Turbulence, Heat and Mass Transfer 8

RANS turbulence treatment for continuous adjoint optimization

M. Popovac[1], C. Reichl[1], H. Jasak[2,3] and H. Rusche[3]

[1]*Austrian Institute of Technology, Energy Department, Giefinggasse 2, 1210 Vienna, Austria, mirza.popovac@ait.ac.at*

[2]*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia, hrvoje.jasak@fsb.hr*

[3]*Wikki GmbH. Goergesstrasse 24, 38118 Braunschweig, Germany, h.rusche@wikki-gmbh.de*

Abstract — This paper discusses the implementational aspects related to the turbulence modelling for continuous adjoint optimization. The starting point is the derivation of equations of the high-Reynolds number k-ϵ model of turbulence in the framework of continuous adjoint optimization. The focus here is on the analysis of the behaviour of different terms in derived adjoint equations, and their implementation into a general-purpose CFD solver based on the finite volume discretization. The success in ensuring computational stability when performing optimization simulations deploying continuous adjoint method method, is presented on several generic test cases.

1. Introduction

The numerical optimization methods are of high importance in various branches of engineering, because they guide the improvement of a system performance through relatively easy design interventions. Since the adjoint optimization method has highly desirable feature that the size of the optimization problem does not depend on the number of optimization parameters, this method has long been used in aerospace and automotive industry [9]. However, most of the early work was done within the framework of computational stress analysis using the finite elements codes. This paper is dealing with the computational fluid dynamics (CFD) framework, where the majority of simulations are performed typically using codes based on the finite volume method.

There are two approaches in the adjoint optimization method: in the continuous approach the adjoint equations are derived analytically from the governing equations, whereas in the discrete approach the adjoint equations are obtained after the discretization of the governing equations [5]. Without any intention to discuss advantages and disadvantages of these two methods [3], the present paper treats the continuous adjoint approach suitable for implementation into a finite volume general purpose CFD code, with the details of this approach presented in several publications ([8], [6]).

As a first attempt in adjoint optimization simulations, the frozen turbulence assumption can be used. Nevertheless, the turbulence contribution to the adjoint equations is very significant, and in some applications frozen turbulence can produce the wrong sign for the local sensitivity [2]. This is the motivation for presenting in this paper the treatment of the RANS turbulence models for continuous adjoint optimization, following the work given in [14] and [15].

The optimization task is formulated here as the minimization of a flow objective function J (expressed in terms of flow state variables and design variables) by intervening through a set of shape design variables b_n (either in the form of the porosity introduced within the cells, or as the displacement of the boundary faces). The design improvement is reached when the objective function is reduced: this is the example of constrained optimization, where the constraints are given by a set of partial differential equations for state variables that govern the fluid flow. The set of equations includes the Reynolds averaged Navier-Stokes and continuity equations, accompanied by an appropriate set of turbulence model equations.

To asses the sensitivity of the objective function J, i.e. its variation with respect to the set of design variables b_m (which is the goal of the optimization method), the total variation of the augmented function L needs to be considered. Due to elliptic character of Navier-Stokes equations, the flow perturbation at any point within the flow domain is propagated throughout the entire domain. As a consequence, the sensitivity calculated directly from the total variation of L would require the calculation of all state variables for each change of design variables. In order to avoid this prohibitively expensive procedure, the main idea behind the adjoint method is to select appropriately the adjoint variables: starting from the total variation expression, the equations for adjoint variables are derived (and the corresponding boundary conditions defined) so that they eliminate the dependency of the sensitivity on the state variables. To that purpose, in the derivation of adjoint equations the Gauss theorem and the integration by parts (among others) are deployed. After some mathematical manipulation, for the specified objective function the sensitivity of the grid nodes with respect to the design variables is to be calculated with thus obtained adjoint variables.

One of the major problems for calculating the sensitivity with adjoint method is the numerical performance of the simulations with adjoint equations. Not only is the complexity of the numerical simulation significantly increased, but even more significant is the problem of the numerical stability. The focus of this paper is on the implementation aspects of the continuous adjoint method which contribute to the improvement of the numerical stability, and in that respect this paper is organized as follows. After this introductory section, the governing equations are summarized in section 2. with the detailed derivation procedure for adjoint equations outlined at the end of the paper (appendix A). The main contribution of this paper is given in the section 3. which explains the implementation details for continuous adjoint method. Finally, the obtained results will be discussed in section 4. while the concluding remarks are summarized in section 5.

2. Governing equations

For a steady state turbulent flow of incompressible Newtonian fluid the governing equations can be written in the residual form as:

$$\begin{aligned} R^{u_i} =& u_j \frac{\partial u_i}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu+\nu_t)\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)\right] + \frac{\partial p_{eff}}{\partial x_i} = 0 \\ R^p =& -\frac{\partial u_i}{\partial x_i} = 0 \end{aligned} \tag{1}$$

where u_i and p are velocity and pressure state variables respectively, ν is the molecular viscosity, whereas ν_t is the turbulent viscosity that represents the net effect of turbulent mixing. In analogy to its molecular counterpart, the turbulent viscosity can be expressed through the velocity scale and the time scale which cannot go below its Kolmogorov value:

$$\begin{aligned} \nu_t =& c_\mu T k \\ T =& max\left[\frac{k}{\epsilon}, c_\tau \left(\frac{\nu}{\epsilon}\right)^{1/2}\right] \end{aligned} \tag{2}$$

Within the RANS two-equation framework of $k-\epsilon$ model [4], this definition of ν_t implies solving additional transport equations for two state variables that characterize turbulent effects: turbulent kinetic energy k and its dissipation rate ϵ. The transport equations for k and ϵ in residual form read:

$$
\begin{aligned}
R^k =& u_j \frac{\partial k}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] - (P_k - \epsilon) = 0 \\
R^\epsilon =& u_j \frac{\partial \epsilon}{\partial x_j} - \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial x_j}\right] - \frac{c_1 P_k - c_2 \epsilon}{T} = 0
\end{aligned}
\tag{3}
$$

where $p_{eff} = p + \frac{2}{3}k$ is the effective pressure, $P_k = \nu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\frac{\partial u_i}{\partial x_j}$ is the production of turbulent kinetic energy, $\sigma_k = 1$ and $\sigma_\epsilon = 1.3$ are the turbulent Prandtl numbers, while $c_\mu = 0.09$, $c_\tau = 6.0$, $c_1 = 1.44$ and $c_2 = 1.92$ are the model constants. These governing equations are complemented by an appropriate near-wall treatment, e.g. standard wall functions [11] or more advanced compound wall treatment [10].

The problem of optimization constrained by the governing state equations (in the present case Eq.(1) and Eq.(3), with the definition from Eq.(2) and appropriate near-wall treatment) is solved using the Lagrangian calculus. The objective function J is augmented by the volume integral of the applied state equations weighted by the adjoint variables:

$$
L = J + \int_\Omega \left(u_i^* R^{u_i} + p^* R^p + k^* R^k + \epsilon^* R^\epsilon\right) d\Omega \tag{4}
$$

where L is the augmented objective function, and acting as the Lagrange multipliers the starred variables u_i^*, p^*, k^* and ϵ^* denote the adjoint to the state variables u_i, p, k and ϵ respectively. Having in mind this condition for which the equations for adjoint variables are derived (Eq.4), it is clear that the physical meaning of the adjoint variables is to carry the information about the variation of state variables with respect to specified objective function. From this consideration follow also the dimensions of the adjoint variables (Eq.4): $[\phi^*] = \frac{[J]}{[R^\phi][\Omega]} = \frac{[J]}{[\phi]}\frac{s}{m^3}$.

2.1. Adjoint equations and boundary conditions

In the derivation of the adjoint k and ϵ equations, the work presented in [15] is followed. The detailed steps are presented in the appendix (A), while in this section only the final expressions will be given. Subjecting the governing equations to a rigorous mathematical apparatus, of which the main ingredients are the integration by parts and Gauss theorem, one can identify on one side the field integrals (terms denoted as FI), and on the other the boundary integrals (terms denoted as BI), which in turn can contain either the values of the variables (BIv: 6a, 6c, 6d 6f) or their gradients (BIg: 6b, 6e 6g). By equating the final expressions to zero, the field integrals FI are yielding the adjoint governing equations, whereas the boundary integrals BI give rise to the respective boundary conditions.

Summarized in Eq.(5) are the momentum and continuity adjoint equations (although, for brevity, their derivation has not been shown in this paper), together with the adjoint k and ϵ

equations[1]:

$$
\begin{aligned}
R^{u_i^*} =& - u_j \left(\frac{\partial u_j^*}{\partial x_i} + \frac{\partial u_i^*}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left[(\nu + \nu_t) \left(\frac{\partial u_j^*}{\partial x_i} + \frac{\partial u_i^*}{\partial x_j} \right) \right] \\
&+ \frac{\partial p^*}{\partial x_i} + k^* \frac{\partial k}{\partial x_i} + \epsilon^* \frac{\partial \epsilon}{\partial x_i} \\
&+ 2 \frac{\partial}{\partial x_j} \left[\left(k^* + c_1 \frac{\epsilon^*}{T} \right) \nu_t \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \right] + \frac{\partial J_\Omega}{\partial u_i} && \text{(5a)} \\
R^{p^*} =& - \frac{\partial u_i^*}{\partial x_i} + \frac{\partial J_\Omega}{\partial p} && \text{(5b)} \\
R^{k^*} =& - u_j \frac{\partial k^*}{\partial x_j} - \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k^*}{\partial x_j} \right] \\
&+ \frac{2 c_\mu T}{\sigma_k} \frac{\partial k}{\partial x_j} \frac{\partial k^*}{\partial x_j} + \frac{2 c_\mu T}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} \frac{\partial \epsilon^*}{\partial x_j} \\
&+ 2 c_\mu T \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_i^*}{\partial x_j} \\
&- 2 k^* \frac{P_k}{\epsilon T} - c_1 \epsilon^* \frac{P_k}{\epsilon T^2} - c_2 \epsilon^* \frac{1}{T^2} - \frac{2}{3} \frac{\partial u_i^*}{\partial x_i} + \frac{\partial J_\Omega}{\partial k} && \text{(5c)} \\
R^{\epsilon^*} =& - u_j \frac{\partial \epsilon^*}{\partial x_j} - \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon^*}{\partial x_j} \right] \\
&- \frac{c_\mu T^2}{\sigma_k} \frac{\partial k}{\partial x_j} \frac{\partial k^*}{\partial x_j} - \frac{c_\mu T^2}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} \frac{\partial \epsilon^*}{\partial x_j} \\
&- c_\mu T^2 \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_i^*}{\partial x_j} \\
&+ k^* + k^* \frac{P_k}{\epsilon} + 2 c_2 \frac{\epsilon^*}{T} + \frac{\partial J_\Omega}{\partial \epsilon} && \text{(5d)}
\end{aligned}
$$

where the last term in all adjoint equations is a volume contribution from the objective function $\frac{\partial J_\Omega}{\partial \phi}$, for the case where the objective function is defined over a volume. This is particularly interesting for the adjoint continuity equation, which is not divergence-free (like it's state counterpart) in case that for specified objective function the volumetric term $\frac{\partial J_\Omega}{\partial p}$ in non-zero.

The bilinear concomitant terms BIv and BIg, originating from the integration by parts, are the boundary integrals which are containing the boundary contribution to the adjoint equations. Hence, they are used to determine the boundary conditions for adjoint governing equations by equating these terms to zero. In addition, analogously to the source term in the adjoint equations that comes from the volume integral of the objective function, there is also the boundary contribution that comes from the objective function $\frac{\partial J_\Gamma}{\partial \phi}$. This contribution is represented separately, in order to underline the dependency of the set of adjoint equations on the specification of the

[1] in the reference paper [15] the terms in adjoint turbulence equations that contain the production P_k are dimensionally incorrect, therefore the derivation of adjoint k and ϵ equations is shown step by step in appendix A

objective function.

$$BIU = \int_\Gamma \{\ u_i^* u_j n_j + (\nu + \nu_t) \left(\frac{\partial u_i^*}{\partial x_j} + \frac{\partial u_j^*}{\partial x_i} \right) n_j$$

$$- 2 \left(k^* + c_1 \frac{\epsilon^*}{T} \right) \nu_t \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) n_j$$

$$+ u_j^* u_j n_i - p^* n_i$$

$$+ \frac{\partial J_\Gamma}{\partial u_i}\ \} \frac{\partial u_i}{\partial b_m} d\Gamma \tag{6a}$$

$$- \int_\Gamma u_i^* (\nu + \nu_t) \frac{\partial}{\partial b_m} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) n_j d\Gamma \tag{6b}$$

$$BIP = \int_\Gamma \{\ - u_i^* n_i + \frac{\partial J_\Gamma}{\partial p}\ \} \frac{\partial p}{\partial b_m} d\Gamma \tag{6c}$$

$$BIK = \int_\Gamma \{\ k^* u_j n_j + \left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k^*}{\partial x_j} n_j$$

$$- 2 u_i^* c_\mu T \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) n_j$$

$$- k^* \frac{2 c_\mu T}{\sigma_k} \frac{\partial k}{\partial x_j} n_j - \epsilon^* \frac{2 c_\mu T}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} n_j$$

$$+ \frac{2}{3} u_i^* n_i$$

$$+ \frac{\partial J_\Gamma}{\partial k}\ \} \frac{\partial k}{\partial b_m} d\Gamma \tag{6d}$$

$$- \int_\Gamma -k^* \left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial}{\partial b_m} \left(\frac{\partial k}{\partial x_j} \right) n_j d\Gamma \tag{6e}$$

$$BIE = \int_\Gamma \{\ \epsilon^* u_j n_j + \left(\nu + \frac{\nu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon^*}{\partial x_j} n_j$$

$$+ u_i^* c_\mu T^2 \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) n_j$$

$$+ k^* \frac{c_\mu T^2}{\sigma_k} \frac{\partial k}{\partial x_j} n_j + \epsilon^* \frac{c_\mu T^2}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} n_j$$

$$+ \frac{\partial J_\Gamma}{\partial \epsilon}\ \} \frac{\partial \epsilon}{\partial b_m} d\Gamma \tag{6f}$$

$$- \int_\Gamma \epsilon^* \left(\nu + \frac{\nu_t}{\sigma_\epsilon} \right) \frac{\partial}{\partial b_m} \left(\frac{\partial \epsilon}{\partial x_j} \right) n_j d\Gamma \tag{6g}$$

With the boundary expressions defined above, the geometry configuration characteristic for the duct flows is adopted, where the boundary consists of the inlet, outlet and wall segments $\Gamma = \Gamma_{in} \cup \Gamma_{out} \cup \Gamma_{wall}$, the treatment of the boundary conditions is analysed for each of these segments individually [15]. On the other hand, all the remaining terms which collect only the boundary contribution from the walls that are depending on the sensitivity of the geometrical quantities (such as the surface integral in Eq.7) define the sensitivity derivatives. This is the quantification of the shape optimization (sensitivity map [6]).

Typically the nodal coordinates are fixed along inlet and outlet surfaces, i.e. $\frac{\delta x_k}{\delta b_m} = 0$. At the inlet Dirichlet conditions are applied for $u_i, k,$ and ϵ, which means that their sensitivities are zero so their BIv terms vanish. This leaves the integrals that involve $\frac{\partial p}{\partial b_m}$ for defining adjoint velocity at the inlet: $BIUv = \frac{\partial J_\Gamma}{\partial p}$. This condition is fulfilled at the inlet by zeroing the adjoint velocity tangential component (tangential unit vector t_j), and for the normal component (normal unit vector n_i) imposing $u_i^* n_i = \frac{\partial J_\Gamma}{\partial p} n_i$. At the same time, by imposing $k^* = 0$ and $\epsilon^* = 0$ the terms $BIKg$ and $BIEg$ are eliminated ($BIUg$ is eliminated with previous boundary definition for u_i^*). Since there is no specific condition for p^*, zero Neumann boundary condition can be applied at the inlet, in analogy to its state counterpart.

For the state variables u_i, k and ϵ zero Neumann condition is typically applied at the outlet, and Dirichlet condition is applied for p. This means $BIP = 0$ and $BIUg, BIKg, BIEg = 0$, and the outlet boundary condition for adjoint velocity is obtained from $BIP = 0$. This expression will give the definition of p^* over the outlet surface, together with the component of the adjoint velocity normal to the outlet surface, while the tangential component is zeroed. Finally, the conditions $BIKg = 0$ and $BIEg = 0$ give rise to the outlet boundary conditions for k^* and ϵ^* which combine both the variable and their gradients: k^* is computed from $-2c_\mu \frac{k}{\epsilon}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right) u_i^* n_j + \frac{2}{3} u_j^* n_j + u_j n_j k^* + \left(\nu + \frac{\nu_t}{\sigma_k}\right) \frac{\partial k^*}{\partial x_j} n_j = 0$, whereas ϵ^* is computed from $c_\mu \frac{k^2}{\epsilon^2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right) u_i^* n_j + u_j n_j \epsilon^* + \left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right) \frac{\partial \epsilon^*}{\partial x_j} n_j = 0$.

As for the wall boundary conditions, the approach analogous to classical turbulence near-wall treatment has been developed 15]. Namely, the adjoint $k^* = \epsilon^* = 0$ and $u_i^* = 0$ fulfil the no-penetration condition, whereas from the remaining terms the adjoint friction velocity is defined: $u_\tau^* = \sqrt{\frac{1}{U^+}\left[2u_j^* t_j u_\tau - \left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial k^*}{\partial x_j} n_j \frac{\delta k}{\delta u_\tau} - \left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon^*}{\partial x_j} n_j \frac{\delta \epsilon}{\delta u_\tau}\right]}$. This expression is used in the wall function manner, in order to compute the adjoint viscous diffusivity along the wall boundaries. Finally, using the operator $L_i^m() = \frac{\partial ()}{\partial x_k} t_k^l \left(n_j t_i^l - t_j^l n_i\right) \frac{\delta x_j}{\delta b_m}$ the sensitivity derivatives are computed.

3. Implementation

The adjoint optimization method presented here has been implemented into the general purpose open-source CFD library suite OpenFOAM version *foam-extend-3.1*[2] [13]. From the implementation point of view, the straightforward way is to code in term by term from Eq.(5) and Eq.(6), and for that purpose OpenFOAM offers an excellent platform with its object-oriented structure. However, this way proves to be highly unstable from the numerical performance point of view. In order to improve the numerical stability, we will have a closer look at the physical meaning of the terms in adjoint equations.

A distinctive feature of the adjoint governing equations (as given by Eq.5) is that the convective term comes with the negative sign, which means that for the adjoint variables the flow information is conveyed up the flow. Furthermore, in the adjoint momentum equation there is a contribution from all adjoint equations that are being solved: in the present case these are the adjoint k and ϵ, and this is how the adjoint velocity (and thus also the assesment of the objective function) is sensing the turbulent contribution. Finally, one can note an additional convection term in the adjoint momentum equation, which can be particularly troublesome in the adjoint optimization numerical simulations. The same remark can be made also for the cross-gradient terms in the turbulent adjoint equations.

[2]www.extend-project.de

3.1. Limited time scale

The starting point was to use the the time scale limit, because it is proven to reduce the numerical instabilities in the standard turbulent flow simulations [1]. For the adjoint equations, its impact is multiplied: there are several terms in adjoint equations with T in denominator, where the time scale limitation with Kolmogorov values is highly beneficial for the computational stability.

3.2. Under-relaxation of ”convective term”

The second adjoint convection term is identified to be the troublemaker [7]. However, instead of its convective form (adjoint velocity advected by the primal velocity), it can be turned into d(u.v)=u.dv+v.du, which means it can be viewed as the source term (just like ka.dk and ea.de) plus the gradient of the sensitivity, i.e. this is the contribution of the adjoint velocity and sensitivity which can be treated as the source term - in the present case the under-relaxation has been used.

3.3. Effective flux

The gradients in the second row of adjoint k and eps equations can be viewed as the contribution to the effective flux for the respective adjoint quantities. In addition, assuming that de-unit=dk-unit (the unit vector of the gradient is the same), than can both terms be added to the effective flux.

3.4. Scaled production

The terms in the third row of adjoint k and eps equations are similar to the Pk expression, and in fact if the same scaling is used also for the adjoint velocity, then can these two terms be expressed through Pk. This is beneficial, because the explicit dependency on the adjoint quantity is reduced, and the problem is that the adjoint equations are very sensitive and therefore they can numerically cause problems.

3.5. Boundary conditions

There are several remarks on the implementation of the adjoint equations and their boundary conditions: (1) the wall friction contribution from k and ϵ is not treated explicitly (directly from Eq.38) but implicitly through the diffusivity for adjoint velocity by changing the effective wall turbulent viscosity (last term in Eq.18a); (2) the cross-gradient in adjoint k and ϵ equations, involving gradKgradKStar and gradEpsilongradEpsilonStar respectively (fifth term in 18c, and seventh term in 18d), are treated through the convection by changing the kFlux and epsilonFlux; (3) the outlet boundary condition are first evaluated from the zeroGradient condition (which is the approximation that extrapolates it from the in-domain cell) in order to fill in the matrix, but then they are exactly calculated (from the adjoint boundary condition requirements) and imposed on the outlet face in order to satisfy the objective requirement; (4) the boundary condition that appears for the outlet, which involves both the value and the gradient of the variable (Robin type), is very sensitive - the performance is improved if the expression is averaged over the outlet.

4. Results

The results presented here include the minimization of the dissipated power within a curved duct and an axial diffuser.

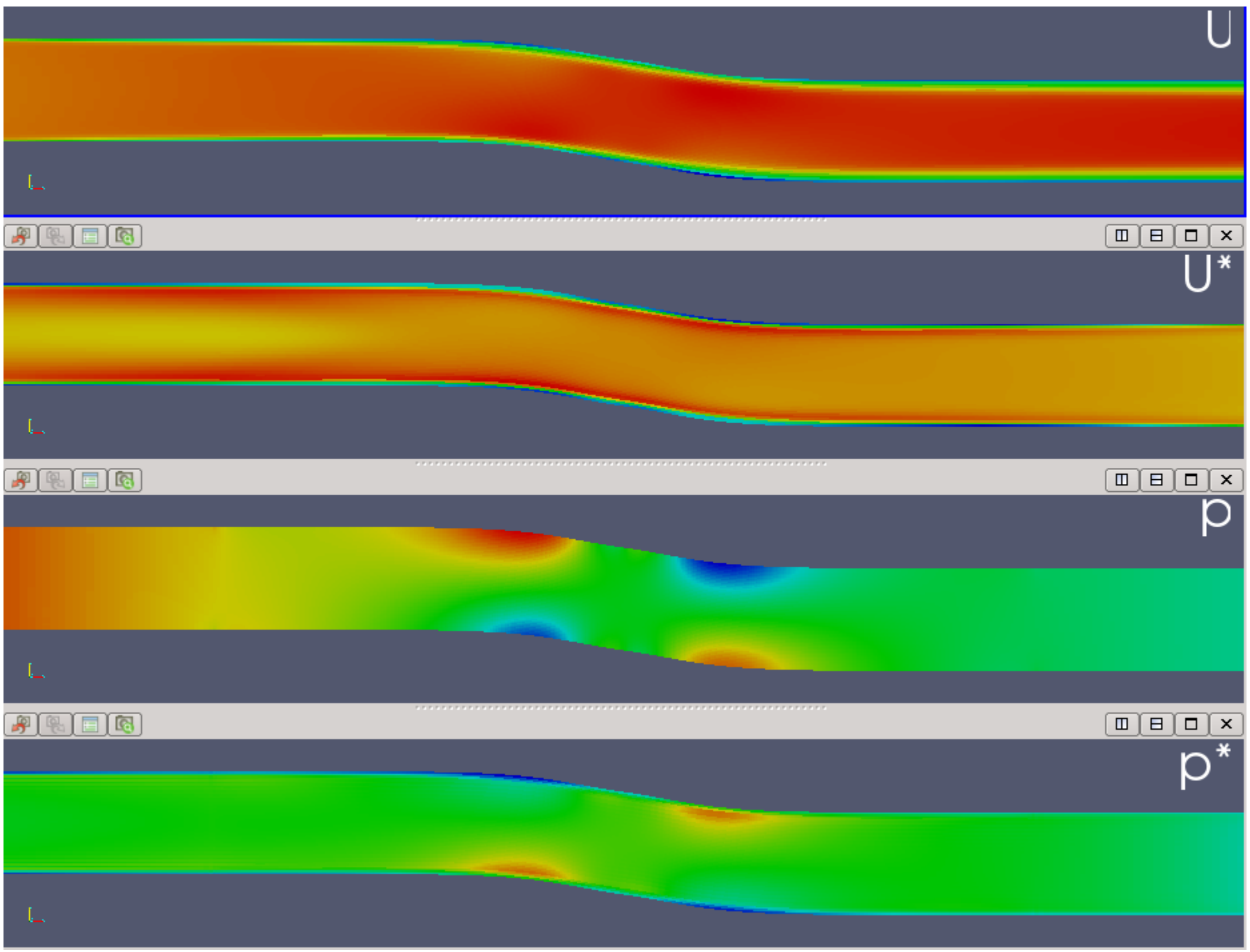

Figure 1: State variables and their adjoint counterparts for a curved duct.

5. Conclusion

Using the adjoint variables the sensitivity of the objective function is calculated without direct dependency on the sensitivity of the state variables. This is the main strength of adjoint method: the sensitivity is calculated with the same cost irrespective of the size of the design variable set.

Solving additional set of adjoint equations is significantly increasing the complexity of the numerical fluid flow simulations. This is even more pronounced for already highly demanding simulations of realistic engineering flows, where the the introduction of the adjoint equations can ruin the numerical stability. This is why an efficient implementation of these additional equations is very important for making the application of the adjoint optimization approach practically possible in realistic engineering problems.

In this paper the implementation of adjoint method has been discussed, focusing on the treatment of the terms that can impede the stability of the simulation: convection, wall, BC.

A Appendix

In this paper the derivation of the adjoint equations and their boundary conditions is performed following the work presented in [15]: in order to scrutinize the expressions presented therein, however, the derivation steps will be discussed here in more details. For the turbulence model equations all derivations steps will be shown here, whereas for the momentum and continuity equations only the final equations will be shown for brevity.

The mathematical manipulation required for the derivation of adjoint equations include: (i) the transformation of the total sensitivity of a variable $\frac{\delta}{\delta b_m}$ into the sum of its partial sensitivity $\frac{\partial}{\partial b_m}$ and the grid sensitivity $\frac{\delta x_k}{\delta b_m}$; (ii) the Gauss theorem $\int_\Omega \frac{\partial \phi}{\partial x_k} d\Omega = \int_\Gamma \phi n_k d\Gamma$; (iii) the integration by parts $\int_\Omega \phi \frac{\partial \psi}{\partial x_k} d\Omega = \int_\Omega \frac{\partial(\phi\psi)}{\partial x_k} d\Omega - \int_\Omega \psi \frac{\partial \phi}{\partial x_k} d\Omega = \int_\Gamma \phi\psi n_k d\Gamma - \int_\Omega \psi \frac{\partial \phi}{\partial x_k} d\Omega$; (iv) the chain rule $\frac{\partial(\phi\psi)}{\partial x_k} = \phi \frac{\partial \psi}{\partial x_k} + \psi \frac{\partial \phi}{\partial x_k}$ (v) the permutation of the partial derivative operators is allowed $\frac{\partial}{\partial x_j}\left(\frac{\partial \phi}{\partial b_m}\right) = \frac{\partial}{\partial b_m}\left(\frac{\partial \phi}{\partial x_j}\right)$; (vi) the indices under an individual integral can be exchanged $\int_\Omega \frac{\partial \phi_i}{\partial x_j} d\Omega = \int_\Omega \frac{\partial \phi_j}{\partial x_i} d\Omega$; (vii) invoking the continuity equation in the terms where it appears $\frac{\partial u_i}{\partial x_i} = 0$.

A 1. Augmented objective function

Applying the Leibniz integral rule to Eq.(4) yields the sensitivity of augmented objective function with respect to the design variables, since for all state variables $\phi = u_i, p, k, \epsilon$ (with starred adjoint counterparts $\phi^* = u_i^*, p^*, k^*, \epsilon^*$) one can write $\frac{\delta(\phi^* R^\phi)}{\delta b_m} = \phi^* \frac{\delta R^\phi}{\delta b_m} + R^\phi \frac{\delta \phi^*}{\delta b_m} = \phi^* \frac{\delta R^\phi}{\delta b_m}$, given that the state equations are taken in the residual form $R^\phi = 0$. In the next step the total sensitivities are recasted into the divergence form: $\frac{\delta R^\phi}{\delta b_m} = \frac{\partial R^\phi}{\partial b_m} + \frac{\partial R^\phi}{\partial x_k}\frac{\delta x_k}{\delta b_m}$. Finally, by making use of the Gauss theorem for the second volume integral, the sensitivity of the above augmented objective function can be further rearranged as:

$$\begin{aligned} \frac{\delta L}{\delta b_m} = \frac{\delta J}{\delta b_m} &+ \int_\Omega \left(u_i^* \frac{\partial R^{u_i}}{\partial b_m} + p^* \frac{\partial R^p}{\partial b_m} + k^* \frac{\partial R^k}{\partial b_m} + \epsilon^* \frac{\partial R^\epsilon}{\partial b_m} \right) d\Omega \\ &+ \int_\Gamma \left(u_i^* R^{u_i} + p^* R^p + k^* R^k + \epsilon^* R^\epsilon \right) n_k \frac{\delta x_k}{\delta b_m} d\Gamma \end{aligned} \tag{7}$$

whereby applying the concept of material derivative it can also be shown that: $\frac{\delta(d\Omega)}{\delta b_m} = \frac{\partial}{\partial x_k}\left(\frac{\delta x_k}{\delta b_m}\right) d\Omega$ [8].

In general case, the objective function can be defined both over a surface (surface based objective) or over a volume (volume based objective) $J = \int_\Gamma J_\Gamma d\Gamma + \int_\Omega J_\Omega d\Omega$. Therefore, in order to obtain the sensitivity of the objective function, the concept of material derivative is applied for both the volume and surface integral:

$$\begin{aligned}\frac{\delta J}{\delta b_m} &= \int_\Omega \frac{\partial J_\Omega}{\partial b_m} d\Omega + \int_\Omega \frac{\partial J_\Omega}{\partial x_k}\frac{\delta x_k}{\delta b_m} d\Omega + \int_\Omega J_\Omega \frac{\delta(d\Omega)}{\delta b_m} \\ &+ \int_\Gamma \frac{\partial J_\Gamma}{\partial b_m} d\Gamma + \int_\Gamma \frac{\partial J_\Gamma}{\partial x_k}\frac{\delta x_k}{\delta b_m} d\Gamma + \int_\Gamma J_\Gamma \frac{\delta(d\Gamma)}{\delta b_m}\end{aligned} \tag{8}$$

where $\frac{\partial J_{\Omega,\Gamma}}{\partial b_m} = \frac{\partial J_{\Omega,\Gamma}}{\partial \phi}\frac{\partial \phi}{\partial b_m}$ is summated over all state variables $\phi = u_i, p, k$ and ϵ. Given that the objective volume is not subject of the spatial deformation, for the surface based objective it must be taken care of whether the objective surface and design surface are separated or not [12].

A 2. Variation step

As an example of the variation terms appearing in the volume integral of Eq.(7), the turbulent viscosity and production of k will be shown first for, as they are appearing in the diffusion and source term of momentum, k and ϵ equations:

$$\frac{\partial T}{\partial b_m} = max\left[\frac{\partial}{\partial b_m}\left(\frac{k}{\epsilon}\right), c_\tau \frac{\partial}{\partial b_m}\left(\frac{\nu}{\epsilon}\right)^2\right] = \frac{1}{\epsilon}\frac{\partial k}{\partial b_m} - \frac{max(k, \frac{c_\tau}{2}\sqrt{\nu/\epsilon})}{\epsilon^2}\frac{\partial \epsilon}{\partial b_m} \tag{9a}$$

$$\frac{\partial \nu_t}{\partial b_m} = c_\mu\left(\frac{k}{\epsilon} + T\right)\frac{\partial k}{\partial b_m} - c_\mu \frac{k}{\epsilon^2} max\left(k, \frac{c_\tau}{2}\sqrt{\frac{\nu}{\epsilon}}\right)\frac{\partial \epsilon}{\partial b_m} \tag{9b}$$

$$\frac{\partial P_k}{\partial b_m} = \left[c_\mu\left(\frac{k}{\epsilon} + T\right)\frac{\partial k}{\partial b_m} - c_\mu \frac{k}{\epsilon^2} max\left(k, \frac{c_\tau}{2}\sqrt{\frac{\nu}{\epsilon}}\right)\frac{\partial \epsilon}{\partial b_m}\right]\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} \tag{9c}$$

$$+\nu_t\left[\frac{\partial}{\partial x_i}\left(\frac{\partial u_j}{\partial b_m}\right) + \frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial b_m}\right)\right]\frac{\partial u_i}{\partial x_j} \tag{9d}$$

$$+\nu_t\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial b_m}\right) \tag{9e}$$

where, coming from the variation of the time scale T (9a), in the expression for the turbulent viscosity there are two terms representing the variation of k and ϵ (9b), whereas for the production of k there are three terms (9c), (9d) and (9e) coming from the variations of the turbulent viscosity, rate of strain and the velocity gradient. For the rest of the derivation stronger condition will be taken: $k/\epsilon = T$ and $k^2/\epsilon^2 = T^2$.

The same procedure is performed for the variations of Eq.(1) for the continuity and momentum equations, as well as Eq.(3) for the transport equations for k and ϵ. In the case of the k transport equation, the variation and its subsequent multiplication by the corresponding adjoint variable k^*, the following expression is obtained:

$$
\begin{aligned}
k^* \frac{\partial R^k}{\partial b_m} =& k^* \frac{\partial k}{\partial x_j} \frac{\partial u_j}{\partial b_m} + k^* u_j \frac{\partial}{\partial x_j} \left(\frac{\partial k}{\partial b_m} \right) && \text{(10a)} \\
& - k^* \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial}{\partial x_j} \left(\frac{\partial k}{\partial b_m} \right) \right] && \text{(10b)} \\
& - k^* \frac{\partial}{\partial x_j} \left[\frac{2 c_\mu}{\sigma_k} \frac{k}{\epsilon} \frac{\partial k}{\partial x_j} \frac{\partial k}{\partial b_m} - \frac{c_\mu}{\sigma_k} \frac{k^2}{\epsilon^2} \frac{\partial k}{\partial x_j} \frac{\partial \epsilon}{\partial b_m} \right] && \text{(10c)} \\
& - k^* \left(2 c_\mu \frac{k}{\epsilon} \frac{\partial k}{\partial b_m} - c_\mu \frac{k^2}{\epsilon^2} \frac{\partial \epsilon}{\partial b_m} \right) \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_i}{\partial x_j} && \text{(10d)} \\
& - k^* \nu_t \left[\frac{\partial}{\partial x_i} \left(\frac{\partial u_j}{\partial b_m} \right) + \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial b_m} \right) \right] \frac{\partial u_i}{\partial x_j} && \text{(10e)} \\
& - k^* \nu_t \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial b_m} \right) && \text{(10f)} \\
& + k^* \frac{\partial \epsilon}{\partial b_m} && \text{(10g)}
\end{aligned}
$$

where (10a) are the terms coming from the convection, in addition to standard diffusivity term (10b) an extra term originating from the expansion of ν_t (10c) is yielded, while the sources in the k transport equation yielded the last four terms: (10d), (10e) and (10f) related to the production, and (10g) related to the dissipation.

In the analogous procedure, the variation of the ϵ transport equation and its multiplication by the corresponding adjoint variable ϵ^*, the following expression is obtained:

$$
\begin{aligned}
\epsilon^* \frac{\partial R^\epsilon}{\partial b_m} =& \epsilon^* \frac{\partial \epsilon}{\partial x_j} \frac{\partial u_j}{\partial b_m} + \epsilon^* u_j \frac{\partial}{\partial x_j} \left(\frac{\partial \epsilon}{\partial b_m} \right) && \text{(11a)} \\
& - \epsilon^* \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon} \right) \frac{\partial}{\partial x_j} \left(\frac{\partial \epsilon}{\partial b_m} \right) \right] && \text{(11b)} \\
& - \epsilon^* \frac{\partial}{\partial x_j} \left[\frac{2 c_\mu}{\sigma_\epsilon} \frac{k}{\epsilon} \frac{\partial \epsilon}{\partial x_j} \frac{\partial k}{\partial b_m} - \frac{c_\mu}{\sigma_\epsilon} \frac{k^2}{\epsilon^2} \frac{\partial \epsilon}{\partial x_j} \frac{\partial \epsilon}{\partial b_m} \right] && \text{(11c)} \\
& - c_1 \epsilon^* \frac{\epsilon}{k} \left(2 c_\mu \frac{k}{\epsilon} \frac{\partial k}{\partial b_m} - c_\mu \frac{k^2}{\epsilon^2} \frac{\partial \epsilon}{\partial b_m} \right) \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial u_i}{\partial x_j} && \text{(11d)} \\
& - c_1 \epsilon^* \frac{\epsilon}{k} \nu_t \left[\frac{\partial}{\partial x_i} \left(\frac{\partial u_j}{\partial b_m} \right) + \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial b_m} \right) \right] \frac{\partial u_i}{\partial x_j} && \text{(11e)} \\
& - c_1 \epsilon^* \frac{\epsilon}{k} \nu_t \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial b_m} \right) && \text{(11f)} \\
& - c_1 \epsilon^* \frac{P_k}{k} \frac{\partial \epsilon}{\partial b_m} + c_1 \epsilon^* P_k \frac{\epsilon}{k^2} \frac{\partial k}{\partial b_m} && \text{(11g)} \\
& + 2 c_2 \epsilon^* \frac{\epsilon}{k} \frac{\partial \epsilon}{\partial b_m} - c_2 \epsilon^* \frac{\epsilon^2}{k^2} \frac{\partial k}{\partial b_m} && \text{(11h)}
\end{aligned}
$$

where (11a) are the terms coming from the convection, again there is the standard diffusivity term (11b) and extra term originating from the expansion of ν_t (11c), while the sources in the ϵ transport equation yielded the last five terms: (11d), (11e), (11f) and (11g) related to the production and its model coefficient, and (11h related to the dissipation and its model coefficient.

The expressions for the variation of the momentum and continuity equations (not included here for brevity), as well as the variation of the transport equations for k and ϵ (10 and 11) are inserted into the Eq.(7). In the next step the terms under the volume integral of Eq.(7) are grouped according to the variations of state variables $\int_\Omega \left[I\left(\frac{\partial u_i}{\partial b_m}\right) + I\left(\frac{\partial p}{\partial b_m}\right) + I\left(\frac{\partial k}{\partial b_m}\right) + I\left(\frac{\partial \epsilon}{\partial b_m}\right)\right] d\Omega$. Subsequently, these integrals are being transformed by deploying the mathematical apparatus listed at the beginning of this section ($i - vii$): for brevity, this step will be shown in the following subsections only for k and ϵ equations. In the last step, based on these individual integrals the adjoint equations and their boundary conditions are being formed by equating the obtained expressions to zero.

The variation integral of the turbulent kinetic energy k reads:

$$
\begin{aligned}
I\left(\frac{\partial k}{\partial b_m}\right) = \int_\Omega d\Omega \, \{ & \underbrace{\frac{2}{3} u_i^* \frac{\partial}{\partial x_i}\left(\frac{\partial k}{\partial b_m}\right)}_{IK1} - \underbrace{u_i^* \frac{\partial}{\partial x_j}\left[2c_\mu \frac{k}{\epsilon}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial k}{\partial b_m}\right]}_{IK2} \\
& + \underbrace{k^* u_j \frac{\partial}{\partial x_j}\left(\frac{\partial k}{\partial b_m}\right)}_{IK3} - \underbrace{k^* \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial k}{\partial b_m}\right)\right]}_{IK4} \\
& - \underbrace{k^* \frac{\partial}{\partial x_j}\left[\frac{2c_\mu}{\sigma_k}\frac{k}{\epsilon}\frac{\partial k}{\partial x_j}\frac{\partial k}{\partial b_m}\right]}_{IK5} - \underbrace{k^*\left(2c_\mu \frac{k}{\epsilon}\frac{\partial k}{\partial b_m}\right)\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j}}_{IK6} \qquad (12) \\
& - \underbrace{\epsilon^* \frac{\partial}{\partial x_j}\left[\frac{2c_\mu}{\sigma_\epsilon}\frac{k}{\epsilon}\frac{\partial \epsilon}{\partial x_j}\frac{\partial k}{\partial b_m}\right]}_{IK7} - \underbrace{c_1 \epsilon^* \frac{\epsilon}{k}\left(2c_\mu \frac{k}{\epsilon}\frac{\partial k}{\partial b_m}\right)\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j}}_{IK8} \\
& + \underbrace{c_1 \epsilon^* P_k \frac{\epsilon}{k^2}\frac{\partial k}{\partial b_m}}_{IK9} - \underbrace{c_2 \epsilon^* \frac{\epsilon^2}{k^2}\frac{\partial k}{\partial b_m}}_{IK10} \, \}
\end{aligned}
$$

The variation integral of the turbulent kinetic energy dissipation rate ϵ:

$$
\begin{aligned}
I\left(\frac{\partial \epsilon}{\partial b_m}\right) = \int_\Omega d\Omega \{ & \underbrace{u_i^* \frac{\partial}{\partial x_j}\left[c_\mu \frac{k^2}{\epsilon^2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial \epsilon}{\partial b_m}\right]}_{IE1} + \underbrace{k^* \frac{\partial}{\partial x_j}\left[\frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon^2}\frac{\partial k}{\partial x_j}\frac{\partial \epsilon}{\partial b_m}\right]}_{IE2} \\
& + \underbrace{k^* \left(c_\mu \frac{k^2}{\epsilon^2}\frac{\partial \epsilon}{\partial b_m}\right)\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j}}_{IE3} + \underbrace{k^* \frac{\partial \epsilon}{\partial b_m}}_{IE4} + \underbrace{\epsilon^* u_j \frac{\partial}{\partial x_j}\left(\frac{\partial \epsilon}{\partial b_m}\right)}_{IE5} \\
& - \underbrace{\epsilon^* \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial \epsilon}{\partial b_m}\right)\right]}_{IE6} + \underbrace{\epsilon^* \frac{\partial}{\partial x_j}\left[\frac{c_\mu}{\sigma_\epsilon}\frac{k^2}{\epsilon^2}\frac{\partial \epsilon}{\partial x_j}\frac{\partial \epsilon}{\partial b_m}\right]}_{IE7} \\
& + \underbrace{c_1 \epsilon^* \frac{\epsilon}{k}\left(c_\mu \frac{k^2}{\epsilon^2}\frac{\partial \epsilon}{\partial b_m}\right)\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j}}_{IE8} \\
& - \underbrace{c_1 \epsilon^* \frac{P_k}{k}\frac{\partial \epsilon}{\partial b_m}}_{IE9} + \underbrace{2 c_2 \epsilon^* \frac{\epsilon}{k}\frac{\partial \epsilon}{\partial b_m}}_{IE10} \}
\end{aligned} \tag{13}
$$

A 3. Integration by parts for k

To devise the final form of the k adjoint equation and the related boundary conditions, the integral (12) is transformed through the integration by parts. The integrals related to the variation of the turbulent kinetic energy $I\left(\frac{\partial k}{\partial b_m}\right)$ read:

$$
\begin{aligned}
IK1 &= \int_\Omega \frac{2}{3} u_i^* \frac{\partial}{\partial x_i}\left(\frac{\partial k}{\partial b_m}\right) d\Omega \\
&= \underbrace{\int_\Gamma \frac{2}{3} u_i^* \frac{\partial k}{\partial b_m} n_i d\Gamma}_{BIK1v} - \underbrace{\int_\Omega \frac{2}{3}\frac{\partial u_i^*}{\partial x_i}\frac{\partial k}{\partial b_m} d\Omega}_{\substack{FIK1 \\ continuity}}
\end{aligned} \tag{14a}
$$

$$
\begin{aligned}
IK2 &= \int_\Omega -u_i^* \frac{\partial}{\partial x_j}\left[2 c_\mu \frac{k}{\epsilon}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial k}{\partial b_m}\right] d\Omega \\
&= \underbrace{\int_\Gamma -u_i^* 2 c_\mu \frac{k}{\epsilon}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial k}{\partial b_m} n_j d\Gamma}_{BIK2v} + \underbrace{\int_\Omega \frac{\partial u_i^*}{\partial x_j} 2 c_\mu \frac{k}{\epsilon}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial k}{\partial b_m} d\Omega}_{FIK2}
\end{aligned} \tag{14b}
$$

$$
\begin{aligned}
IK3 &= \int_\Omega k^* u_j \frac{\partial}{\partial x_j}\left(\frac{\partial k}{\partial b_m}\right) d\Omega \\
&= \int_\Gamma k^* u_j \frac{\partial k}{\partial b_m} n_j d\Gamma - \int_\Omega \frac{\partial (k^* u_j)}{\partial x_j}\frac{\partial k}{\partial b_m} d\Omega \\
&= \underbrace{\int_\Gamma k^* u_j \frac{\partial k}{\partial b_m} n_j d\Gamma}_{BIK3v} - \underbrace{\int_\Omega k^* \frac{\partial u_j}{\partial x_j}\frac{\partial k}{\partial b_m} d\Omega}_{continuity} - \underbrace{\int_\Omega u_j \frac{\partial k^*}{\partial x_j}\frac{\partial k}{\partial b_m} d\Omega}_{FIK3}
\end{aligned} \tag{14c}
$$

$$
\begin{aligned}
IK4 &= \int_\Omega -k^* \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial k}{\partial b_m}\right)\right] d\Omega \\
&= \int_\Gamma -k^* \left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial k}{\partial b_m}\right) n_j d\Gamma + \int_\Omega \frac{\partial k^*}{\partial x_j}\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial k}{\partial b_m}\right) d\Omega \\
&= \underbrace{\int_\Gamma -k^* \left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial}{\partial b_m}\left(\frac{\partial k}{\partial x_j}\right) n_j d\Gamma}_{\substack{BIK4g \\ permutation}} + \underbrace{\int_\Gamma \frac{\partial k^*}{\partial x_j}\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial b_m} n_j d\Gamma}_{BIK4v} \\
&\quad - \underbrace{\int_\Omega \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial k^*}{\partial x_j}\right]\frac{\partial k}{\partial b_m} d\Omega}_{FIK4}
\end{aligned} \tag{14d}
$$

$$
\begin{aligned}
IK5 &= \int_\Omega -k^* \frac{\partial}{\partial x_j}\left[\frac{2c_\mu}{\sigma_k}\frac{k}{\epsilon}\frac{\partial k}{\partial x_j}\frac{\partial k}{\partial b_m}\right] d\Omega \\
&= \underbrace{\int_\Gamma -k^* \frac{2c_\mu}{\sigma_k}\frac{k}{\epsilon}\frac{\partial k}{\partial x_j}\frac{\partial k}{\partial b_m} n_j d\Gamma}_{BIK5v} + \underbrace{\int_\Omega \frac{\partial k^*}{\partial x_j}\frac{2c_\mu}{\sigma_k}\frac{k}{\epsilon}\frac{\partial k}{\partial x_j}\frac{\partial k}{\partial b_m} d\Omega}_{FIK5}
\end{aligned} \tag{14e}
$$

$$
\begin{aligned}
IK6 &= \int_\Omega -k^* \left(2c_\mu \frac{k}{\epsilon}\frac{\partial k}{\partial b_m}\right)\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} d\Omega \\
&= \int_\Omega -k^* \frac{2}{k} c_\mu \frac{k^2}{\epsilon}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j}\frac{\partial k}{\partial b_m} d\Omega = \underbrace{\int_\Omega -2k^* \frac{P_k}{k}\frac{\partial k}{\partial b_m} d\Omega}_{FIK6}
\end{aligned} \tag{14f}
$$

$$
\begin{aligned}
IK7 &= \int_\Omega -\epsilon^* \frac{\partial}{\partial x_j}\left[\frac{2c_\mu}{\sigma_\epsilon}\frac{k}{\epsilon}\frac{\partial \epsilon}{\partial x_j}\frac{\partial k}{\partial b_m}\right] d\Omega \\
&= \underbrace{\int_\Gamma -\epsilon^* \frac{2c_\mu}{\sigma_\epsilon}\frac{k}{\epsilon}\frac{\partial \epsilon}{\partial x_j}\frac{\partial k}{\partial b_m} n_j d\Gamma}_{BIK7v} + \underbrace{\int_\Omega \frac{\partial \epsilon^*}{\partial x_j}\frac{2c_\mu}{\sigma_\epsilon}\frac{k}{\epsilon}\frac{\partial \epsilon}{\partial x_j}\frac{\partial k}{\partial b_m} d\Omega}_{FIK7}
\end{aligned} \tag{14g}
$$

$$
IK8 = \int_\Omega -c_1 \epsilon^* \frac{\epsilon}{k}\left(2c_\mu \frac{k}{\epsilon}\frac{\partial k}{\partial b_m}\right)\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} d\Omega \tag{14h}
$$

$$
IK9 = \int_\Omega c_1 \epsilon^* P_k \frac{\epsilon}{k^2}\frac{\partial k}{\partial b_m} d\Omega \tag{14i}
$$

$$
\begin{aligned}
IK8 + IK9 &= \int_\Omega \left[-c_1 \epsilon^* \frac{\epsilon}{k}\left(2c_\mu \frac{k}{\epsilon}\right)\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} + c_1 \epsilon^* P_k \frac{\epsilon}{k^2}\right]\frac{\partial k}{\partial b_m} d\Omega \\
&= \int_\Omega \left[-2c_1 \epsilon^* \frac{\epsilon}{k} c_\mu \frac{k^2}{\epsilon}\frac{1}{k}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} + c_1 \epsilon^* P_k \frac{\epsilon}{k^2}\right]\frac{\partial k}{\partial b_m} d\Omega \\
&= \underbrace{\int_\Omega -c_1 \epsilon^* P_k \frac{\epsilon}{k^2}\frac{\partial k}{\partial b_m} d\Omega}_{FIK8+9}
\end{aligned} \tag{14j}
$$

$$IK10 = \underbrace{\int_\Omega -c_2\epsilon^* \frac{\epsilon^2}{k^2}\frac{\partial k}{\partial b_m} d\Omega}_{FIK10} \tag{14k}$$

A 4. Integration by parts for ϵ

To devise the final form of the ϵ adjoint equation and the related boundary conditions, the integral (13) is transformed through the integration by parts. The integrals related to the variation of the turbulent kinetic energy dissipation $I\left(\frac{\partial\epsilon}{\partial b_m}\right)$ read:

$$\begin{aligned} IE1 &= \int_\Omega u_i^* \frac{\partial}{\partial x_j}\left[c_\mu \frac{k^2}{\epsilon^2}\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)\frac{\partial \epsilon}{\partial b_m}\right] d\Omega \\ &= \underbrace{\int_\Gamma u_i^* c_\mu \frac{k^2}{\epsilon^2}\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)\frac{\partial \epsilon}{\partial b_m} n_j d\Gamma}_{BIE1v} - \underbrace{\int_\Omega \frac{\partial u_i^*}{\partial x_j} c_\mu \frac{k^2}{\epsilon^2}\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)\frac{\partial \epsilon}{\partial b_m} d\Omega}_{FIE1} \end{aligned}$$

$$\begin{aligned} IE2 &= \int_\Omega k^* \frac{\partial}{\partial x_j}\left[\frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon^2}\frac{\partial k}{\partial x_j}\frac{\partial \epsilon}{\partial b_m}\right] d\Omega \\ &= \underbrace{\int_\Gamma k^* \frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon^2}\frac{\partial k}{\partial x_j}\frac{\partial \epsilon}{\partial b_m} n_j d\Gamma}_{BIE2v} - \underbrace{\int_\Omega \frac{\partial k^*}{\partial x_j}\frac{c_\mu}{\sigma_k}\frac{k^2}{\epsilon^2}\frac{\partial k}{\partial x_j}\frac{\partial \epsilon}{\partial b_m} d\Omega}_{FIE2} \end{aligned} \tag{15a}$$

$$\begin{aligned} IE3 &= \int_\Omega k^* \left(c_\mu \frac{k^2}{\epsilon^2}\frac{\partial \epsilon}{\partial b_m}\right)\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} d\Omega \\ &= \int_\Omega k^* c_\mu \frac{k^2}{\epsilon}\frac{1}{\epsilon}\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j}\frac{\partial \epsilon}{\partial b_m} d\Omega = \underbrace{\int_\Omega k^* \frac{P_k}{\epsilon}\frac{\partial \epsilon}{\partial b_m} d\Omega}_{FIE3} \end{aligned} \tag{15b}$$

$$IE4 = \underbrace{\int_\Omega k^* \frac{\partial \epsilon}{\partial b_m} d\Omega}_{FIE4} \tag{15c}$$

$$\begin{aligned} IE5 &= \int_\Omega \epsilon^* u_j \frac{\partial}{\partial x_j}\left(\frac{\partial \epsilon}{\partial b_m}\right) d\Omega \\ &= \int_\Gamma \epsilon^* u_j \frac{\partial \epsilon}{\partial b_m} n_j d\Gamma - \int_\Omega \frac{\partial(\epsilon^* u_j)}{\partial x_j}\frac{\partial \epsilon}{\partial b_m} d\Omega \\ &= \underbrace{\int_\Gamma \epsilon^* u_j \frac{\partial \epsilon}{\partial b_m} n_j d\Gamma}_{BIE5v} - \underbrace{\int_\Omega \epsilon^* \frac{\partial u_j}{\partial x_j}\frac{\partial \epsilon}{\partial b_m} d\Omega}_{continuity} - \underbrace{\int_\Omega u_j \frac{\partial \epsilon^*}{\partial x_j}\frac{\partial \epsilon}{\partial b_m} d\Omega}_{FIE5} \end{aligned} \tag{15d}$$

$$
\begin{aligned}
IE6 &= \int_\Omega -\epsilon^* \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial \epsilon}{\partial b_m}\right)\right] d\Omega \\
&= \int_\Gamma -\epsilon^* \left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial \epsilon}{\partial b_m}\right) n_j d\Gamma + \int_\Omega \frac{\partial \epsilon^*}{\partial x_j}\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial}{\partial x_j}\left(\frac{\partial \epsilon}{\partial b_m}\right) d\Omega \\
&= \underbrace{\int_\Gamma -\epsilon^* \left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial}{\partial b_m}\left(\frac{\partial \epsilon}{\partial x_j}\right) n_j d\Gamma}_{\substack{BIE6g \\ permutation}} + \underbrace{\int_\Gamma \frac{\partial \epsilon^*}{\partial x_j}\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon}{\partial b_m} n_j d\Gamma}_{BIE6v} \\
&\quad \underbrace{- \int_\Omega \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\epsilon}\right)\frac{\partial \epsilon^*}{\partial x_j}\right]\frac{\partial \epsilon}{\partial b_m} d\Omega}_{FIE6}
\end{aligned} \tag{15e}
$$

$$
\begin{aligned}
IE7 &= \int_\Omega \epsilon^* \frac{\partial}{\partial x_j}\left[\frac{c_\mu}{\sigma_\epsilon}\frac{k^2}{\epsilon^2}\frac{\partial \epsilon}{\partial x_j}\frac{\partial \epsilon}{\partial b_m}\right] d\Omega \\
&= \underbrace{\int_\Gamma \epsilon^* \frac{c_\mu}{\sigma_\epsilon}\frac{k^2}{\epsilon^2}\frac{\partial \epsilon}{\partial x_j}\frac{\partial \epsilon}{\partial b_m} n_j d\Gamma}_{BIE7v} - \underbrace{\int_\Omega \frac{\partial \epsilon^*}{\partial x_j}\frac{c_\mu}{\sigma_\epsilon}\frac{k^2}{\epsilon^2}\frac{\partial \epsilon}{\partial x_j}\frac{\partial \epsilon}{\partial b_m} d\Omega}_{FIE7}
\end{aligned} \tag{15f}
$$

$$
IE8 = \int_\Omega c_1 \epsilon^* \frac{\epsilon}{k}\left(c_\mu \frac{k^2}{\epsilon^2}\frac{\partial \epsilon}{\partial b_m}\right)\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} d\Omega \tag{15g}
$$

$$
IE9 = \int_\Omega -c_1 \epsilon^* \frac{P_k}{k}\frac{\partial \epsilon}{\partial b_m} d\Omega \tag{15h}
$$

$$
\begin{aligned}
IE8 + IE9 &= \int_\Omega \left[c_1 \epsilon^* \frac{\epsilon}{k} c_\mu \frac{k^2}{\epsilon^2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} - c_1 \epsilon^* \frac{P_k}{k}\right]\frac{\partial \epsilon}{\partial b_m} d\Omega \\
&= \int_\Omega \left[c_1 \epsilon^* \frac{\epsilon}{k} c_\mu \frac{k^2}{\epsilon}\frac{1}{\epsilon}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)\frac{\partial u_i}{\partial x_j} - c_1 \epsilon^* \frac{P_k}{k}\right]\frac{\partial \epsilon}{\partial b_m} d\Omega \\
&= \underbrace{\int_\Omega \left(c_1 \epsilon^* \frac{\epsilon}{k}\frac{P_k}{\epsilon} - c_1 \epsilon^* \frac{P_k}{k}\right)\frac{\partial \epsilon}{\partial b_m} d\Omega = 0}_{FIE8+9}
\end{aligned} \tag{15i}
$$

$$
IE10 = \underbrace{\int_\Omega 2 c_2 \epsilon^* \frac{\epsilon}{k}\frac{\partial \epsilon}{\partial b_m} d\Omega}_{FIE10} \tag{15j}
$$

References

1. P.A. Durbin. On the k-3 stagnation point anomaly. *International Journal of Heat and Fluid Flow*, 17(1):89-90, 1996.
2. K.C. Giannakoglou, D.I. Papadimitriou, E.M. Papoutsis-Kiachagias, C. Othmer. Adjoint methods in CFD-based optimization - gradient computation and beyond. In *European Congress on Computational Methods in Applied Sciences and Engineering - ECCOMAS 2012 (Edited by J. Eberhardsteiner et.al.)*, 10-24, 2012.
3. M.B. Giles, N.A. Pierce. An Introduction to the Adjoint Approach to Design. *Flow, Turbulence and Combustion*, 65:393415, 2000.
4. W.P. Jones, B.E. Launder. The Prediction of Laminarization with a Two-Equation Model of Turbulence. *International Journal of Heat and Mass Transfer*, 15:301-314, 1972.
5. S.K. Nadarajah, A. Jameson. A Comparison of the Continuous and Discrete Adjoint Approach to Automatic Aerodynamic Optimization. *AIAA-2000-0667*.
6. C. Othmer. A continuous adjoint formulation for the computation of topological and surface sensitivities of ducted flows. *International Journal for Numerical Methods in Fluids*, 58(8):861877, 2008.
7. C. Othmer. Adjoint methods for car aerodynamics. *Journal of Mathematics in Industry*, 4:6, 2014.
8. D. Papadimitriou, K. Giannakoglou. A Continuous Adjoint Method with Objective Function Derivatives Based on Boundary Integrals for Inviscid and Viscous Flows. *Computers and Fluids*, 36:325-341, 2007.
9. O. Pironneau. On optimum design in fluid mechanics. *Journal of Fluid Mechanics*, 64:97-110, 1974.
10. M. Popovac, K. Hanjalic. Compound Wall Treatment for RANS Computation of Complex Turbulent Flows and Heat Transfer. *Flow Turbulence and Combustion*, 78:177-202, 2007.
11. D.B. Spalding. A Single Formula for the ”Law of the Wall”. *Journal of Applied Mechanics*, 28(3):455-458, 1961.
12. A. Stueck, T. Rung. Adjoint RANS with filtered shape derivatives for hydrodynamic optimisation. *Computers and Fluids*, 47(1):22-32, 2011.
13. H.G. Weller, G. Tabora, H. Jasak, C. Fureby. A tensorial approach to computational continuum mechanics using object-oriented techniques. *Computers in Physics*, 12:620-631, 1998.
14. A.S. Zymaris, D.I. Papadimitriou, K.C. Giannakoglou, C.Othmer. Continuous Adjoint Approach to the Spalart-Allmaras Turbulence Model for Incompressible Flows. *Computers and Fluids*, 38:1528-1538, 2009.
15. A.S. Zymaris, D.I. Papadimitriou, K.C. Giannakoglou, C.Othmer. Adjoint wall functions: A new concept for use in aerodynamic shape optimization. *Journal of Computational Physics*, 229(13):5228-5245, 2010.