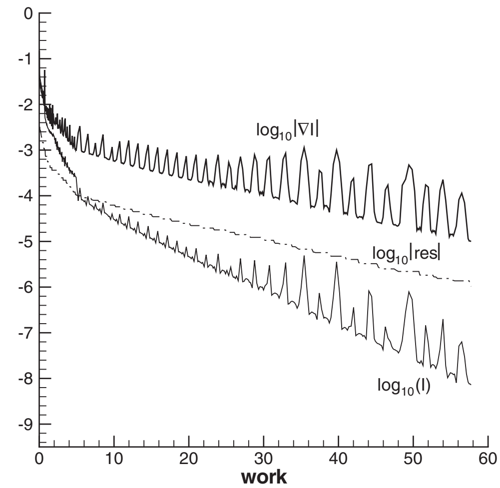

Figure 9. MAFD progressive optimization of References [9, 10] using the Bézier–Bernstein representation.

6. CONCLUSIONS

A method to derive a set of orthogonal shape functions by modifying an airfoil-like Bézier–Bernstein polynomial is proposed. The method is able to provide a set of symmetrical and anti-symmetric shape functions that can be used in optimization to represent the body surface. The solution of an inverse design problem demonstrates the superior performance of the orthogonal representation. In particular, the computational time required by a gradient-based design optimization using the orthogonal shape functions is 6–10 times lower than that required when using the Bézier–Bernstein representation.

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REFERENCES

1. Mohammadi B. A new optimal shape design procedure for inviscid and viscous turbulent flows. *International Journal for Numerical Methods in Fluids* 1997; **25**(5):183–203.
2. Farin G. *Curves and Surfaces for Computer Aided Geometric Design. A Practical Guide* (3rd edn). Academic Press: New York, 1993.
3. Obayashi S, Tsukahara T. Comparison of optimization algorithms for aerodynamic shape design. *AIAA Paper 96-2394*, 1996.
4. Hicks RM, Henne PA. Wing design by numerical optimization. *Journal of Aircraft* 1978; **15**(7):407–412.
5. Kuruvila G, Ta'asan S, Salas MD. Airfoil design and optimization by the one-shot method. *AIAA Paper 95-0478*, 1995.
6. Chang C, Torres FJ, Tung C. Geometric analysis of wing sections. *NASA-TM-110346*, 1995.
7. Robinson GM, Kean AJ. Concise orthogonal representation of supercritical airfoils. *Journal of Aircraft* 2001; **38**(3):580–583.

8. Dadone A, Grossman B. Progressive optimization of inverse fluid dynamic design problems. *Computers and Fluids* 2000; **29**:1–32.
9. Catalano LA, Dadone A, Daloiso VSE. Progressive optimization on unstructured grids using multigrid-aided finite difference sensitivities. *International Journal for Numerical Methods in Fluids* 2005; **47**(10–11):1383–1391.
10. Catalano LA, Dadone A, Daloiso VSE. Turbine cascade design via multigrid-aided finite-difference progressive optimization. *European Journal of Computational Mechanics* 2008; **17**(1–2):203–220.
11. Catalano LA, Daloiso VSE. Accurate computation of 2D turbulent compressible flows on unstructured grids. *AIAA Paper 2003-3828*, 2003.
12. Catalano LA, Daloiso VSE. Upwinding and implicit residual smoothing on cell-vertex unstructured grids. *International Journal for Numerical Methods in Fluids* 2005; **47**(8–9):895–902.

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