Multidisciplinary Sensitivity Derivatives Using Complex Variables

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Abstract

A new method for computing single and multidisciplinary sensitivity derivatives using complex variables has been developed. Extremely accurate derivatives are computed from high fidelity aerodynamic, structural, and aero-structural analyses. This report briefly reviews the various techniques to obtain single discipline sensitivity derivatives and how they may be used to evaluate multidisciplinary derivatives. The advantages and disadvantages of the complex variable approximation are compared with these existing techniques. It is shown that this new method has all the advantages of existing direct-discrete approaches and the finite-difference approximation, while avoiding some of their shortcomings. In addition, existing software can be easily modified to incorporate this technique, which makes it a valuable tool for multidisciplinary applications. To demonstrate the accuracy of the complex variable approximation, a low aspect ratio ONERA M6 wing, that has been used in previous optimization studies, is examined. Aerodynamic, structural, and aero-structural sensitivity derivatives have been computed for a variety of design variables. Design variables appropriate for both aerodynamic and structural optimization have been selected.

Introduction and Background Remarks

Numerical optimization procedures are based on mathematical techniques for finding the extremum of an objective function subjected to various constraints. When the costs associated with evaluating the objective function and constraints are excessive (as in the case of nonlinear aerodynamic analyses), zeroth-order methods are usually prohibitively expensive and, thus, gradient-based design optimization procedures are frequently adopted. These procedures require the gradients of the objective function and constraints (dependent variables) with respect to the shape-design (independent) variables. These gradients, commonly referred to as sensitivity derivatives, provide the mechanism for changing the design variables to improve the objective function without violating the given constraints.

In the mid 1970s, researchers began exploring the use of numerical optimization techniques for the design of aircraft components. These early studies primarily focused on airfoil and wing design using low fidelity fluid models for the analyses and finite-difference calculations for gradient information. The inability of these fluid models to accurately predict nonlinear phenomena limited their applicability. By the mid 1980s, computational resources were available that permitted aerodynamic simulations using the higher fidelity Euler and Navier-Stokes equations about isolated components and moderately complex configurations. Then Sobieski[37] challenged the aerodynamics community to extend these algorithms to include the shape sensitivity analysis for the geometry. This plea ignited studies aimed at developing methods that would allow for the use of nonlinear aerodynamics in shape optimization. A review on the early aerodynamic shape optimization work has been reviewed by Labrujere and Sloof[22] and a concise review on the use of sensitivity analysis in aerodynamic shape optimization has been reported by Taylor et al.[43] and by Newman et al.[29] A recent paper by Jameson[19], furthermore, delineates the evolution of computational fluid dynamics as a design tool.

For aerodynamic optimization, the state equation is a system of nonlinear partial differential equations (PDE) expressing the conservation of mass, momentum, and energy. Differentiation of the system of PDE (i.e., sensitivity analysis) can be performed at one of two levels. In the first method, termed the continuous or variational approach, the PDE are differentiated prior to discretization, either directly or by introducing Lagrange multipliers which are defined as a set of continuous linear equations adjoint to the governing PDE. Subsequently, these directly differentiated or adjoint equations are discretized and solved. In the second method, termed the discrete approach, the PDE are differentiated after discretization. The discrete approach may also be cast in either a direct or an adjoint formulation, and the reader should refer to Hou et al.[17] for a comprehensive presentation of both discrete formulations. For more detailed recent discussions of the continuous approaches to aerodynamic design optimization, the interested reader is directed, for example, to Refs. 4, 7, 18, 20, and 35 for the adjoint formulations and to Ref. 9 for the direct formulation.

The task of constructing exactly or analytically all of the required linearizations and derivatives by hand for either the direct or adjoint approach and then building the software for evaluating these terms can be extremely tedious. This problem is compounded by the inclusion of even the most elementary turbulence model (for viscous flow) or the use of a sophisticated grid generation package for adapting (or regenerating) the computational mesh to the latest design. One solution to this problem has been found in the use of a technique known as automatic differentiation. Application of this technique to an existing source code, that evaluates output functions, automatically generates another source code that evaluates both output functions and derivatives of those functions with respect to specified code input or internal parameters. A precompiler software tool, called ADIFOR (Automatic Differentiation of FORtran, Bischof et al.[8]), has been developed and utilized with much success to obtain complicated derivatives from advanced CFD and grid generation codes, for use within aerodynamic design optimization procedures.[12,13,42,44] The use of ADIFOR produces code that, when executed, evaluates these derivatives of the output functions via a discrete-direct approach, referred to as forward-mode automatic differentiation. More recently, automatic differentiation software has emerged that enables the derivatives to be evaluated with a discrete-adjoint approach.[10,25] This type of automatic differentiation is known as reverse-mode.[26]

The best known method for computing the sensitivity information between coupled systems is via the solution of the global sensitivity equations derived by Sobieski.[39] This system of equations, which is obtained by directly differentiating the state vector of each discipline, may sometimes be ill-conditioned and the memory requirements associated with the storage of the coefficient matrix may be prohibitive. The ill-conditioned global sensitivity equations, as well as those associated with higher-order spatially accurate aerodynamic sensitivity analysis, may be reformulated and solved by the incremental iterative technique.[21,32] The incremental iterative technique allows the linear sensitivity equations to be solved iteratively where the coefficient matrix may be any convenient approximation that will converge the system. This allows a better conditioned, and reduced memory requirement, coefficient matrix to be used. Examples on the use of this technique for aerodynamic shape sensitivity analysis may be found in Refs. 15, 21, and 44, and for multidisciplinary sensitivity analysis in Ref. 5. Furthermore, Arslan and Carlson[5] demonstrated the need for multidisciplinary sensitivity analysis, within the design optimization process, by showing that the sensitivity derivatives produced by an aerodynamic-only calculation had different magnitudes, and in some cases different signs, from that obtained with the coupled aero-structural sensitivity analysis. Similar findings have been reported by Barthelemy and Bergen[6] and by Newman et al. [28] A detailed survey of the research being conducted in the field of multidisciplinary sensitivity analysis and optimization may be found in Ref. 38.

In the current work, a new method for performing both aerodynamic and multidisciplinary sensitivity analysis is presented. This method is based on ideas that where explored over three decades ago by Lyness and Moler[24] and Lyness[23], and recently revisited by Squire and Trapp[40]. This technique uses complex variables to approximate derivatives of real functions. The advantages and disadvantages of the current method are discussed and compared with the existing methods presented above. This method is demonstrated via the computation of aerodynamic, structural, and multidisciplinary sensitivity derivatives.

Sensitivity Derivatives Using Complex Variables

For a central finite-difference approximation to the derivative, one may expand the function in a Taylor series about the point x using a forward step and a backward step, and then subtracting to yield the formula,

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

This expression for the derivative has a truncation error of $O(h^2)$. The advantage of the finite-difference approximation, to obtain sensitivity derivatives, is that any existing code may be used without modification. The disadvantages of this method are the computational time required and the possible inaccuracy of the derivatives. The former is due to the fact that for every derivative, Eq. (1) requires two well-converged solutions for the function evaluations. In the case of nonlinear aerodynamics, these solutions may become extremely expensive. The latter is attributed to the sensitivity of the derivatives to the choice of the step size. To minimize the truncation error one selects a smaller step size, however, an exceedingly small step size may produce significant subtractive cancellation errors. The optimal choice for the step size is not known a priori, and may vary from one function to another, and from one design variable to the next.

Instead, if the function is expanded in a Taylor series using a complex step as

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

Solving this equation for the imaginary part of the function yields

$$\frac{df}{dx} \approx \frac{Im[f(x+ih)]}{h} \tag{3}$$

This expression for the derivative also has a truncation error of $O(h^2)$. Thus, by evaluating the function with a complex argument, both the function and its derivative are obtained, without subtractive cancellation error. The real part is the function value.

The disadvantage of the complex variable approximation is the increased runtime required by the evaluating routines when run with complex arguments. With current compiler options, this run time is on the order of three times the cost of the original solver. However, automatic differentiated versions of analysis software, using say ADIFOR, incur about the same time penalties.

The advantages of the complex variable approximation for obtaining the derivatives are numerous. First, like the finite-difference approximation to the derivatives, very little modification to the original software is required. All the original features and capabilities of the software are retained. Thus, user experience with the current software is not lost, and ongoing advancements and enhancements can be readily introduced into subsequent versions without extensive modifications or re-differentiation. This is in direct contrast to hand or automatically differentiated codes where any modification to the original software will require re-differentiation. This advantage is extremely useful in the problem formulation stages of the design process when new objective functions and constraints are being explored. Second, this method is equivalent to a discrete-direct approach, either from automatic differentiation or hand differentiated codes solved in incremental iterative form, in the way that the state vector and its derivatives are being solved for simultaneously. When solving the state equation, the state vector resides in the real part and the derivatives in the imaginary part. Hence, fully converged flow solutions are not required to obtain derivatives of sufficient accuracy for design. This is not the case for the finite-difference approximation to the derivatives. Finally, the complex variable approximation to the derivative is not sensitive to the step size selection, and requires step sizes that avoid excessive truncation error, without regard to the cancellation error.

Aero-Structural Analysis and Sensitivity Derivatives

Briefly described are the aerodynamic and structural analysis codes used in the current work. In addition, previous sensitivity analysis research performed with these codes are discussed. Finally, some issues concerning the interdisciplinary transfer of information across boundary interfaces are presented.

Aerodynamic Analysis

The aerodynamic analysis is conducted using the three-dimensional unstructured Euler/Navier-Stokes code described in Refs. 1-4 and known as FUN3D. This is an implicit, upwind, finite-volume code in which the dependent variables are stored at the vertices of the mesh. Both compressible and incompressible versions of this code exist, and have been previously hand differentiated using an adjoint approach for inviscid, laminar, and turbulent flows.[2,4,33]

Note that in an adjoint approach, the sensitivity derivatives are evaluated by performing a product of the costate variables with the derivatives of the residual with respect to the design variables. Because the complex variable technique can be easily applied to obtain the derivatives of the residuals with respect to each of the design variables, the current methodology can be applied as part of an adjoint method for obtaining sensitivity derivatives.

For complex flow physics, such as chemically reacting or time dependent flows, the complex variable approach may be utilized and may provide the best approach for determining sensitivity information for these complicated codes. The current methodology may also be employed for a wide range of applications such as obtaining numerical flux Jacobians for complex flux functions or for Newton-Krylov schemes.[46]

Structural Analysis

The finite-element structural analysis program used in the present work has been documented in Ref. 27. Since the stiffness matrix for linear static structural analysis is symmetric and positive-definite, a Choleski factorization is used to solve the system of equations. Further details of the solution algorithm may be found in Ref. 41. The solution to this system of equation produces the vector of nodal displacements. From this deformation field, element stresses can be computed. Furthermore, the available element types consist of truss members, beam elements, constant strain triangles with the ability to model multi-layer composites, triangular and quadrilateral plate/shell elements.

This finite-element structural analysis code has been previously differentiated using the automatic differentiation software tool ADIFOR. Details on the usage and development of the supplementary code are documented in Ref. 16. The new software is capable of computing the displacement derivatives with respect to shape design variables. These displacement derivatives may then be used to compute element stress derivatives.

In the current work, the structural derivatives are obtained using the complex variable approximation. The computational time required to compute structural derivatives using the code from Ref. 16 and the current method are comparable. In addition to shape and sizing derivatives, derivatives with respect to material properties can be evaluated without code modification. This is not the case for ADIFOR versions of this software, which would require re-differentiation. An interesting example that would use material properties as design variables, is the aeroelastic tailoring of composite wings. The design variables could be the fiber orientation in the composite layers.

Interdisciplinary Data Transfer

To resolve the nonlinear fluid flow around an arbitrary object, both the surface and the volume exterior to that surface must be discretized. For the structural analysis, the discretization encompasses the surface of the object and the volume interior to the surface. In practice the nonlinear aerodynamic analysis requires a higher degree of resolution than linear structural analysis. Therefore, the interdisciplinary transfer of data between the fluid and the structure becomes an important concern in the aeroelastic analysis of a flexible wing. This aero-structures interaction has been an active area of research.[11,14,31,36,45]

In the current work, the aerodynamic surface mesh is taken to be the wing skin and the wing box structure is constructed from a subset of these nodes. These discretizations are illustrated in Fig. 1. Figure 1b only shows the front and rear spars, and the rib stations. It should be noted that this one-to-one correspondence between the aerodynamic surface mesh and the wing skin is excessive for linear structures, and considerably increases the number of degrees-of-freedom in the structural analysis. However, the object of this work is to demonstrate that accurate multidisciplinary sensitivity derivatives can be computed with the current method. Future computations will incorporate methods for the aero-structures interaction when different discretizations are used.

Once the surface deformations have been determined, either from the structural analysis or when the design process requires modifications to the surface geometry, the aerodynamic mesh must be adapted to reflect these changes. For the inviscid computations in the current work, the spring analogy method described in Ref. 33 is used. For discrete approaches to shape design optimization, the sensitivity of the mesh to the geometric design variables are required. In the design studies of Refs. 2, 4, 33 these terms were achieved by directly differentiating the mesh movement algorithm. In Ref. 30, these terms were obtained via automatic differentiation of the mesh movement algorithm. In the current work, the grid sensitivity derivatives are computed with the complex variable approximation.

Results and Discussion

In the current work, the ONERA M6 wing that was used in the optimization studies of Refs. 2 and 33 was adopted. The unstructured aerodynamic mesh and structural wing box used in this study are shown in Fig. 1. The unstructured mesh has 2,800 nodes (13,576 tetrahedrons) with 814 nodes on the wing surfaces. The wing skin is the aerodynamic surface mesh, and the wing box structure has a front and rear spar with 7 rib stations. Total degrees-of-freedom of the structural analysis is 2,340. For the computations reported in the current work, a transonic Mach number of 0.84, and a fixed angle-of-attack of 3.06˚ were assumed. The aerodynamic forces have been dimensionalized with free-stream data at an altitude of 35,000 ft. For the structural analysis, all members are considered to be made of Aluminum 6061-T6 with a modulus of elasticity, a Poisson's ratio, and a density of 10^7 lb/in^2, 0.33, and 0.097 lb/in^3, respectively.

To verify the accuracy of the derivatives computed with the complex variable approximation, these derivatives are compared with central finite-difference values. All computations are performed in 64-bit arithmetic. To study the sensitivity of derivatives to step size selection for aero-structural analysis, a study was carried out that repetitively reduced the step size from 10^{-2} to 10^{-9}. The results of this study are shown in Table 1. Tabulated are the aero-structural derivatives of lift coefficient, drag coefficient, and vertical leading edge tip deflection with respect to the flow Mach number. Careful inspection of this table illustrates that both the finite-difference and the complex variable approximation to the derivatives suffer from truncation errors for the larger step sizes. However, the complex variable approximations continuously converge as the step size is reduced, whereas the finite-difference derivatives begin to show signs of cancellation error. In addition, the step size at which cancellations errors can be seen are different for the aerodynamic and structural derivatives. The data from Table 1 is depicted in Figs. 2-4. In these figures, the Log of the difference between the finite-difference values and the complex variable approximations is shown. In the figures, the values have been normalized by derivatives obtained using the complex variable approximation at the smallest step size. Figures 2-4 clearly illustrate that the accuracy of the complex variable approximation is of order h^2, and that the finite-difference approximation suffers from cancellation errors for the smaller step sizes. It should be noted that even at the smallest step size, the finite-difference derivatives are still somewhat accurate. This may or may not be the case for other functions and/or design variables.

Rigid-wing aerodynamic derivatives and aero-structural derivatives, with respect to the flow Mach number, are compared in Table 2. This table, and the ones that follow, demonstrate that accurate single and multidisciplinary sensitivity derivatives can easily be obtained with the current method. Additionally, it is observed that the aero-structural derivatives have only a slightly different magnitude from a rigid-wing calculation. It is realized however, that the ONERA M6 wing chosen in this study is a low aspect ratio wing. Low aspect ratio wings, like those found on fighter aircraft, tend to be more rigid. This is in direct contrast to high aspect ratio wings commonly found on transport aircraft. It is anticipated that these differences in derivatives will be more pronounce, on more flexible high aspect ratio wings.

Derivatives for a geometric shape design variable are given in Table 3. Here, the design variable is the thickness to chord ratio along the semispan of the wing. Once again, relatively small differences are observed between the aerodynamic and aero-structural derivatives. To demonstrate the ability of this method to compute single and multidisciplinary derivatives for general design variables, Table 4 illustrates structural and aero-structural derivatives with respect to a structural sizing design variable. This design variable is the thickness of the front spar. The structural derivative is computed with fixed aerodynamic loads; that is, the aerodynamic solution from a fully converged rigid- wing analysis is used as the load vector, and no interaction between the aerodynamic and structural disciplines is performed. In this case, the displacement derivatives between the structural and aero-structural analyses differ significantly. It is believed that this indicates that the derivatives are sensitive to the rigidity of this low aspect ratio wing, and that as the wing becomes more flexible, differences between the single and multidisciplinary derivatives will become more pronounced.

Concluding Remarks

A new method for computing single and multidisciplinary sensitivity derivatives using complex variables has been developed in the present work. High fidelity aerodynamic and structural analyses do not pose any problems with this new method. The advantages and disadvantages of the complex variable approximation were compared with existing techniques for obtaining sensitivity derivatives. It is shown that this method has all the advantages of existing direct-discrete approaches and the finite-difference approximation, while avoiding some of their shortcomings. In addition, existing software can be modified in a very short amount of time to take advantage of the current approach. Furthermore, this new method is capable of producing extremely accurate aerodynamic and structural derivatives with respect to a variety of design variables. In the current study, design variables appropriate for both aerodynamic and structural design optimization were selected. The configuration used for investigation was a low aspect ratio ONERA M6 wing immersed in a transonic flow.

Because the complex variable technique can be easily applied to obtain the derivatives of the residuals with respect to each of the design variables, the current methodology can be applied as part of an adjoint method for obtaining sensitivity derivatives. Additionally, for complex flow physics, such as chemically reacting or time dependent flows, the complex variable approach may be utilized and may provide the best approach for determining sensitivity information for these complicated codes. The current methodology may also be employed for a wide range of applications such as obtaining numerical flux Jacobians for complex flux functions or for Newton-Krylov schemes.

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Tables

Table 1: Step size study for aero-structural sensitivity derivatives.

Step Size	Method	$\frac{dC_L}{dM_\infty}$	$\frac{dC_D}{dM_\infty}$	$\frac{du_{tip}}{dM_\infty}$
10^{-2}	FD	0.2438345595346350	0.0473888119395907	4.951177921532102
	CV	0.2417537088868154	0.0468956863511756	4.921529894646712
10^{-3}	FD	0.2427874017231074	0.0471446387450332	4.935708384067983
	CV	0.2427292825871235	0.0471329668154663	4.934947366389689
10^{-4}	FD	0.2427446700740965	0.0471386234831769	4.935128732540539
	CV	0.2427391459755011	0.0471353577947664	4.935082100725648
10^{-5}	FD	0.2427392465600975	0.0471353820986550	4.935083469348456
	CV	0.2427392446184733	0.0471353817037700	4.935083448138266
10^{-6}	FD	0.2427392450515820	0.0471353818268238	4.935083461998779
	CV	0.2427392456049049	0.0471353819428597	4.935083461612343
10^{-7}	FD	0.2427392430115471	0.0471353815700847	4.935083355306347
	CV	0.2427392456147688	0.0471353819452511	4.935083461747105
10^{-8}	FD	0.2427392842285769	0.0471353822292797	4.935084851886984
	CV	0.2427392456148695	0.0471353819452758	4.935083461748483
10^{-9}	FD	0.2427392037374076	0.0471354084236042	4.935089892299516
	CV	0.2427392456148686	0.0471353819452752	4.935083461748470

Table 2: Aerodynamic and aero-structural sensitivity derivatives with respect to the flow Mach number (step = 10^{-5}).

	Aerodynamic		Aero-Structures		% Diff.
	FD	CV	FD	CV	
$\frac{dC_L}{dM_\infty}$	0.22636731821	0.22636732953	0.24273924656	0.24273924461	-7.2325
$\frac{dC_D}{dM_\infty}$	0.04805136334	0.04805135917	0.04713538209	0.04713538170	1.9062
$\frac{du_{tip}}{dM_\infty}$	N/A	N/A	4.93508346934	4.93508344813	N/A

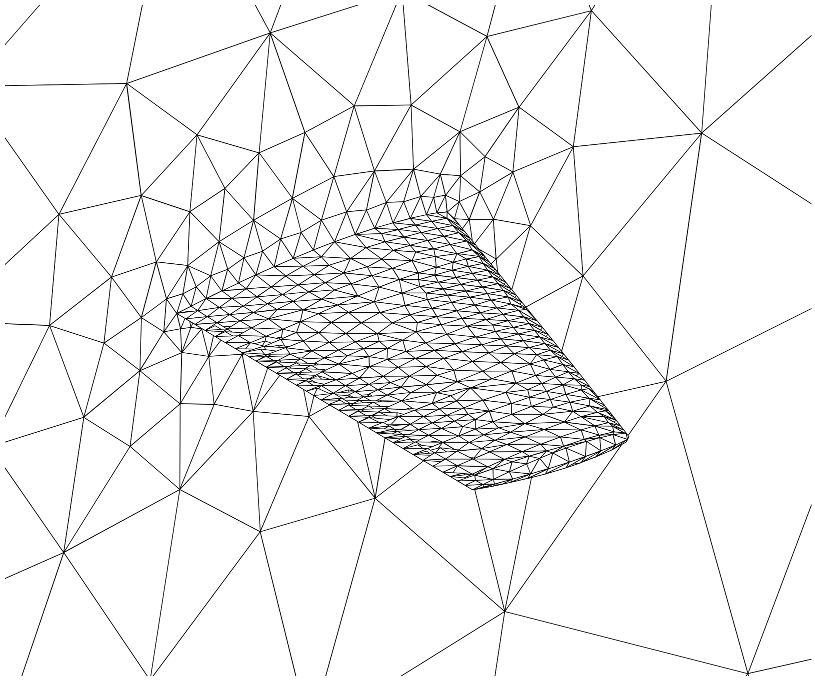
Table 3: Aerodynamic and aero-structural sensitivity derivatives with respect to the thickness to chord ratio (step = 10^{-5}).

	Aerodynamic		Aero-Structures		% Diff.
	FD	CV	FD	CV	
$\frac{dC_L}{dM_\infty}$	-0.0012626581	-0.0012626723	-0.0012606910	-0.0012606965	0.1558
$\frac{dC_D}{dM_\infty}$	0.00182673592	0.00182673442	0.00182538997	0.00182539692	0.0737
$\frac{du_{tip}}{dM_\infty}$	N/A	N/A	-0.0327008248	-0.0327008307	N/A

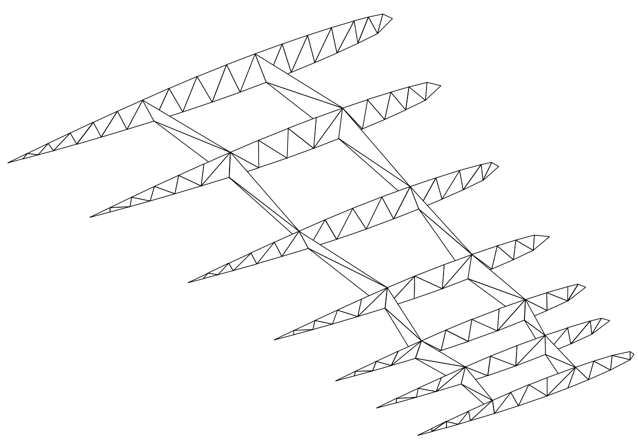
Table 4: Stuctural and aero-structural sensitivity derivatives with respect to the thickness of the front spar (step = 10^{-5}).

	Structures		Aero-Structures		% Diff.
	FD	CV	FD	CV	
$\frac{dC_L}{dM_\infty}$	N/A	N/A	0.05970608795	0.05970608833	N/A
$\frac{dC_D}{dM_\infty}$	N/A	N/A	-0.0015429784	-0.0015429780	N/A
$\frac{du_{tip}}{dM_\infty}$	-8.2870475943	-8.2870474564	-7.0183977216	-7.0183975963	18.076

Figures



(a) Unstructured grid used for aerodynamic design.



(b) Structures mesh: front spar, rear spar, and rib stations.

Figure 1: Discretizations used for the aero-structural analysis.

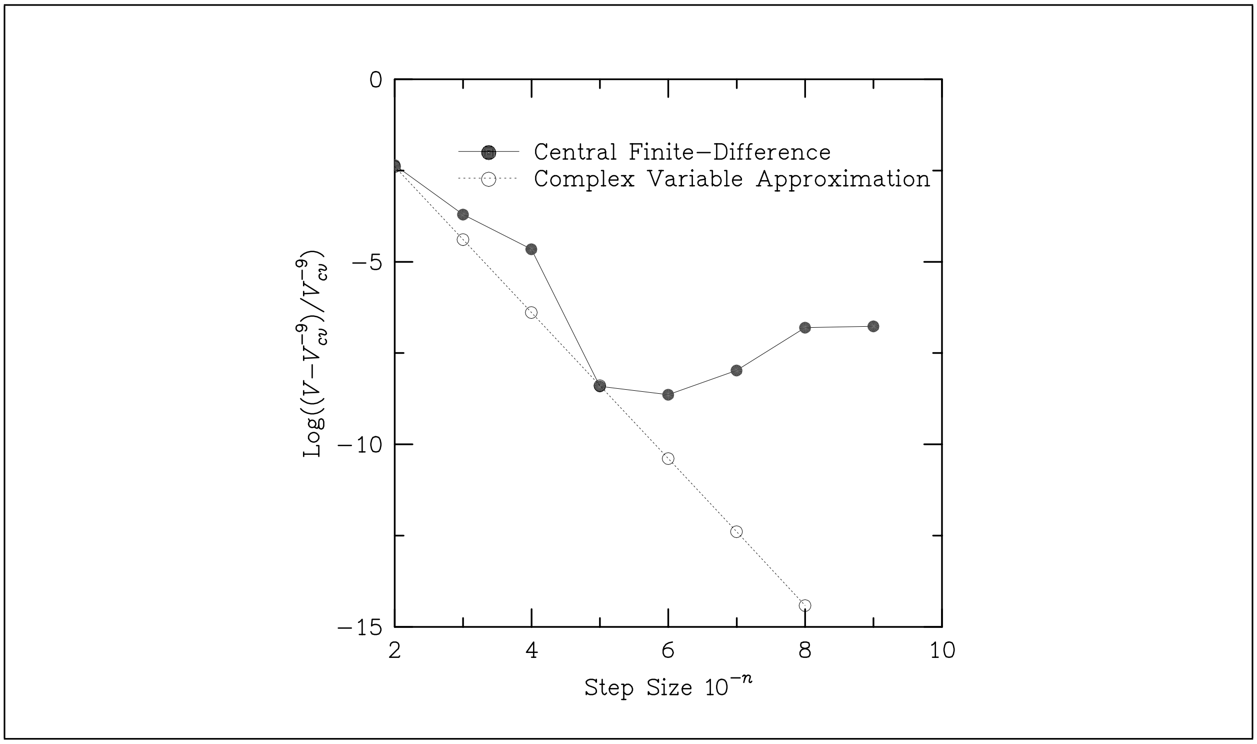


Figure 2: Sensitivity of derivatives to the step size for the lift coefficient.

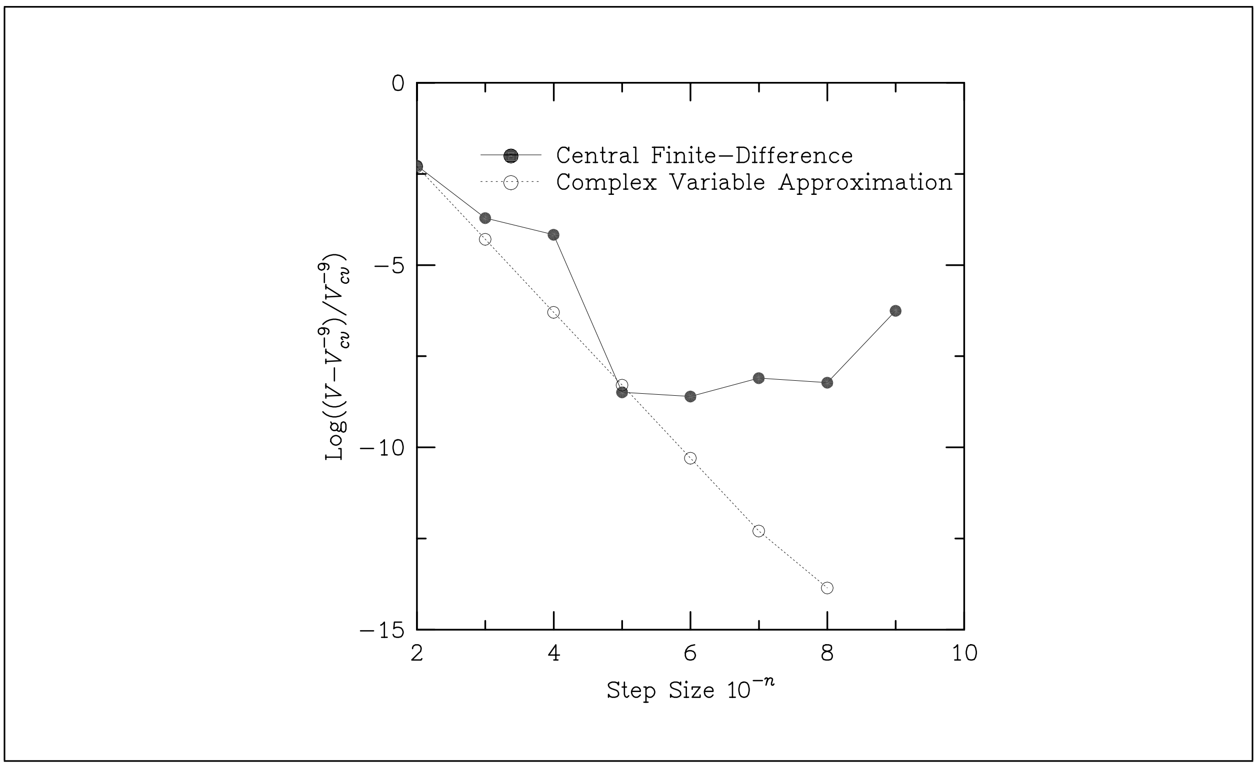


Figure 3: Sensitivity of derivatives to the step size for the drag coefficient.

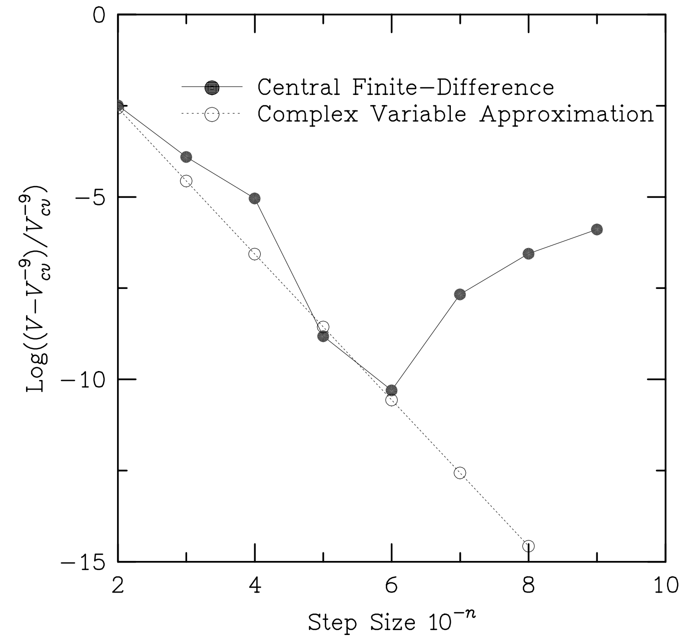


Figure 4: Sensitivity of derivatives to the step size for the tip deflection.