Summary

A technique for obtaining sensitivity derivatives using complex variables is described and demonstrated. The method is very easy to implement and is applicable for computing derivatives for turbulent flow applications. In fact, the methodology is applicable to any simulation code using real-valued variables.

Although the specification of a step-size parameter is required, the resulting sensitivity derivatives are highly accurate and not prone to errors caused by subtractive cancellation. In this regard, two additional digits of accuracy are obtained each time the step size is lowered by one order of magnitude, enabling highly accurate derivatives without the need to adjust the step size. Lastly, second-derivative information is easily computed using available data, although these computations are subject to cancellation errors.

The drawbacks of the current methodology are that the required memory essentially doubles over the original flow solver because of the use of complex variables in the code. Also, the computer time increases by as much as a factor of three.

Acknowledgments

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References

[1]Anders, J.B., Anderson, W.K., and Murthy, A.V., "The use of Heavy Gas for Increased Reynolds Numbers in Transonic Wind Tunnels," AIAA paper 98-2882, June 1998.

[2]Anderson, W.K., and Bonhaus, D.L., "An Implicit Upwind Algorithm for Computing Turbulent Flows on Unstructured Grids," *Computers and Fluids*, Vol. 23, No. 1, 1994, pp. 1-21.

[3]Anderson, W.K., and Bonhaus, D.L., "Aerodynamic Design on Unstructured Grids for Turbulent Flows," NASA TM 112867, June 1997.

[4]Anderson, W.K., and Bonhaus, D.L., "Airfoil Design on Unstructured Grids for Turbulent Flows," *AIAA Journal*, Vol. 37, No. 2, 1999, pp. 185-191.

[5]Anderson, W.K. and Venkatakrishnan, V., "Aerodynamic Design Optimization on Unstructured Grids with a Continuous Adjoint Formulation," *Computers and Fluids*, Vol. 28, No. 4-5, 1999, pp. 443-480.

[6]Anderson, W.K. Rausch, R.D., and Bonhaus, D.L., "Implicit/Multigrid Algorithms for Incompressible Turbulent Flows on Unstructured Grids," *Journal of Computational Phys*ics, Vol. 128, 1996, pp. 391-408.

[7]Baysal, O., and Eleshaky, M.E., "Aerodynamic Sensitivity Analysis Methods for the Compressible Euler Equations," *Journal of Fluids Engineering*, Vol. 113, 1991, pp. 681-688.

[8]Beux, F., and Dervieux, A., "Exact-Gradient Shape Optimization of a 2D Euler Flow," Finite Elements in Analysis and Design, Vol. 12, 1992, pp. 281-302.

[9]Bischof, C., Carle, A., Corliss, G., Grienwank, A., and Hoveland, P., "ADIFOR: Generating Derivative Codes from Fortran Programs," *Scientific Programming*, Vol. 1, No. 1, pp. 11-29, 1992.

[10]Borggaard, J.T., Burns, J., Cliff, E.M., and Gunzburger, M.D., "Sensitivity Calculations for a 2-D Inviscid Supersonic Forebody Problem," Identification and Control Systems Governed by Partial Differential Equations, SIAM Publications, Philadelphia, 1993, pp. 14-24.

[11]Carle, A., Fagan, M., and Green, L.L., "Preliminary Results from the Application of Automated Adjoint Code Generation to CFL3D," AIAA Paper 98-4807, September 1998.

[12]Cook, P., McDonald, M., and Firmin, M., "Airfoil RAE 2822 - Pressure Distributions and Boundary Layer Wake Measurement," AGARD AR-138, Paper A6, 1979.

[13]Elliott, J., and Peraire, J., "Aerodynamic Design Using Unstructured Meshes," AIAA Paper 96-1941, June 1996.

[14]Elliott, J., and Peraire, J., "Aerodynamic Optimization on Unstructured Meshes with Viscous Effects," AIAA Paper 97-1849, June 1997.

[15]Green, L.L., Newman, P.A., and Haigler, K.J., "Sensitivity Derivatives for Advanced CFD Algorithms and Viscous Modeling Parameters via Automatic Differentiation," *Journal of Computational Physics*, Vol. 125, 1996, pp. 313-324.

[16]Grossman, B., and Walters, R.W., "An Analysis of Flux-Split Algorithms for Euler's Equations with Real Gases." AIAA Paper 87-1117, June 1987.

[17]Hou, G.J.-W., Taylor, A.C., and Korivi, V.M., "Discrete Shape Sensitivity Equations for Aerodynamic Problems," *International Journal for Numerical Methods in Engineering*, Vol. 37, 1994, pp. 2251-2266.

[18]Iollo, A., Salas, M., and Ta'asan, S., "Shape Optimization Governed by the Euler Equations Using an Adjoint Method," ICASE Report 93-78, Nov. 1993.

[19]Jameson, A., "Essential Elements of Computational Algorithms for Aerodynamic Analysis and Design," ICASE Report 97-68, Dec. 1997.

[20]Jameson, A., Pierce, N.A., and Martinelli, L., "Optimum Aerodynamic Design Using the Navier-Stokes Equations," AIAA Paper 97-0101, January 1997.

[21]Jou, W.H., Huffman, W.P., Young, D.P., Melvin, R.G., Bieterman, M.B., Hilmes, C.L., and Johnson, F.T., "Practical Considerations in Aerodynamic Design Optimization," AIAA Paper 95-1730, June 1995.

[22]Lyness, J.N., "Numerical Algorithms Based on the Theory of Complex Variables," Proc. ACM 22nd Nat. Conf., Thomas Book Co., Washington, D.C., 1967, pp. 124-134.

[23]Lyness, J.N., and Moler, C.B., "Numerical Differentiation of Analytic Functions," *SIAM Journal of Numerical Analysis*, Vol. 4, 1967, pp. 202-210.

[24]Marcum, D.L., "Generation of Unstructured Grids for Viscous Flow Applications," AIAA Paper 95-0212, January 1995.

[25]Mohammadi, B., "Optimal Shape Design, Reverse Mode of Automatic Differentiation and Turbulence," AIAA Paper 97-0099, January 1997.

[26]Newman, J.C., and Taylor, A.C., "Three-Dimensional Aerodynamic Shape Sensitivity Analysis and Design Optimization Using the Euler Equations on Unstructured Grids," AIAA Paper 96-2464, June 1996.

[27]Newman, J.C., Anderson, W.K., and Whitfield, D.L., "Multidisciplinary Sensitivity Derivatives Using Complex Variables," MSSU-COE-ERC-98-09, Engineering Research Center Report, Mississippi State University, July 1998.

[28]Newman, J.C., Anderson, W.K., and Whitfield, D.L., "A Step-Size Independent Approach for Multidisciplinary Sensitivity Analysis and Design Optimization," AIAA Paper 99-3101, June 1999.

[29]Nielsen, E.J., and Anderson, W.K., "Aerodynamic Design Optimization on Unstructured Meshes Using the Navier-Stokes Equations," AIAA Paper 98-4809, September 1998.

[30]Nielsen, E.J., "Aerodynamic Design Sensitivities on an Unstructured Mesh Using the Navier-Stokes Equations and a Discrete Adjoint Formulation," Ph.D. Thesis, Virginia Polytechnic Institute and State University, Dec. 1998.

[31]Nielsen, E.J., Anderson, W.K., and Kaushik, D.K., "Implementation of a Parallel Framework for Aerodynamic Design Optimization on Unstructured Meshes," Paper presented at Eleventh International Parallel CFD Conference, May 1999.

[32]Pirzadeh, S., "Viscous Unstructured Three-Dimensional Grids by the Advancing-Layers method," AIAA Paper 94-0417, January 1994.

[33]Reuther, J., Jameson, A., Farmer, J., Martinelli, L., and Saunders, D., "Aerodynamic Shape Optimization of Complex Aircraft Configurations via an Adjoint Formulation," AIAA Paper 96-0094, January 1996.

[34]Samareh, J., "Geometric Modeling and Grid Generation for Design and Optimization," ICASE/LaRC/NSF/ARO Workshop on Computational Aerosciences in the 21st Century, April 22-24, 1998.

[35]Schmitt, V., and Charpin, F., "Pressure Distributions on the ONERA-M6 Wing at Transonic Mach Numbers," Experimental Data Base for Computer Program Assessment, AGARD-AR-138, May 1979, pp. B1-1-B1-44.

[36]SF_6. SFBR-1, Allied Chemical Corp., c. 1976.

[37]Sherman, L.L., Taylor, A.C., Green, L.L., Newman, P.A., Hou, G.J.-W., and Korivi, V.M., "First- and Second-Order Aerodynamic Sensitivity Derivatives via Automatic Differentiation with Incremental Iterative Methods," AIAA Paper 94-4262, September 1994.

[38]Soemarwoto, B., "Multipoint Aerodynamic Design by Optimization," Ph.D. Thesis, Delft University of Technology, Dec. 1996.

[39]Spalart, P.R., and Allmaras, S.R., "A One-Equation Turbulence Model for Aerodynamic Flows," AIAA Paper 92-0439, January 1991.

[40]Squire, W., and Trapp, G., "Using Complex Variables to Estimate Derivatives of Real Functions," *SIAM Review*, Vol. 10, No. 1, March 1998, pp. 110-112.

[41]Wrenn, G.A., "An Indirect Method for Numerical Optimization Using the Kresselmeier-Steinhauser Function," NASA CR 4220, March 1989.

Comparisons with ADIFOR

One of the most recently developed techniques for obtaining discretely consistent sensitivity derivatives from complicated engineering codes is ADIFOR (Automatic Differentiation for FORtran).[9] ADIFOR is a precompiler that accepts an existing code as input and creates new source code with necessary modifications for computing sensitivity derivatives. Because complex variables and ADIFOR can both produce sensitivity derivatives which are discretely consistent with the flow solver, it is useful to attempt a comparison.

A two-dimensional inviscid version of the current unstructured mesh methodology has been precompiled using ADIFOR and comparisons are made with the complex-variable approach. The geometry is a NACA 0012 airfoil at a Mach number of 0.8 and an angle of attack of 1.25°. For this study, only the free-stream Mach number is considered as a design variable and the only two sensitivity derivatives of interest are for the lift and drag coefficients. In Table 6, the derivatives obtained using complex variables, ADIFOR, and the adjoint formulation are compared with each other as well as with a central difference formula. As seen in the table, complex-variables, ADIFOR, and the adjoint method all give identical results whereas the derivatives obtained using finite differences show some sensitivity to the step size. Also, note that in this case, the step size that yields the highest accuracy is 1×10^{-6}. This is in contrast to the example shown in Figs. 3 and 4 where a step size of 1×10^{-5} gave the best results in terms of accuracy.

In Table 7, a comparison of several features of the complex-variable approach and ADIFOR is made. In this table, the column marked as CV denotes the complex-variable approach and AD denotes ADIFOR. In each column, a check mark indicates an advantage for the method denoted at the top of the column. If both columns contain a check mark, then neither the complex-variable approach nor ADIFOR have a clear advantage over the other. In general, the complex-variable approach compares quite favorably to ADIFOR, and actually holds the advantage in most areas. The largest advantages of the complex-variable approach over ADIFOR are that it requires very little "training" and that the resulting code is easy to read and therefore easy to maintain. In addition, although the complex-variable approach requires editing of the computer code, ADIFOR usually requires code modifications to the source in order to be successfully precompiled. In this area, both approaches suffer from the possibility of introducing new errors into an existing (and presumably debugged) code. In comparing the execution times, the complex-variable approach will require an essentially fixed cost for each design variable. The cost for ADIFOR, however, appears to be most expensive when considering a single design variable. The execution time using ADIFOR improves as more design variables are added. However, with ADIFOR, the memory increases linearly with the addition of new design variables whereas for the complex-variable approach, the memory is fixed.

While the complex-variable approach has several advantages over ADIFOR, the latter approach has the very significant advantage of extensibility to C programs and reverse mode differentiation. Because the C programming language does not have a native complex data type, incorporating the complex-variable approach into a C code would require additional coding. The largest advantage for ADIFOR over the complex-variable method is that there is a related effort to produce reverse mode differentiation through ADJIFOR.[11] The complex-variable approach does not offer this capability.

Table 6 Derivatives of lift and drag coefficients with respect to Mach number using various techniques.

Methodology	$\frac{\partial C_l}{\partial M_\infty}$	$\frac{\partial C_d}{\partial M_\infty}$
Complex Variable	2.576118	0.5683333
ADIFOR	2.576118	0.5683333
Adjoint	2.576118	0.5683333
Finite Difference $h = 1 \times 10^{-4}$	2.515242	0.5642697
Finite Difference $h = 1 \times 10^{-5}$	2.474685	0.5630385
Finite Difference $h = 1 \times 10^{-6}$	2.576150	0.5683350

Table 7 Comparison between complex-variable approach and ADIFOR.

	CV	AD	Comments
Restart capability	✓		AD does not maintain derivative history. Automatically taken into account by complex approach.
Code ownership	✓		AD license requires that permission be obtained to distribute code once it has been precompiled.
Learning curve	✓		Subjective, although "verified" by several researchers with knowledge of both CV and AD.
Modification for new design variables and outputs	✓		AD requires reprocessing. CV only requires that the complex part of the quantity be printed.
Speed of execution	✓	✓	For small numbers of design variables, CV appears faster. With increasing design variables, ADIFOR cost amortized.
Memory	✓		Memory for CV fixed. Increases linearly with design variables for AD.
Maintenance	✓		CV code essentially identical to the baseline version. AD very difficult to read.
Time to develop derivative versions	✓	✓	Depends on length of code for CV. AD may require extensive code preparation for successful precompiling.
Extensibility		✓	AD offers upgrade path to ADIC and ADJIFOR. CV offers no real path to reverse mode differentiation.
Accuracy of derivatives	✓	✓	Both techniques can provide machine levels of accuracy.

evaluations can lead to large errors in the derivatives because of the division by h^2.

Second derivatives have been obtained for the geometry shown in Fig. 14. In this figure, 39 B-spline control points are used to describe the initial geometry. All of the control points are depicted as open circles with the "active" control points shown as filled circles. In this figure, a few numbers have been placed above selected control points for reference purposes. The flow conditions for this inviscid case are a free-stream Mach number of 0.72 and an angle of attack of 1°. The cost function is associated with attempting to obtain a specified pressure distribution and is given by

$$I = \oint_{\Gamma} \frac{1}{2}(C_p - C_p^*)^2 ds \tag{10}$$

where the integral is taken over the surface of the airfoil, C_p is the pressure coefficient on the airfoil, and C_p^* is the desired, or target, pressure coefficient. Here, the initial and target pressure distributions are shown in Fig. 15.

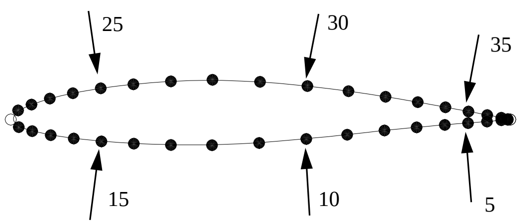

Figure 14. Initial geometry used for obtaining second derivatives.

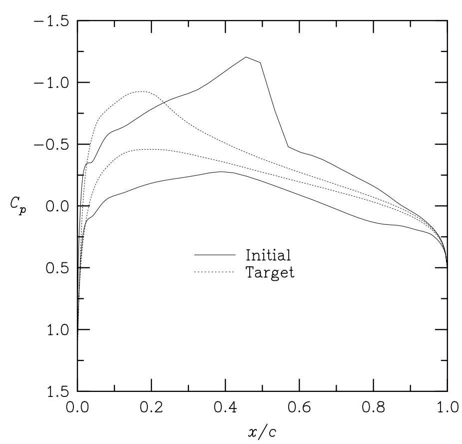

Figure 15. Initial and target pressure distributions.

A plot depicting the second derivatives of the cost function with respect to each of the design variables is shown in Fig. 16. Here, the design variable is the y-position of each of the control points shown as filled circles in Fig. 14. Second derivatives are shown which have been obtained using 3 step sizes ranging over 3 orders of magnitude. Although no cross derivative information is available, it can be seen using Figs. 14, 15 and 16 that the curvature of the design space is much higher in the vicinity of the leading edge of the upper surface than it is away from this region. In fact, the highest curvature, which is associated with design variable number 24, is about 100 times as high as the lowest curvature located at design variable 28. The area where the curvature is the highest is where supersonic flow is present.

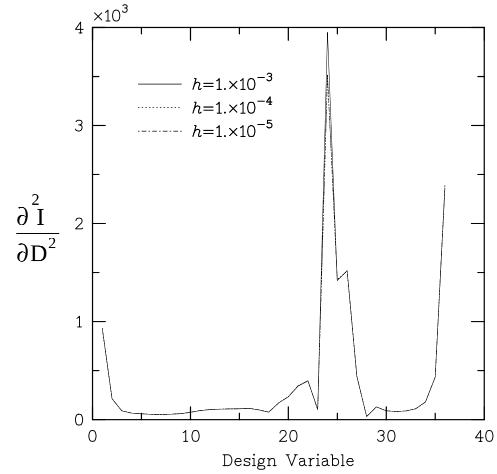

Figure 16. Second derivatives for each design variable.

A comparison of second derivatives which have been obtained using both complex variables and finite differences is shown in Table 5. In this table, second derivatives of the cost function with respect to design variables 10, 25, and 30 are shown for 3 different step sizes. As seen in the table, both complex variables and finite differences give similar approximations to the derivatives and both approaches exhibit some sensitivity to the step size.

In an attempt to accelerate the convergence of the design process, the diagonal contributions obtained at the beginning of the design have been used as the initial approximation to the Hessian needed for the quasi-Newton method outlined in Ref. 41. Although not shown, no significant improvement in the reduction of the cost function was obtained when compared to using the identity matrix as the initial guess for the Hessian.

Table 5 Comparison of second derivatives obtained using complex variables and finite differences.

Design Variable	Step Size	Complex Variables	Finite Difference
10	1×10^{-5}	74.8455	74.7628
	1×10^{-4}	74.7929	74.7924
	1×10^{-3}	74.7765	74.8087
25	1×10^{-5}	1429.49	1428.64
	1×10^{-4}	1429.35	1429.56
	1×10^{-3}	1418.76	1435.73
30	1×10^{-5}	91.2012	91.1143
	1×10^{-4}	91.1459	91.1466
	1×10^{-3}	91.0860	91.2058

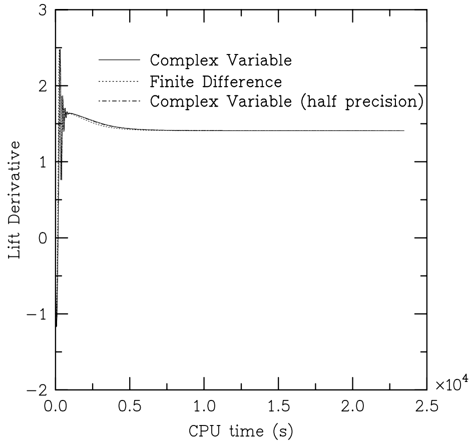

Figure 11. Computer time to obtain lift derivative for camber #4.

Two-Dimensional Flow for a Complicated Equation of State

The next example is for the flow over an airfoil in a non-ideal gas. The purpose is to demonstrate the versatility of the complex-variable approach in determining sensitivity derivatives of very complicated functions. In this case, the complexity enters through the fact that the gas, sulfur hexafluoride, is neither thermally nor calorically perfect. The equation of state for sulfur hexafluoride is given as[36]

$$p = \frac{RT}{v-d} + \sum_{i=2}^{5} \frac{a_i + b_i T + c_i e^{-kT/T_c}}{(v-d)^i} \qquad (8)$$

where R is the specific gas constant, T is the temperature, T_c is the temperature at the critical point, v is the specific volume and the remainder of the terms are constants. To determine the pressure at each iteration of the solution process, the temperature is first determined by solving the following non-linear equation at each point for the local temperature

$$\varepsilon(T, v) = \varepsilon^{\circ}(T, v^{\circ}) + \sum_{i=2}^{5} \frac{a_i + [1 + (kT/T_c)c_i e^{-kT/T_c}]}{(i-1)(v-d)^{i-1}} \qquad (9)$$

In this equation, ε is the actual internal energy and ε° is the ideal gas internal energy which is only a function of temperature. Equation (9) is solved at each mesh point using several iterations of Newtons method. Note that unlike an ideal gas, the solution for a real gas depends on the free-stream reference pressure in addition to the Mach number and Reynolds number.

For this computation, the flow solver has been modified to include two "equivalent" γ's as described in Ref. 16. One of these is associated with the pressure at each point in the flowfield while the other is for the speed of sound. The process required to account for the real gas effects is similar to that needed for other thermodynamic models such as equilibrium air. It should be pointed out that the modifications to the code that are required to get the derivatives using the complex-variable approach took only a single day, including the thermodynamics and turbulence models. This is due to the fact that the only real modifications required were to declare the floating point variables in these routines as complex.

In Fig. 12, the computed pressure distribution is compared with experimental data from Ref. 1 for a free-stream Mach number of 0.7, an angle of attack of 1°, a Reynolds number of 30×10^6 based on the chord of the airfoil and a reference pressure of 3.34 atmospheres. The mesh used for the computation contains 38,637 nodes with a normal spacing at the wall of 1.0×10^{-6}.

As noted earlier, the results for a real gas depend on the free-stream pressure so that the lift and drag coefficients will change in response to changes in the free-stream reference value. Using a forward-difference formula with a step size of 1×10^{-5}, the derivatives of the lift and drag coefficients with respect to changes in the free-stream pressure are -6.600×10^{-4} and -6.400×10^{-6} respectively. The corresponding values obtained using the complex-variable approach are -6.606×10^{-4} and -6.404×10^{-6}. Contours of the sensitivity derivatives of Mach number with respect to the free-stream pressure are shown in Fig. 13. As expected, the effect of changing the free-stream pressure is most strongly felt in the region of the shock near the leading edge of the airfoil.

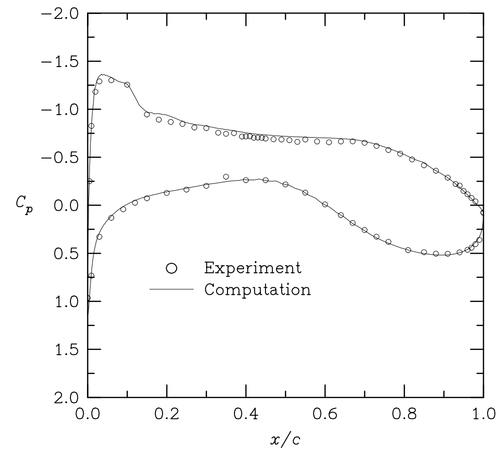

Figure 12. Pressure distribution for sulfur hexafluoride; $M_\infty = 0.7$**,** $\alpha = 1^{\circ}$**,** $Re = 30 \times 10^6$**,** $p_\infty = 3.34$ **atm.**

Figure 13. Sensitivity derivatives of Mach number with respect to free-stream pressure.

Obtaining Second Derivatives Using Complex Variables

In Eq. (6), a formula for obtaining second derivatives is given which requires no additional computations over those required for obtaining first derivatives. In this formula however, it is apparent that the determination of second derivatives will be susceptible to subtractive cancellation error. In addition, unconverged function

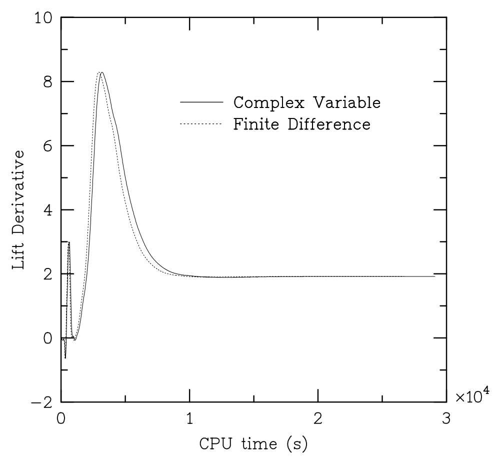

Figure 8. Computer time required to obtain lift derivative for point B.

Three-Dimensional Turbulent Flow over an ONERA M6 Wing

Three-dimensional results have been obtained for turbulent flow over the ONERA M6 wing[35] depicted in Fig. 9. The mesh has been generated using the methodology described in Ref. 32 and contains 16,391 nodes and 90,892 tetrahedra. This mesh is obviously too coarse for accurate resolution of the physics but the flow solvers can easily be run to machine zero, which is necessary to verify the accuracy of the derivatives. The flow conditions for this case are a free-stream Mach number of 0.3, an angle of attack of 2.0°, and a Reynolds number of 5×10^6 based on the mean aerodynamic chord. The geometry has been parameterized using the free-form deformation technique described in Ref. 34, although the control points in the B-spline net have been further grouped into more intuitive design variables as shown in Fig. 10.

A comparison of sensitivity derivatives obtained using finite differences, the adjoint methodology, and complex variables is shown in Table 4. The step sizes used for these results are the same as those used for the two-dimensional cases: 1×10^{-5} for finite differences and 1×10^{-7} for the complex variables. As in the two-dimensional case, the derivatives obtained with the adjoint and complex-variable approaches are in excellent agreement whereas slight discrepancies are evident in the finite-difference results.

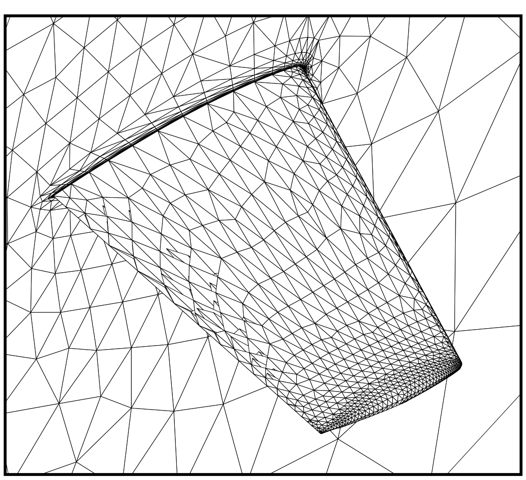

Figure 9. Grid used for assessment of three-dimensional design sensitivities.

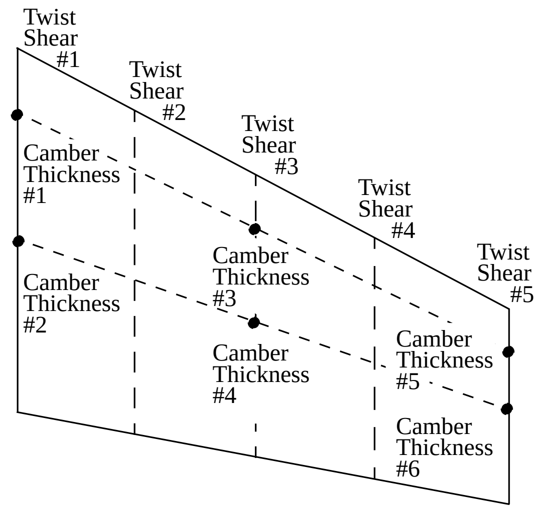

Figure 10. Location of design variables for wing.

Table 4 Comparison of derivatives for three-dimensional wing

Design Variable	Finite Difference	Adjoint	Complex Variables
Camber #4	1.409643	1.409592	1.409592
Thickness #3	0.041174	0.041195	0.041194
Twist #3	-0.010392	-0.010372	-0.010372
Shear #3	0.045804	0.045844	0.045844

As with the two-dimensional results, a comparison has also been made of the computer time required to obtain a derivative using the complex-variable approach and a central-difference formula. In this test, the design variable is the fourth camber variable shown in Fig. 10. Figure 11 depicts the comparison in computer times for both the complex-variable approach and the use of finite differences. As seen, the timing between the two approaches is comparable so that the cost of the complex-variable approach is similar to that of a central-difference approximation to the derivative.

As previously mentioned, the use of complex variables increases the memory requirement of the code by approximately a factor of two because of the complex declaration of the floating point variables. For three-dimensional computations, this could place an unwanted restriction on the size of the problem. In order to mitigate the penalty of extra memory, the flux Jacobians have been stored using “half precision” so that 32 bits are used for both the real and imaginary parts; i.e. 64 total bits are used to store each contribution to the flux Jacobian. Because the Jacobians are responsible for the largest amount of storage in the code, the use of half-precision Jacobians yields approximately 32% savings over storing the Jacobians with full precision. In terms of computer time, Fig. 11 indicates that the use of half precision Jacobians has not yielded any significant savings. Note that the use of half precision Jacobians could also have been used for the baseline flow solver so that a similar savings in memory could be realized. In this case, of course, the complex version of the code still requires about twice the memory of the baseline flow solver.

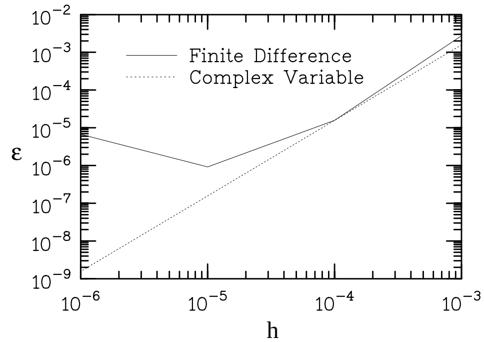

Figure 3. Errors in derivatives of lift coefficient due to step size.

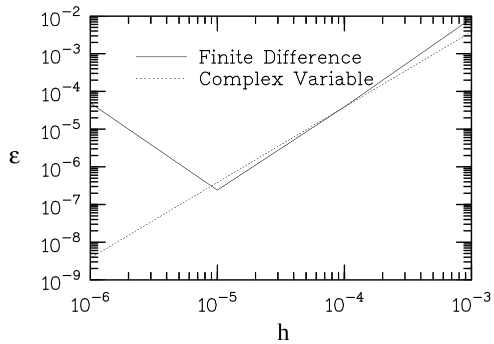

Figure 4. Errors in derivatives of drag coefficient due to step size.

approach and a central-difference technique. The design variable used for this study is point B shown in Fig. 2 and all runs have been started using free-stream values so that each case begins at a common datum. It is apparent that the cost of the complex-variable approach is almost identical to that of a central-difference approximation to the derivative. However, while the cost of the central-difference formula is fixed at twice that of a single flow solution, the actual cost of the complex-variable approach depends somewhat on the computer code, the compiler, and hardware considerations such as cache size. In practice, the computer times for the complex-variable approach range from 2-3.5 times that of the original flow solver. In addition, because of the complex declaration of the floating point variables, the memory for the complex-variable version of the code is roughly twice that of the baseline flow solver. In this regard, the complex-variable approach does not offer a saving of resources when compared to using finite-differences. The primary advantage of the complex-variable approach over the use of finite-differences is through the accuracy of the resulting derivatives. However, although the step size chosen for the finite-difference approximation yields accurate results for the current design variables, it has been observed in practice that different design variables may require different step sizes in order to achieve accurate derivatives. In this regard, the use of complex variables offers a significant advantage over finite-differences because the step size can be chosen based on accuracy requirements without concern for subtractive cancellation errors.

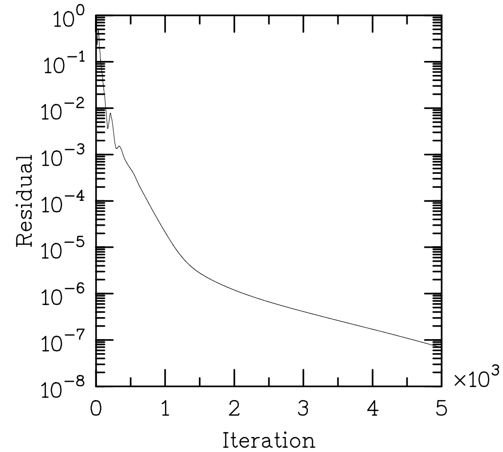

Figure 5. Residual history for transonic airfoil.

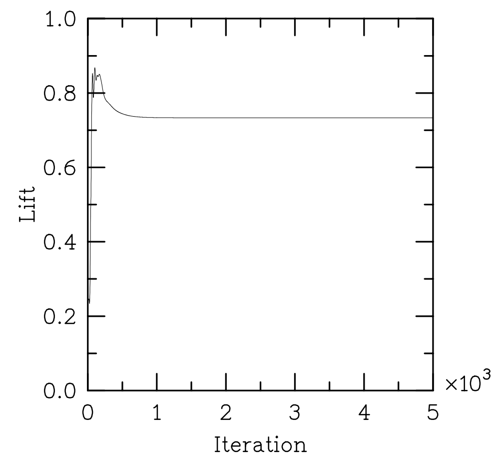

Figure 6. Lift history for transonic airfoil.

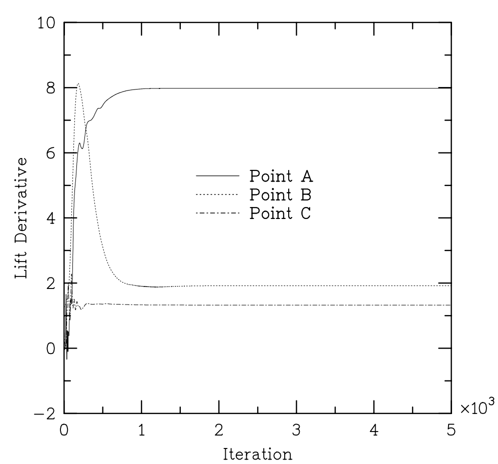

Figure 7. History of lift derivatives for transonic airfoil.

Two-Dimensional Transonic Turbulent Flow Over an Airfoil

The first case presented is for a transonic flow over the RAE 2822 airfoil.[12] The free-stream Mach number is 0.75 while the angle of attack and Reynolds number are 2.81° and 6.2 million respectively. The mesh has been generated using the program described in Ref. 24 and contains 14,127 nodes with a wall spacing of 1×10^{-5}. The computed pressure distribution is shown in Fig.1 along with the experimental data taken from Ref. 12. For this case, a shock is present on the upper surface of the airfoil which leads to a region of separated flow immediately aft of the shock.

For demonstrating the accuracy of the derivatives obtained using the complex-variable approach, comparisons are made with results obtained using finite differences as well as the adjoint approach described in Refs. 3, 4, 29, and 30. In the results shown below, the geometry of the airfoil has been described using a third-order B-spline, where the location of the defining control points are shown as circles in Fig. 2.

Derivatives of the lift and drag coefficients have been obtained with respect to the vertical positions of the three control points shown as solid circles in Fig. 2. In Tables 1 and 2, the sensitivity derivatives obtained using the complex-variable approach are compared with those obtained using both finite differences as well as the adjoint approach. For the finite-difference method, a step size of 1×10^{-5} is used and has been chosen based on the results of an accuracy study shown later. The step size used for the complex-variable method is 1×10^{-7} so that the resulting derivatives should be accurate to approximately machine precision. As seen in the tables, the agreement between the adjoint and complex-variable approaches is excellent.

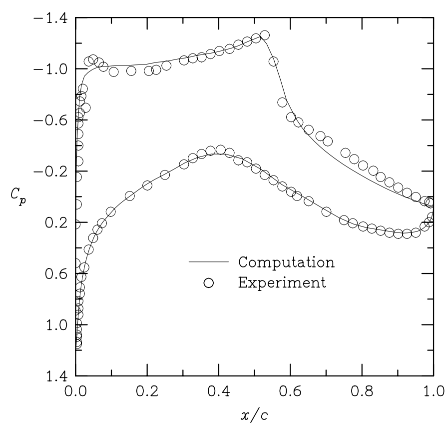

Figure 1. Pressure distribution for transonic RAE 2822.

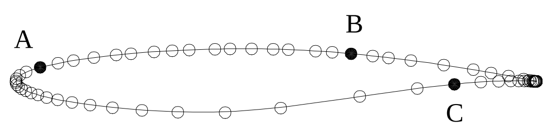

Figure 2. Design variables for RAE 2822.

The finite-difference results shown in Tables 1 and 2 differ somewhat from the derivatives obtained using both the adjoint and complex-variable approaches. In the finite-difference results, the largest errors appear in the derivatives with respect to control point B. Here, the lift and drag derivatives differ from the complex-variable and adjoint approaches by about 0.15% and 0.3% respectively. However, results are shown in Table 3 which indicate that for this design variable, the finite-difference derivatives are dependent on the step size.

Table 1 Sensitivity derivatives for lift coefficient for RAE 2822

Design Variable	Finite Difference	Adjoint	Complex Variables
Point A	7.98260	7.98144	7.98143
Point B	1.92469	1.92185	1.92185
Point C	1.32831	1.32826	1.32826

Table 2 Sensitivity derivatives for drag coefficient for RAE 2822

Design Variable	Finite Difference	Adjoint	Complex Variables
Point A	-0.273960	-0.273954	-0.273954
Point B	-0.031486	-0.031580	-0.031580
Point C	0.100724	0.100713	0.100714

Table 3 Sensitivity of finite-difference derivatives to step size for point B

	Step Size		
	1×10^{-6}	1×10^{-5}	5×10^{-5}
Lift Derivative	1.91870	1.92469	1.91501
Drag Derivative	-0.026180	-0.031486	-0.031911

Figures 3 and 4 show the errors in the derivatives of the lift and drag coefficients with changing step sizes obtained using both finite differences and the complex-variable formulation. Here, the error is defined as

$$\varepsilon = \log\frac{(\varphi - \varphi_C)}{\varphi_C} \tag{7}$$

where φ is the derivative determined using the current step size parameter and φ_C is the derivative obtained using the complex-variable approach with a step size of 1×10^{-7}. It is apparent that the accuracy of the finite-difference formulation depends on the step size and does not recover second-order accuracy as the step size is reduced; this behavior is due to subtractive cancellation error. With the complex-variable approach, the accuracy of the derivatives is increased by two digits each time the step size is lowered one order of magnitude, thus demonstrating that the complex-variable approach recovers true second-order accuracy and is not susceptible to subtractive cancellation errors.

The iterative convergence history for the residual, the lift coefficient, and the derivatives of the lift coefficient are shown in Figs. 5, 6, and 7, respectively. Note that only the first 5000 iterations have been shown although the results have been run to machine zero. From the figures, it is evident that the residual is reduced by approximately five orders of magnitude in about 1000 iterations, at which point the lift coefficient is converged to 4 digits of accuracy. It can be seen in Figs. 6 and 7 that the convergence of the derivatives resembles that of the lift history in that when the lift coefficient is converged, the derivatives are also converged. Although not shown, the convergence of a central-difference approximation converges in a similar manner.

In terms of computer time, Fig. 8 depicts the lift coefficient as a function of computer time for both the complex-variable given in Ref. 27 where an inviscid flow solver has been coupled with a structural analysis code for obtaining multidisciplinary sensitivity derivatives. It has been demonstrated in this reference that accurate aero-structural sensitivity derivatives can be obtained with minimal changes to the existing analysis codes. The complex variable approach has been further applied for aero-structural sensitivity analysis in Ref. 28.

The purpose of the present paper is to extend the work described in Ref. 27 to obtaining sensitivity derivatives for turbulent flows. In addition, several features, as well as drawbacks, of this approach will be more clearly discussed and demonstrated.

The current approach uses complex variables to aid in the determination of the derivatives. The resulting information includes the discretely consistent derivatives of all the flow variables with respect to the design variables similar to that obtained using either finite differences or automatic differentiation. However, unlike finite differences, the present approach is not subject to subtractive cancellation errors. Also, the computer code does not require preprocessing with an automatic differentiation procedure so the resulting code is virtually identical to the original code. This feature enables easy maintenance of the resulting software.

Complex-Variable Approach for Sensitivity Derivatives

The simplest, and perhaps most commonly used method for obtaining derivatives is a central-difference approach:

$$\frac{df}{dx} = \frac{f(x+h) - f(x-h)}{2h} + \vartheta(h^2) \tag{1}$$

where f is the function of interest, x is the independent variable, and h is a small perturbation parameter. The use of Eq. (1) simply requires that the function be evaluated at two nearby states and the results subtracted. This feature is very attractive when the function is sufficiently complicated that obtaining an analytic derivative is cumbersome and error-prone. In addition, when used in the context of obtaining derivatives for cost functions that depend on the solution of the Navier-Stokes equations, the above procedure is particularly attractive because it does not require any modifications to existing computer codes. However, the drawback of this technique is that it is prone to subtractive cancellation errors. While it is desirable to use a step size as small as possible to minimize the truncation error, too small of a step size can lead to errors in the derivatives caused by subtractive cancellation of the terms in the numerator of Eq. (1). As a result of having to adjust the step size in order to obtain accuracy while at the same time minimizing subtractive cancellation errors, it is not unusual that this technique requires a different step size for each design variable. In addition, with a small step size, the solution to the Navier-Stokes equations must be very well converged so that the cost function can be evaluated with sufficient precision.

In the complex-variable approach, a series expansion is also used with the exception that a complex perturbation is taken

$$f(x+ih) = f(x) + ih\frac{df}{dx} - \frac{h^2}{2}\frac{d^2f}{dx^2} - \frac{ih^3}{6}\frac{d^3f}{dx^3} + \frac{h^4}{24}\frac{d^4f}{dx^4} + \dots \tag{2}$$

The real and imaginary parts of this equation yield

$$\mathrm{Im}(f(x+ih)) = h\frac{df}{dx} - \frac{h^3}{6}\frac{d^3f}{dx^3} + \vartheta(h^5) \tag{3}$$

$$\mathrm{Re}(f(x+ih)) = f(x) - \frac{h^2}{2}\frac{d^2f}{dx^2} + \vartheta(h^4) \tag{4}$$

From Eqs. (3) and (4), the first and second derivatives may be obtained as

$$\frac{df}{dx} = \frac{\mathrm{Im}(f(x+ih))}{h} + \vartheta(h^2) \tag{5}$$

$$\frac{d^2f}{dx^2} = \frac{2[f(x) - \mathrm{Re}(f(x+ih))]}{h^2} + \vartheta(h^2) \tag{6}$$

From Eq. (5), it is apparent that obtaining the derivative using the complex-variable approach does not involve subtracting the values of two functions. This feature is one of the primary advantages of the complex-variable approach because it eliminates any concerns about subtractive cancellation errors. The advantage of this property has been demonstrated in Ref. 27 where aero-structural sensitivity derivatives have been obtained using both finite differences as well as the complex-variable approach. In this reference, it is demonstrated that the finite-difference approach is sensitive to the step size while for the complex-variable approach, two decimal places of accuracy are obtained each time the step size is reduced by an order of magnitude.

To incorporate the complex-variable approach into an existing flow solver, the only requirement is that the floating point variables be declared as complex and a complex perturbation be added to the design variable of interest. The resulting flow solver is then run and the derivatives of any function dependent on the flow solution is determined by examining the complex part divided by the step size (see Eq. (5)). However, there are several functions such as `min()`, `max()`, and `abs()` that require some care in order to evaluate correctly for complex arguments. In most cases though, the transformation of the basic code into a complex version can be accomplished in a very short time (usually a single day). The resulting code is virtually identical to the initial code and is therefore easy to follow and easy to maintain; each time a new routine is added to the flow solver, a similar one is added to the complex version.

Note that during the course of a design, the basic flow solver would be employed the majority of the time. Therefore, the unperturbed function evaluation, $f(x)$, is available at all points visited in the design space. When the complex version of the flow solver is then run to obtain derivatives, the real part of this solution can be used in Eq. (6) to obtain second derivatives. These derivatives may be used for the diagonal contributions to the Hessian and are obtained without additional cost. However, this computation is prone to cancellation errors.

There are two primary disadvantages in applying the complex-variable approach for obtaining sensitivity derivatives. The first is that the required memory essentially doubles due to the use of complex declarations of the floating point variables. Secondly, the execution time is increased over the original flow solver. Both of these issues will be further addressed in a later section.

Results

In this section, some initial results for obtaining sensitivity derivatives for turbulent flows are demonstrated. The flow solver used for all of the results given below is an unstructured, implicit, upwind scheme described in Refs. 2 and 6. The turbulence model of Spalart and Allmaras[39] is used for determining the eddy viscosity.

Sensitivity Analysis for the Navier-Stokes Equations on Unstructured Meshes Using Complex Variables

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Abstract

The use of complex variables for determining sensitivity derivatives for turbulent flows is examined. Although a step size parameter is required, the numerical derivatives are not subject to subtractive cancellation errors and therefore exhibit true second-order accuracy as the step size is reduced. As a result, this technique guarantees two additional digits of accuracy each time the step size is reduced one order of magnitude. This behavior is in contrast to the use of finite differences, which suffer from inaccuracies due to subtractive cancellation errors. In addition, the complex-variable procedure is easily implemented into existing codes.

Introduction

There are currently several ongoing efforts to develop aerodynamic design optimization techniques using the Navier-Stokes equations (see e.g. Refs. 3, 4, 14, 19, 20, 25, 29, 30 and 38). Many of the prominent techniques being utilized are gradient-based methodologies in which a specific cost function is minimized subject to both geometric and flow-field related constraints. A primary requirement of these techniques is the determination of the gradients of the cost function and the constraints with respect to the design variables. These gradients are subsequently used to reduce the cost function in a systematic manner while not violating the constraints.

The techniques available for obtaining sensitivity derivatives can be generally classified into either direct or adjoint methodologies. Both techniques can be further divided into either discrete or continuous approaches. More information on these techniques can be found in Refs. 3-5, 7-11, 13-15, 17-21, 25-30, 33, 37, and 38.

The direct approach, which includes techniques such as finite differencing, forward differentiation,[9] and sensitivity equations,[10] yields the most information in that the derivatives of all of the flow variables in the domain are obtained with respect to each design variable. The derivatives of the cost function, as well as any constraints which depend on the flow variables, may then be obtained using these quantities. The primary advantage of the direct approach is that the derivatives of all quantities that depend on the flowfield can be obtained. The disadvantage of this approach is that the procedure must be repeated for each design variable separately. For cases in which there are many design variables, this can be prohibitively expensive.

The other methodology which has received much attention is the adjoint approach. Here, an adjoint system of equations is solved and the results are then used to determine the sensitivity derivatives. This approach has an advantage over the direct approach in that after the solution of the adjoint equations is obtained, the derivatives of the cost function with respect to all the design variables can be evaluated with the same operation count as a single matrix-vector product where the size of the matrix is determined by the number of design variables. Provided that the cost of the matrix-vector product is not large, the adjoint approach can yield a significant savings over the direct approach when there are many design variables. The disadvantage of this approach, however, is that an adjoint equation must be solved for each flow-field constraint so that if there are many such constraints, this technique is very expensive.

The choice of either the direct or adjoint approach depends on the problem at hand and it is likely that both approaches will contribute significantly to design efforts underway. In addition, Hessian information can be obtained in an efficient manner by combining both techniques.[21,37] Therefore, it is desirable to have both direct and adjoint techniques available.

In Refs. 3, 4, 29, 30, and 31 an adjoint approach has been described for obtaining sensitivity derivatives for turbulent flows on unstructured meshes. In these references, two- and three-dimensional flow solvers have been accurately differentiated for both compressible and incompressible flows. The focus of the present study is to develop an approach for obtaining the derivatives which is equivalent to direct differentiation.

In the 1960's, Lyness[22] and Lyness and Moler[23] suggested that complex variables be more prominently utilized in the development of numerical algorithms. One of the techniques demonstrated in these references was the determination of numerical derivatives for complicated functions. The resulting technique is very general, easy to apply, and is not sensitive to subtractive cancellation errors that often arise in finite differencing. To date, this technique has not been widely exploited and has only recently been reviewed in Ref. 40 for determining derivatives for functions of a single variable.

Although this technique offers much potential for simplifying the computation of derivatives such as flux Jacobians or in performing matrix-vector products using only function evaluations, perhaps the largest benefit to be gained is in the differentiation of entire codes used for analysis purposes, so that discretely consistent derivatives can be obtained.

The first use of this technique for large-scale computations is

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