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IMPROVING ACCURACY AND ROBUSTNESS OF A DISCRETE DIRECT DIFFERENTIATION METHOD AND DISCRETE ADJOINT METHOD FOR AERODYNAMIC SHAPE OPTIMIZATION

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Abstract. *This paper describes the recent activities developed at ONERA in the field of aerodynamic shape optimization using gradient based methods. Both discrete direct differentiation method and discrete adjoint method have been considered for the computation of the derivatives of a function with respect to (w.r.t.) the design parameters. The numerical methods for flow computations (solving RANS equations) and for gradient computations are briefly described. The linearization of Wilcox ($k-\omega$) model for improving accuracy of standart gradient computation method - with " frozen " turbulent viscosity - is presented. Also described are two techniques for robustness enhancement of iterative resolution of discrete adjoint equation.*

1 INTRODUCTION

The aim of aerodynamic design optimization is the minimization of an objective function subject to a set of constraints. A classical example and a main application in aerodynamic design is the drag-reduction of an aircraft under constraints relating to the lift, the geometry or the momentums. Optimization methods using computational fluid dynamics became popular tools during the last decade, reducing the costs associated with wind-tunnel tests. Among the methods currently used are gradient-based optimizers in which the gradients of the functions with respect to (w.r.t.) the design variables are used to update the design variables, in order to systematically reduce the cost function to arrive at a local minimum. An important step in this process is the determination of these gradients which are also referred to as sensitivity derivatives. As objective and

constraints functions are non-linear functions of the conservative variables vector and the geometric variables vector which are connected by the flow equations, the computation of derivatives is not easy and several techniques have been investigated for evaluating these sensitivities.
The (discrete) direct differentiation methods and the (continuous or discrete) adjoint variable methods have been proposed around 1990 [1,2,3]. They only involve linear system resolution, in contrast with the old and expensive finite difference method which requires flow computation for shifed meshes. Both discrete direct differentiation method and discrete adjoint vector method have been developed at ONERA. The basic numerical method is briefly described in the first part. The second part presents linearization of Wilcox $(k-\omega)$ model for improving accuracy of gradient computations. The third part describes two techniques for enhancing the robustness of the iterative resolution of the adjoint equation.

2 NUMERICAL METHODS

The basic choices were already described[4,5]. They are summarized in this section.

2.1 Equations of the direct and adjoint variable methods

The discrete residual of the steady state flow equations can be written as

$$R(W,X) = 0 \tag{1}$$

where W is the conservative variable vector, X is the vector of grid points defining the computational mesh. For aerodynamic shape optimization, the computational grid will assume the functional form $X = X(\alpha)$, where α is the design variable vector (its length is n_c, one of its components is noted α_i). Furthermore, because of the implicit dependence of the flow field on the design variables, the residual R has the following form :

$$R = R(W(\alpha), X(\alpha)) = 0 \tag{2}$$

The objective function $\mathcal{J}$ and the constraint functions $\mathcal{G}_k$ depend on the design parameters through the flow field and the mesh :

$$\mathcal{J}(\alpha) = J(W(\alpha), X(\alpha)) \qquad \mathcal{G}_k(\alpha) = G_k(W(\alpha), X(\alpha)) \tag{3}$$

The number of functions is noted n_f. The issue is to compute efficiently the gradient of the n_f functions w.r.t. the n_c design parameters. Differentiation of equation (2) w.r.t. the design variables yields the following equation :

$$\frac{\partial R}{\partial W}\frac{dW}{d\alpha_i} = -\frac{\partial R}{\partial X}\frac{dX}{d\alpha_i} \tag{4}$$

The direct differentiation method consists in solving equation (4) for all design parameters α_i (i.e. resolution of n_c linear systems). Then the total derivative of the objective function

$\mathcal{J}$ or the constraint function $\mathcal{G}_k$ is computed by the formula :

$$\frac{d\mathcal{J}}{d\alpha_i} = \frac{\partial J}{\partial X}\frac{dX}{d\alpha_i} + \frac{\partial J}{\partial W}\frac{dW}{d\alpha_i} \tag{5}$$

Alternately, the sensitivity coefficients may be obtained using the adjoint variable approach which can be introduced by different simple algebraic computations[4]. If we define the adjoint vector λ_J, linked with function $\mathcal{J}$, that satisfies the following adjoint equation

$$(\frac{\partial R}{\partial W})^T \lambda_J = -(\frac{\partial J}{\partial W})^T, \tag{6}$$

the sensitivity derivative of the objective function J w.r.t. the design variable vector can be expressed by the following equations :

$$\frac{d\mathcal{J}}{d\alpha_i}(\alpha) = \frac{\partial J}{\partial X}\frac{dX}{d\alpha_i} + \lambda_J^T(\frac{\partial R}{\partial X}\frac{dX}{d\alpha_i}) \tag{7}$$

It appears that the adjoint variable formulation requires the resolution of n_f linear systems in order to get the functions sensitivities w.r.t. the design variables. As concerning the direct differentiation approach, n_c linear systems of the same size have to be solved in order to calculate these sensitivities. So the formulation of the optimization problem dictates which method should be used to produce the sensitivity coefficients most efficiently. As concerning industrial problems, it is to note that the number of design variables is generally much larger than the number of constraint functions, that is why in those cases the adjoint variable formulation is preferred.
Equations (4) and (6) have to be inverted in some way. A direct inversion would require an exact Jacobian for the LHS that would result in having a large, sparse and very complex matrix to invert. To avoid that, those equations are put in an incremental iterative form. They are both converted to the following systems of linear equations and solved by an implicit method, almost the same as the one used for the flow calculation. It is worthy of note that this formulation makes an exact Jacobian appear on the right hand side and an approximate Jacobian appear on the left hand side.

$$\frac{\partial R}{\partial W}^{T(APP)} \left(\lambda_J^{(l+1)} - \lambda_J^{(l)}\right) = -\left(\frac{\partial R}{\partial W}^{T(EXA)} \lambda_J^{(l)} + \frac{\partial J}{\partial W}\right) \tag{8}$$

$$\frac{\partial R}{\partial W}^{(APP)} \left((\frac{dW}{d\alpha_i})^{(l+1)} - (\frac{dW}{d\alpha_i})^{(l)}\right) = -\left(\frac{\partial R}{\partial W}^{(EXA)} \frac{dW}{d\alpha_i}^{(l)} + (\frac{\partial R}{\partial X}\frac{dX}{d\alpha_i})\right) \tag{9}$$

The linear systems at each step (l), are solved approximately using 2 or 4 iterations of lower-upper block relaxation.

2.2 Turbulence model. Space discretization

Only turbulent flows modeled by (RANS) approach are taken into consideration in this article. The closure of the mean flow system uses either Wilcox (k, ω) model[6] or Spalart-Allmaras model[7]. The general framework of our code is the finite volume cell-centered approach with structured meshes. The discretization of the different terms of the equations is defined below :
- mean flow convective flux : Roe flux combined with Van Albada flux limiting function [8,9,10] ;
- turbulent variables convective flux : first order Roe flux[8] ;
- mean flow and turbulent variables diffusive flux : centred formula using interface-centred evaluation of gradient terms ;
- turbulent variables source term : centered formula using cell-centered evaluation of gradient terms.
Both convective fluxes use Harten-type correction to prevent the absolute values of eigenvalues from vanishing. They are noted Ψroe and Ψtroe. These values are indicated on some plots. The so-defined discrete convective fluxes are differentiable. The choice of upwind convective fluxes for discrete direct differentiation and discrete adjoint method is known to lead to a well conditioned exact jacobian matrix, $\frac{\partial R}{\partial W}^{(EXA)}$.

2.3 Standard linearization

Considering gradient computations - with both, direct differentiation and adjoint method - following approximations are done most often :
- the eddy viscosity and turbulent viscosity are considered constant (these values, evaluated at cell-centers, are considered independent of the shape parameters) ;
- the thin layer assumption is used for the linearization of the mean flow diffusive flux.
The first assumption is used by almost all authors. It means that direct linearized and adjoint equations - (4) and (6) - are 5-field equation even if the number of fields of the space residual is six (Spallart-Allmaras turbulence model) or seven (Wilcox (k, ω) model). This point will be discussed in more detail in section 3, where the "constant viscosity" assumption will not be considered anymore.
The definition of the other matrix of the problem, $\frac{\partial R}{\partial W}^{(APP)}$, can be found in references [4] or [11].

3 GRADIENT COMPUTATION INCLUDING LINEARIZATION OF WILCOX (k,ω) TURBULENCE MODEL

3.1 Discussion

Most authors interested in gradient computation methods have used the so-called "constant viscosity" assumption. Nevertheless a limited number of authors have considered

turbulence model linearization and discussed its benefit in term of accuracy. The following models have been differentiated in order to compute the accurate jacobian matrix $\frac{\partial R}{\partial W}^{(EXA)}$:
- Baldwin-Lomax model was differentiated by LeMoigne et al.[12] and also Kim et al.[13] ;
- Spalart-Allmaras model was differentiated by Nielsen, Anderson and their coworkers[14,15] and by Giles et al.[16] ;
- Several two-equation models were differentiated by Kim et al.[17,18].
Several 2D test cases were presented in these articles. The reader is referred to these articles for more information about improvement of gradient accuracy.

3.2 Linearization of Wilcox (k,ω) model

The Wilcox (k,ω) model was differentiated in direct mode, in order to compare the robustness and accuracy of a full linearization - differentiation of (RANS) equations plus turbulence model- compared to those of the standard linearization - differentiation of (RANS) equations, constant turbulent viscosity. The different terms of the turbulent variable equations were differentiated in the following way :
- convective flux : no approximation ;
- diffusive flux : no approximation ;
- source term : using a decomposition of the term along mesh-lines.
The terms of implicit stage matrix -$\frac{\partial R}{\partial W}^{(APP)}$- for the coupled problem can be found in[11].

3.3 Validation

The test case is a transonic flow around the NACA64A212 airfoil. The upstream flow characteristics are : $M_\infty = 0.71, \quad Re = 2.\ 10^6, \quad a_\infty = 2.5^o$. The flow is transonic. The mesh size is 257*65. There is only one design parameter, whose positive variation causes the thickening of the rear part of the suction side. The flow sensitivity is studied and also the derivatives of three aerodynamic functions w.r.t. the shape parameter : the lift (noted CL), the far-field drag and the near-field drag (noted $CDff$ and $CDnf$) as defined in [19]. Finite-differences for flow- and functions-sensitivities are calculated from flow calculations on shifted-meshes with a centered formula (actually, flow fields $W(-.01)$ and $W(+.01)$ were computed using corresponding meshes, $X(-.01)$ and $X(+.01)$).
Several variable sensitivity plots in the cells adjacent to the wall are presented in figures 1 to 3. The sensitivity of ($\rho\omega$) near the trailing edge is presented in figures 4 -finite difference- and 5 -solution of linearized equation. From those figures and the corresponding plots for the other variables, it appears that the flow sensitities of all variables (mean flow and turbulent variables) is quite correctly computed using the full linearization approach, the accuracy being higher for the mean flow variables. When comparing mean flow sensitivities obtained by standard and full linearization approach, it appears that the accuracy is improved by full linearization. It can be seen in particular in figures 1 and 2 :

the standard linearization leads to an significant error at the upper-side, near the shock, whereas the full linearization leads to an accurate solution at this location.
The function sensitivities are presented in table 1. The accuracy improvement due to full linearization is confirmed by these results. Indeed, the full linearization derivatives are closer to the finite difference values, than the standard linearization derivatives for all three functions. The gap beetween full linearization values and finite difference reference value for $CDff$ and $CDnf$ is difficult to explain. It may be caused by the lack of convergence in flow computations or by the remaining approximations in the "exact" jacobian $\frac{\partial R}{\partial W}^{(EXA)}$

Fonction	finite diff.	"frozen μ_t" lin.	full (RANS)+$(k-\omega)$ lin.
CL	3.82 10-1	3.99 10-1	3.83 10-1
$CDff$	2.34 10-3	2.85 10-3	2.68 10-3
$CDnf$	3.19 10-3	3.87 10-3	3.67 10-3

Table 1: NACA64A212. Comparison of aerodynamic function-sensitivities.

4 ROBUSTNESS ENHANCEMENT OF ADJOINT GRADIENT COMPUTATION METHOD

4.1 Definition of robustness enhancement techniques

The iterative process defined by equations (8) and (9) appeared to diverge for some complex configurations. This lack of convergence was observed even with the standard "frozen μ_t approximation" which is used for all 3D complex configurations. Hence, different techniques were considered in order to enhance the robustness of the resolution of adjoint equation (which is used for the complex applications). Two of them appeared to be efficient. They will be noted (FO) and (AD) :
- (FO) - switch to first order linearization of mean flow convective flux for some domains. Even if the explicit residual R is computed from second order Roe flux plus MUSCL approach (Van Albada limiting function), the jacobian $\frac{\partial R}{\partial W}^{(EXA)}$ may include for some domains the linearization of the basic first-order Roe flux ;
- (AD) - add a dissipative term in $\frac{\partial R}{\partial W}^{(EXA)}$. Even if the residual R includes no artificial dissipation, an artificial dissipation term may be included in $\frac{\partial R}{\partial W}^{(EXA)}$. It is not defined by linearization of a classical artificial dissipation term -as defined in [20] for example-, but by directly applying this kind of formula to the adjoint vector.

4.2 Application to ONERA M6 wing

The test case for this study is the ONERA M6 Wing. The upstream flow characteristics are $M = .84$ $Re = 1.46\ 10^7$. Four angles of attack are considered $a_\infty = 0^o, 1^o, 2^o, 3^o$. The 10-block mesh contains 620042 points. The design parameter is the angle of rotation around the axis ($x = 0$,$z = 0$). The function to derivate is the lift CL. Without the techniques (FO) and (AD), the iterative process defined by equation (8) fails to converge, after a reduction of two to three orders of magnitude of the right hand side of the equation. Different numerical experiments were carried out with (FO) and (AD) techniques.
- Applying (AD) technique improves the best convergence level (to more than three order of magnitude), but all four adjoint gradient computations exhibit finally a divergent behaviour. The most appropriate coefficients for the artificial dissipation have low values - about $k_2 = .004$, k_4=0.00025-, much lower than those used for analysis computation with a centered scheme.
- Applying (FO) technique to two blocks located downstream the wing - blocks 9 and 10, see figure (6)-, which are not adjacent to the wall, enables the convergence of adjoint gradient computation for two of the four computations - $a = 0^o$, $a = 1^0$. The convergence of the two other computations can be obtained with a blend of (FO) and (AD) techniques. The values of the corresponding artificial dissipation coefficients and the convergence plots are presented in figure (7).
- Applying (FO) technique to two blocks located downstream the wing - blocks 1, 9 and 10, see figure (6)- which are not adjacent to the wall, enables the convergence of all four adjoint gradient computation. The corresponding convergence plots are presented in figure (8).

5 CONCLUSIONS

The discrete gradient computation methods developed at ONERA for shape optimization have been presented, as well as recent activities aiming at improving robustness and accuracy.
Further work will include extension of gradient computation to turbomachinery configurations, to other space discretizations and to unsteady flows.

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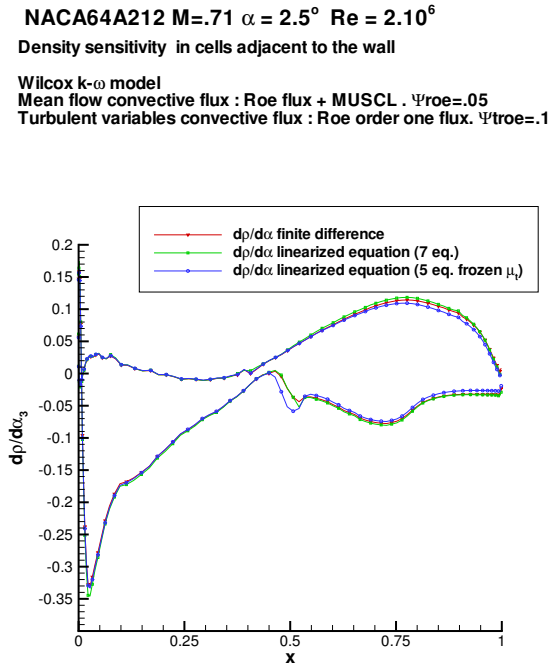

Figure 1: Density sensitivity in cells adjacent to the wall

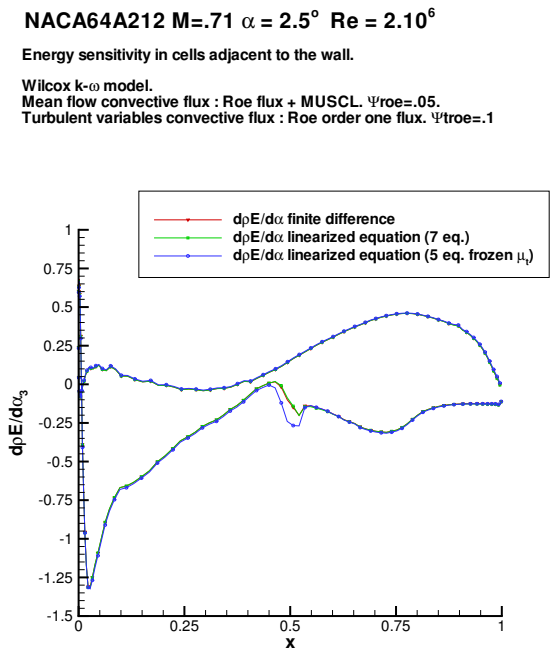

Figure 2: Energy sensitivity in cells adjacent to the wall

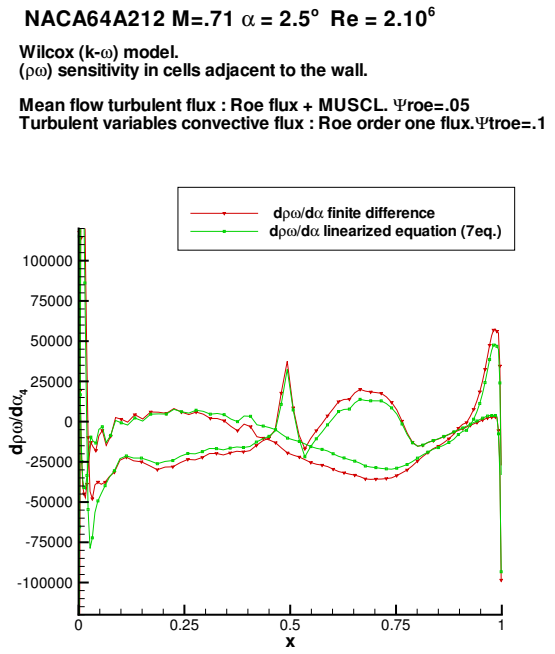

Figure 3: $\rho\omega$ sensitivity in cells adjacent to the wall

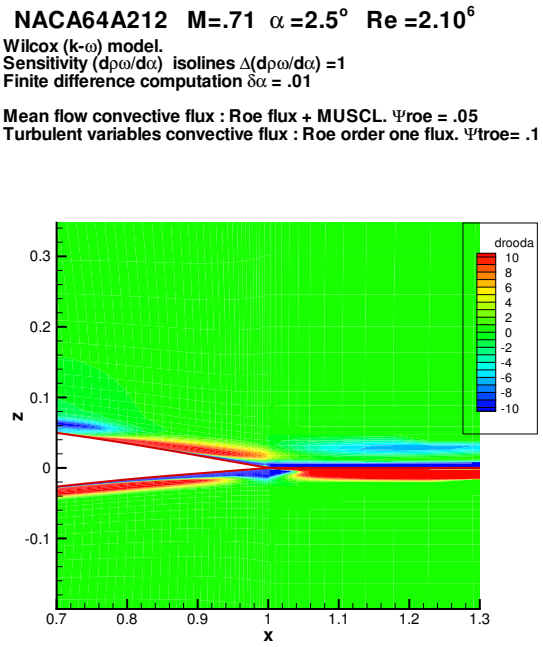

Figure 4: $\rho\omega$ sensitivity near the trailing edge (finite difference)

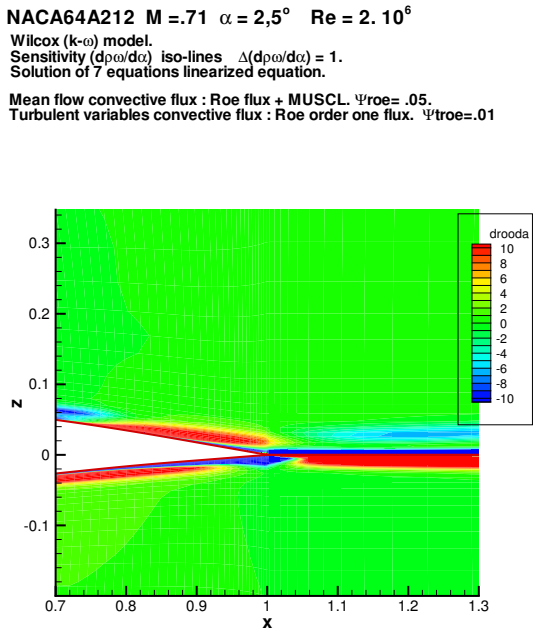

Figure 5: $\rho\omega$ sensitivity near the trailing edge (linearized equation)

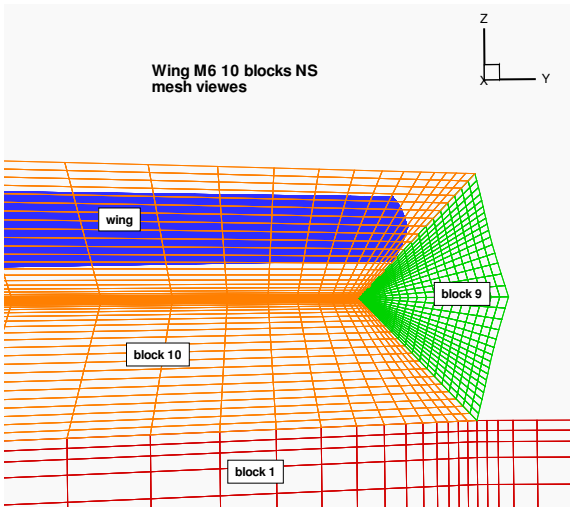

Figure 6: ONERA M6 Wing. Location of blocks for (FO) method

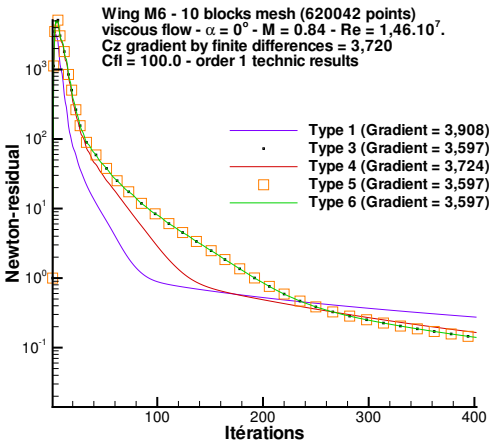

Figure 7: ONERA M6 Wing. Adjoint equation resolution, convergence plots

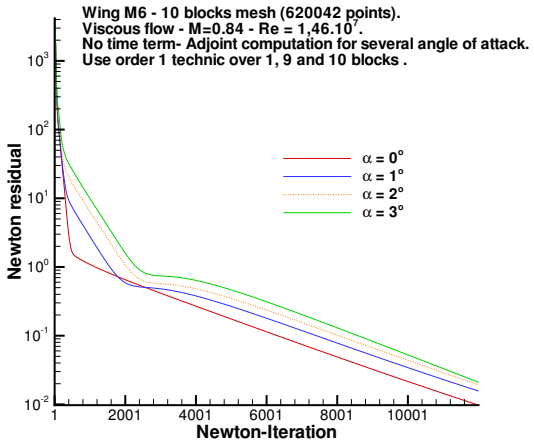

Figure 8: ONERA M6 Wing. Adjoint equation resolution, convergence plots