TOPOLOGICAL DERIVATIVE FORMULATION FOR SHAPE SENSITIVITY IN **INCOMPRESSIBLE TURBULENT FLOWS**

Aleksandar JEMCOV^{1*}, Darrin STEPHENS²

¹Aerospace and Mechanical Engineering and Center for Research Computing, University of Notre

Dame, Indiana, USA

²Applied CCM Pty Ltd, PO BOX 2220, Dandenong North, Victoria, 3175, Australia

* Corresponding author, E-mail address: ajemcov@nd.edu

ABSTRACT

Shape derivative based on topological consideration is presented in this work. The resulting derivative has simpler form compared to corresponding classical shape derivative due to topological derivative formulation. Shape derivative is based on topological derivative in the limit of infinitesimally weak source terms in momentum equation approaching the boundary of the computational domain. The consistency of two derivatives is demonstrated and computational example of the flow in curved duct is used for the illustration of the derivative computations.

Keywords: CFD, adjoint, incompressible, turbulent, topological derivative, shape derivative

NOMENCLATURE

- A PDE operator
- \mathscr{B} Boundary operator
- С Linear operator
- α Arbitrary test function
- D_k Turbulent kinetic energy diffusivity $[m^2/s]$
- D_{ε} Turbulent dissipation diffusivity $\left[\frac{m^2}{s}\right]$
- GTurbulence production
- Η Domain height
- $\mathcal{J}_{\mathcal{L}}^{,J}$ Output functional
- Lagrangian
- Ν Number
- P Parameters
- Q State vector
- BΓ Bilinear concommitant
- b Bilinear boundary operator
- c_1, c_2, c_μ Turbulence model parameters
- $c_k, c^*_{\mu_k}, c_{\varepsilon}, c^*_{\mu_{\varepsilon}}$ Adjoint turbulence model parameter Adjoint wall friction velocity [m/s] u_{tau}^*
- Multiplicative parameter c_s
- Momentum source f
- k Turbulent kinetic energy, $[m2/s^2]$
- boundary normal n
- boundary tangent t
- Density normalized pressure, $[m^2/s^2]$ р
- Velocity, [m/s]u
- y^+ Non-dimensional wall distance
- Ω Computational domain
- Г Boundary of computational domain
- Γ_b, Γ_0 Boundary segments of computational domain
- δ Variational derivative
- Turbulent dissipation, $[m^2/s^3]$ ε
- η Indictor function
- ν Kinematic viscosity, $[m^2/s]$

- Turbulent Kinematic viscosity, $[m^2/s]$ v_t
- ξ Local direction
- φ General variable

Sub/superscripts

- face f
- i Cartesian component of a vector or tensor *i*
- j Cartesian component of a vector or tensor j
- Adjoint variable * *
- Derivative of a variable '

INTRODUCTION

Computing the shape derivatives in turbulent incompressible flows is a basic requirement for any design optimisation gradient based algorithm. Solution of continuous adjoint Navier-Stokes equations is a method of choice for many applications of design optimisation problems where gradient information is required due to its efficiency in computing gradients (Nadarajah and Jameson, 2000), (Jameson et al., 2008), (Anderson and Venkatakrishnan, 1997). Adjoint incompressible equations lead to two different formulations of the sensitivity gradients: shape derivatives and topological derivatives (Othmer, 2008). Both approaches have been used in design optimisation to produce optimal shapes and optimal domains. Despite their differences, Othmer (Othmer, 2008) have shown that they produce consistent gradients close to the boundary of the domain. Therefore, the interesting prospect of using topological derivatives in shape optimisation is investigated in this paper.

In this work, continuous adjoint Navier-Stokes equations that account for the effect of turbulence in computation of the adjoint field (Castro et al., 2007), (Bueno-Orovio et al., 2012), (Zymaris et al., 2010) are used. In addition, a new way of computing the shape sensitivity derivatives is proposed. The new approach is based on the topological formulation of the sensitivity derivative in the limit of vanishing source term in Navier-Stokes equations. The source term used in the formulation is equivalent to a porosity source term with vanishing porosity coefficient. This formulation allows for the classical definition and the topological sensitivity using the adjoint and primal velocity fields that can be transformed to the shape sensitivity derivative through a process of local interpolation. Given the weak source term (porosity asymptotically approaching zero), the Navier-Stokes equations are not modified in the limit of zero strength of source term while the adjoint system of equations can still be used to compute the topological derivative. This is possible due to the fact that adjoint system is formulated with arbitrarily small porosity coefficients and the passage to the zero limit is performed after Lagrangian duality for the Navier-Stokes system is enforced.

GOVERNING EQUATIONS

Consider a CFD problem in abstract formulation:

$$\mathcal{A}(\mathbf{Q}) = 0 \text{ in } \Omega \tag{1}$$
$$\mathcal{B}(\mathbf{Q}) = 0 \text{ on } \Gamma = \Gamma_b \cup \Gamma_a$$

Define functional of interest that we would like to minimize:

$$\mathcal{J}(\mathcal{P}, \mathbf{Q}(\mathcal{P})) = 0 \text{ on } \Gamma_o \tag{2}$$

The output functional J usually represents a measure of



Figure 1: Computational domain.

the performance of an engineering device and it can be defined on the boundary Γ or within the computational domain Ω . Examples of functionals include integral of the force on the surface, dissipated power in the domain, uniformity of the profile of the velocity on the outlet, to name a few. Output functionals \mathscr{J} depend on the independent variable \mathbf{Q} and some parameters \mathscr{P} . The nature of parameters \mathscr{P} is such that they can represent quantities used to input data for the model such as material properties, model constants and/or boundary condition values. They can also define the shape of the computational domain and here we are mostly concerned with functionals that depend on parameters describing the shape of the domain. In other words, we are interested in computing the shape derivatives of functionals \mathscr{J} with respect to parameters \mathscr{P} defining the shape of the domain.

Computing derivative of output functionals \mathcal{J}_i with respect to parameter \mathcal{P}_i is defined analytically as

$$\delta_{\mathscr{P}_{j}}\mathscr{J}_{j}(\mathscr{P}_{j},\mathbf{Q}(\mathscr{P}_{j})) = \lim_{\beta \to 0} \frac{\partial}{\partial \beta} \mathscr{J}_{i}(\mathscr{P}_{j} + \beta \mathscr{R}_{j}) \quad (3)$$

Rules of differentiation are well defined for directional derivatives that are similar to gradient calculations. In other words, chain rule of differentiation can be applied to Eq. (3) resulting in the need to compute derivatives of the independent variable \mathbf{Q} with respect to parameter \mathscr{P} . In this work direct computation of derivatives of independent variable \mathbf{Q} with respect to shape parameters \mathscr{P} is avoided through the introduction of adjoint variables, thus simplifying the problem significantly.

Incompressible turbulent system of Navier-Stokes equations

is given by the following expression:

$$\mathscr{A} = \begin{pmatrix} \mathscr{A}_{1} \\ \mathscr{A}_{2} \\ \mathscr{A}_{3} \\ \mathscr{A}_{4} \end{pmatrix}$$

$$\begin{pmatrix} \partial_{i}u_{i} \\ u_{j}\partial_{j}u_{i} + \partial_{i}p - \partial_{j}\left[(\mathbf{v} + \mathbf{v}_{t})(\partial_{j}u_{i} + \partial_{i}u_{j})\right] + f_{i} \\ u_{j}\partial_{j}k - \partial_{j}(D_{k}\partial_{j}k) - G + \varepsilon \\ u_{j}\partial_{j}\varepsilon - \partial_{j}(D_{\varepsilon}\partial_{j}\varepsilon) - c_{1}G\frac{\varepsilon}{k} + c_{2}\frac{\varepsilon^{2}}{k} \end{pmatrix}$$

$$(4)$$

The system of equations defined in Eq. (4) consist of incompressible continuity and momentum equations supplemented by the $k - \varepsilon$ turbulence model equations responsible for the transport of the turbulent kinetic energy and dissipation. Appropriate boundary conditions and transport properties must accompany the system of equations (4).

Our goal is to derive adjoint system of equations based on Eq. (4) and this is accomplished by introducing the Lagrangian \mathscr{L}

$$\mathscr{L} = \mathscr{J} + \langle \mathbf{Q}^*, \mathscr{A} \rangle \tag{5}$$

Vector of adjoint variables \mathbf{Q}^* plays the role of Lagrangian multipliers whereas integral \mathscr{J} represents the quantity that is being optimized.

$$\mathscr{L} = \mathscr{J} + \int_{\Omega} \left(\begin{array}{cc} p^* & u_i^* & k^* & \varepsilon^* \end{array} \right) \left(\begin{array}{c} \mathscr{A}_1 \\ \mathscr{A}_2 \\ \mathscr{A}_3 \\ \mathscr{A}_4 \end{array} \right) d\Omega \quad (6)$$

In order to define the system of adjoint equations, we seek to compute the total variation of Lagrangian \mathcal{L} by following the rules of the variational calculus:

$$\delta \mathscr{L} = \delta_{\mathscr{P}} \mathscr{L} + \delta_{u_i} \mathscr{L} + \delta_p \mathscr{L} + \delta_k \mathscr{L} + \delta_{\varepsilon} \mathscr{L}$$
(7)

The total variation includes variations of all fields that depend on parameter(s) \mathcal{P} . In principle, expression for the total variation in Eq. (7) can be used to define the shape derivative if all individual variations in that expression are known. However, computing the variation of the Lagrangian with respect to primitive variables p, u_i, k , and ε involves computing the derivatives of the Navier-Stokes system of equations with respect to those variables since they are known only implicitly thorough the solution of the system of equations defined in Eq. (4). Therefore, in order to compute total variation of Lagrangian with N parameters \mathcal{P}_j , N independent problems defined through derivatives of the Navier-Stokes system of equations have to be solved. This is computationally very expensive even though the resulting system of equations is linear. Therefore, a cheaper way of computing variations of the Lagrangian with respect to primitive variables is required. One way of achieving this goal is by simply requiring that variations with respect to state variables vanish. This can be stated trivially as the following expression:

$$\delta_{u_i}\mathcal{L} + \delta_p\mathcal{L} + \delta_k\mathcal{L} + \delta_{\varepsilon}\mathcal{L} = 0 \tag{8}$$

With this requirement the total variation of the Lagrangian takes a simplified form

$$\delta \mathscr{L} = \delta_{\mathscr{P}} \mathscr{J} + \delta_{\mathscr{P}} \int_{\Omega} \mathbf{Q}^* \mathscr{A} d\Omega \tag{9}$$

Since the variation of the Lagrangian with respect to parameter \mathscr{P} explicitly is trivial, the only remaining unknown part is find the way to compute the integral:

$$\delta_{\mathscr{P}} \int_{\Omega} \mathbf{Q}^* \mathscr{A} d\Omega \tag{10}$$

Computation of the total variation of Lagrangian requires that we know the values of Lagrange multipliers \mathbf{Q}^* . Adjoint variables are computed through the introduction of the Lagrange duality principle. Lagrange duality principle for a general linear operator **C** acting on a general variable ϕ is given by the following expression:

$$\left\langle \phi^*, \mathbf{C}\phi' \right\rangle_{\Omega} = \left\langle \phi', \mathbf{C}^*\phi^* \right\rangle_{\Omega} + \mathbf{B}_{\Gamma}$$
 (11)

or in explicit integral form

$$\int_{\Omega} \phi^* \mathbf{C} \phi' d\Omega = \int_{\Omega} \phi' \mathbf{C}^* \phi^* d\Omega + \int_{\Gamma} b(\phi', \phi^*) d\Gamma \qquad (12)$$

where the notation $\delta_{\mathscr{P}}\phi = \phi'$ was used for simplicity. Eq. (12) and Eq. (8) are used to define the expression

$$\delta_{p} \mathscr{J} + \int_{\Omega} \mathbf{Q}^{*} \delta_{p} \mathscr{A} d\Omega$$

$$+ \quad \delta_{u_{i}} \mathscr{J} + \int_{\Omega} \mathbf{Q}^{*} \delta_{u_{i}} \mathscr{A} d\Omega$$

$$+ \quad \delta_{k} \mathscr{J} + \int_{\Omega} \mathbf{Q}^{*} \delta_{k} \mathscr{A} d\Omega$$

$$+ \quad \delta_{\varepsilon} \mathscr{J} + \int_{\Omega} \mathbf{Q}^{*} \delta_{\varepsilon} \mathscr{A} d\Omega = 0 \quad (13)$$

Variational differentiation of operator \mathscr{A} defines the linearisation of non-linear operator \mathscr{A} in some suitably defined neighbourhood defined by a particular value of the state vector **Q**. In other words, if the linearisation of the operator \mathscr{A} in Eq. (4) is known, then Eq. (13) can be used to define adjoint equations that will be used to compute adjoint variables **Q**^{*} needed for the computation of the derivatives in Eq. (10). Following the rules of the differentiation, the differentiated continuity equation with respect to parameter \mathscr{P} is given by

$$\delta_{\mathscr{P}}\mathscr{A}_1 = \partial_i \delta_{\mathscr{P}} u_i \tag{14}$$

while differentiated momentum equation is given by expression

$$\delta_{\mathscr{P}}\mathscr{A}_{2} = u_{j}\partial_{j}\delta_{\mathscr{P}}u_{i} + \delta_{\mathscr{P}}u_{j}\partial_{j}u_{i} + \partial_{i}\delta_{\mathscr{P}}p - \partial_{j}\left[(\mathbf{v} + \mathbf{v}_{t})(\partial_{j}\delta_{\mathscr{P}}u_{i} + \partial_{i}\delta_{\mathscr{P}}u_{j})\right] - \partial_{j}\left[\delta_{\mathscr{P}}\mathbf{v}_{t}(\partial_{j}u_{i} + \partial_{i}u_{j})\right] + \delta_{\mathscr{P}}f_{i}$$
(15)

and the differentiated turbulent kinetic and dissipation equations in $k - \varepsilon$ turbulence model is given by the following two expressions:

$$\begin{split} \delta_{\mathscr{P}}\mathscr{A}_{3} &= \delta_{\mathscr{P}}u_{j}\partial_{j}k + u_{j}\partial_{j}\delta_{\mathscr{P}}k - \partial_{j}(D_{k}\partial_{j}\delta_{\mathscr{P}}k) \\ &- \partial_{j}(\delta_{\mathscr{P}}D_{k}\partial_{j}k) - \delta_{\mathscr{P}}G + \delta_{\mathscr{P}}\varepsilon \end{split}$$
(16)

$$\begin{split} \delta_{\mathscr{P}}\mathscr{A}_{4} &= \delta_{\mathscr{P}}u_{j}\partial_{j}\varepsilon + u_{j}\partial_{j}\delta_{\mathscr{P}}\varepsilon - \partial_{j}(D_{\varepsilon}\partial_{j}\delta_{\mathscr{P}}\varepsilon) \\ &- \partial_{j}(\delta_{\mathscr{P}}D_{\varepsilon}\partial_{j}\varepsilon)c_{1}\delta_{\mathscr{P}}G\frac{\varepsilon}{k} - c_{1}G\frac{\delta_{\mathscr{P}}\varepsilon}{k} \\ &+ c_{1}G\frac{\varepsilon}{k^{2}}\delta_{\mathscr{P}}k + 2c_{2}\frac{\varepsilon}{k}\delta_{\mathscr{P}}\varepsilon - c_{2}\frac{\varepsilon^{2}}{k^{2}}\delta_{\mathscr{P}}k \end{split}$$
(17)

Application of the Lagrange duality principle leads to the following integral that is equivalent to expression in Eq. (13)

$$\int_{\Omega} (\partial_{p} J_{\Omega} + \mathscr{A}_{1}^{*}) \delta_{\mathscr{P}} p d\Omega + \int_{\Gamma} (\partial_{p} J_{\Gamma} + \mathscr{B}_{1}) \delta_{\mathscr{P}} p d\Gamma$$

$$+ \int_{\Omega} (\partial_{u_{i}} J_{\Omega} + \mathscr{A}_{2}^{*}) \delta_{\mathscr{P}} u_{i} d\Omega + \int_{\Gamma} (\partial_{u_{i}} J_{\Gamma} + \mathscr{B}_{2}) \delta_{\mathscr{P}} u_{i} d\Gamma$$

$$+ \int_{\Omega} (\partial_{k} J_{\Omega} + \mathscr{A}_{3}^{*}) \delta_{\mathscr{P}} k d\Omega + \int_{\Gamma} (\partial_{k} J_{\Gamma} + \mathscr{B}_{3}) \delta k_{\mathscr{P}} d\Gamma$$

$$+ \int_{\Omega} (\partial_{\varepsilon} J_{\Omega} + \mathscr{A}_{4}^{*}) \delta_{\mathscr{P}} \varepsilon d\Omega$$

$$+ \int_{\Gamma} (\partial_{\varepsilon} J_{\Gamma} + \mathscr{B}_{4}) \delta_{\mathscr{P}} \varepsilon d\Gamma = 0 \qquad (18)$$

Where functional \mathscr{J} was split into boundary and interior contributions

$$\mathscr{J} = J_{\Gamma} + J_{\Omega} \tag{19}$$

Requiring that each term in Eq. (18) is equal to zero in the domain we define the set of adjoint equations: *Adjoint continuity*:

$$\mathscr{A}_1^* = -\partial_i u_i^* + \partial_p J_\Omega = 0 \tag{20}$$

Adjoint momentum:

$$\mathscr{A}_{2}^{*} = - u_{j}\partial_{j}u_{i}^{*} - u_{j}\partial_{i}u_{j}^{*} - \partial_{j}\left[\mathbf{v}(\partial_{j}u_{i}^{*} + \partial_{i}u_{j}^{*})\right] + \partial_{i}p^{*}]$$

$$+ k^{*}\partial_{i}k + \varepsilon^{*}\partial_{i}\varepsilon + 2\partial_{j}\left[k^{*} + c_{1}\varepsilon^{*}\frac{\varepsilon}{k}\mathbf{v}_{t}(\partial_{j}u_{i} + \partial_{i}u_{j})\right]$$

$$+ f_{i}^{*} + \partial_{u_{i}}J_{\Omega} = 0, \qquad (21)$$

Adjoint k equation:

$$\mathcal{A}_{3}^{*} = - u_{j}\partial_{j}k^{*} - \partial_{j}(D_{k}\partial_{j}k^{*}) + c_{\mu_{k}}^{*}\partial_{j}k\partial_{j}k^{*} - c_{\mu_{k}}^{*}G^{*}k^{*} + c_{\mu_{k}}^{*}\partial_{j}\varepsilon\partial_{j}\varepsilon^{*} + c_{k}\varepsilon^{*} + c_{\mu_{k}}^{*}(\partial_{j}u_{i} + \partial_{i}u_{j})\partial_{j}u_{i}^{*} + \partial_{k}J_{\Omega} = 0,$$
(22)

Adjoint ε equation:

$$\mathscr{A}_{4}^{*} = - u_{j}\partial_{j}\varepsilon^{*} - \partial_{j}(D_{k}\partial_{j}\varepsilon^{*}) - c_{\mu_{\varepsilon}}^{*}\partial_{j}\varepsilon\partial_{j}\varepsilon^{*} + c_{\varepsilon}^{*}\varepsilon^{*} + c_{\mu_{\varepsilon}}^{*}\partial_{j}k\partial_{j}k^{*} + c_{\mu_{\varepsilon}}G^{*}k^{*} + k^{*} - c_{\mu_{\varepsilon}}^{*}(\partial_{j}u_{i} + \partial_{i}u_{j})\partial_{j}u_{i}^{*} + \partial_{\varepsilon}J_{\Omega} = 0,$$
(23)

$$c_{\mu_{k}}^{*} = 2c_{\mu}\frac{k}{\varepsilon},$$

$$c_{k} = -c_{1}c_{\mu}G^{*} - c_{2}\frac{\varepsilon^{2}}{k^{2}},$$

$$c_{\mu_{\varepsilon}}^{*} = c_{\mu}\frac{k^{2}}{\varepsilon^{2}},$$

$$c_{\varepsilon} = 2c_{2}\frac{\varepsilon}{k}.$$

Similar requirement for the boundary terms yields boundary conditions for adjoint equations where unbalanced surface integral terms must be perfectly balanced by terms in the original output functional \mathscr{J} and its derivatives. In addition, adjoint wall functions were defined in (Zymaris *et al.*, 2010) for the case of adjoint $k - \varepsilon$ turbulence model. The wall conditions for the adjoint ε conditions are defined in a similar way as the primal ε equation throug the definition of of the adjoint wall velocity u_{τ}^* :

$$u_{\tau}^{*} = (\mathbf{v} + \mathbf{v}_{t}) \left(\frac{\partial u_{i}^{*}}{\partial x_{j}} + \frac{\partial u_{j}^{*}}{\partial x_{i}} \right) n_{j} t_{i}.$$
(24)

Eq. (24) is used to compute the adjoint viscous fluxes at the wall in the same way as the primal viscous fluxes are computed.

TOPOLOGICAL DERIVATIVE

Directional derivative previously was defined to be

$$\delta \mathscr{L} = \delta_{\mathscr{P}} \mathscr{J} + \delta_{\mathscr{P}} \int_{\Omega} \mathbf{Q}^* \mathscr{A} d\Omega \tag{25}$$

Applying the rules of differentiation

$$\delta_{\mathscr{P}} \int_{\Omega} \mathbf{Q}^* \mathscr{A} d\Omega = \int_{\Omega} \mathbf{Q}^* \delta_{\mathscr{P}} \mathscr{A} d\Omega + \int_{\Omega} \delta_{\mathscr{P}} \mathbf{Q}^* \mathscr{A} d\Omega \quad (26)$$

Variation of adjoint variables is second order contribution and will be ignored

$$\delta_{\mathscr{P}} \int_{\Omega} \mathbf{Q}^* \mathscr{A} d\Omega = \int_{\Omega} \delta_{\mathscr{P}} \mathbf{Q}^* \mathscr{A} d\Omega \qquad (27)$$

We can now compute the derivative

$$\delta_{\mathscr{P}} \int_{\Omega} \mathbf{Q}^* \mathscr{A} d\Omega = \int_{\Omega} \left(\begin{array}{cc} p^* & u_i^* & k^* & \varepsilon^* \end{array} \right) \begin{pmatrix} \delta_{\mathscr{P}} \mathscr{A}_1 \\ \delta_{\mathscr{P}} \mathscr{A}_2 \\ \delta_{\mathscr{P}} \mathscr{A}_3 \\ \delta_{\mathscr{P}} \mathscr{A}_4 \end{pmatrix} d\Omega$$
(28)

If the forcing term in momentum equation is given by

$$f_i = \mathscr{P} u_i \eta \tag{29}$$

then the derivative becomes

$$\delta_{\mathscr{P}} \int_{\Omega} \mathbf{Q}^* \mathscr{A} d\Omega = \int_{\Omega} \left(\begin{array}{cc} p^* & u_i^* & k^* & \varepsilon^* \end{array} \right) \left(\begin{array}{c} 0 \\ u_i \eta \\ 0 \\ 0 \end{array} \right) d\Omega$$
(30)

Total variation of the Lagrangian is

$$\delta \mathscr{L} = \delta_{\mathscr{P}} \mathscr{J} + \int_{\Omega} \delta_{\mathscr{P}} \mathbf{Q}^* \mathscr{A} d\Omega \tag{31}$$

Since there is no explicit dependence of \mathcal{J} on \mathcal{P} , directional derivative at each cell becomes

$$\delta_{\mathscr{P}}\mathscr{L}_{j} = u_{i}u_{i}^{*}\eta\Omega_{j}.$$
(32)

Therefore, in order to evaluate this directional derivative we need to compute primal and adjoint velocities. Topological derivative in Eq. (31) depends only on the primal and adjoint fields, volume and characteristic function η that defines the location of the source term within the domain. There are no restrictions on where that location can be as long as the source term is within the computational domain Ω . Therefore, we can consider the source term distribution defined very close to the boundary Γ_0 that is being modified.



Figure 2: Sources distribution.

The connection between the topological derivative and the shape derivative can be seen if we consider the limit of the source term moving closer and closer to the boundary of the domain. In Figure 2 we consider one such situation in which we would like to compute the topological derivative infinitesimally close to the boundary Γ_0 . Using the values of the computed sensitivity in its current location, linear extrapolation is used to define the value close to the boundary:

$$(u_i u_i^*)_f = (u_i + \xi_j \partial_j u_i \triangle u_i)(u_i^* + \xi_j \partial_j u_i^* \triangle u_i^*)\eta$$
(33)

$$\Delta u_i = u_i - u_{if}, \ \Delta u_i^* = u_i - u_{if}^* \tag{34}$$



Figure 3: Sources distribution.

If the source term is approaching the surface in the direction of the local normal, then local direction ξ can be expressed as $\xi = ||\xi||\mathbf{n}$ thus leading to the expression

$$(u_i u_i^*)_f = ||\xi||^2 (n_j \partial_j u_i \triangle u_i) (n_j \partial_j u_i^* \triangle u_i^*) \eta$$
(35)

Taking into account boundary conditions close to the wall and the following inequalities

$$||\partial_{j}u_{i}u_{i}|| > ||u_{i}||, \ ||\partial_{j}u_{i}^{*}u_{i}^{*}|| > ||u_{i}^{*}||$$
(36)

gives an expression for topological derivative infinitesimally close to the boundary of the domain

$$(u_i u_i^*)_f \approx ||\xi||^2 (n_j \partial_j u_i u_i) (n_j \partial_j u_i^* u_i^*) \eta \tag{37}$$

Equation (37) is consistent with the definition of the shape derivative defined as (Othmer, 2008)

$$\delta_{\mathscr{P}}\mathscr{L}_{S} = -(\mathbf{v} + \mathbf{v}_{t})n_{j}\partial_{j}u_{i}u_{i}n_{j}\partial_{j}u_{i}^{*}u_{i}^{*}A_{j}$$
(38)

up to a multiplicative parameter c_s and neglecting the contributions of adjoint turbulent fields to shape derivative value. Using the expression in Eq. (37) the shape derivative is defined as

$$\delta_{\mathscr{P}}\mathscr{L}_{S_i} = c_s u_i u_i^* \Omega_j \eta \tag{39}$$

Multiplicative parameter c_s can be shown to correspond to the following expression

$$c_s = \frac{\mathbf{v} + \mathbf{v}_t}{||\boldsymbol{\xi}||^2} \tag{40}$$

Equation (39) will be used to move the boundary Γ_0 in order to optimise the shape. Therefore, action of moving boundary replaces the source term distribution in momentum equation and for small changes in the shape the source term becomes negligible. This corresponds to vanishing source term limit in the momentum equation.

COMPUTATIONAL ALGORITHM

Computational algorithm for computing the shape derivatives consists of following steps:

- 1. Compute primal field **Q** using governing equations defined in Eq. (4) in the limit $f_i \rightarrow 0$
- 2. Compute adjoint field \mathbf{Q}^* using adjoint equations defined in Eq. (20), Eq. (21), Eq. (22), and Eq. (23) in the limit $f_i^* \to 0$
- 3. Compute shape derivative using the definition from the equation Eq. (39)

NUMERICAL RESULTS

In order to demonstrate the shape derivative computation, turbulent incompressible flow in a two-dimensional S-shaped duct is used as an example. The computational mesh is given in figure (4). The height of the first layer of cells is selected so that the value of y^+ is within the range of 30 to 50 enabling the use of wall functions for near wall modelling of turbulent fields. The inlet boundary condition is specified as a uniform velocity value equal to 5m/s while the outlet pressure boundary condition correspond to zero gauge pressure condition. Kinematic viscosity is specified to be $v = 1 \times 10^{-5} [m^2/s]$ while the height of the domain is H = 0.1 m giving the Reynolds number of 50,000. Results of the computation of the prime field are given in figures (5) and (6).

Output functional that was used to compute shape derivatives corresponds to dissipated power functional given by the following expression:

$$\mathscr{J} = -\int_{\Gamma} \left(p + \frac{1}{2} ||U||^2 \right) u_i n_i d\Gamma$$
(41)

This functional represents a measure of the dissipated energy within the duct and this particular form of the functional is selected so that admissible boundary conditions are possible for adjoint equations. Shape parameters \mathcal{P}_i are positions of centroids of finite volume faces on all wall boundaries. Computed shape sensitivity is given in the figure (7). The computed sensitivity field indicates that in order to decrease losses based on Eq. (41) the face centroids should be moved in such way so that duct becomes straight. This is intuitively correct result since the losses due to total pressure changes within the duct will be at their local minimum if the duct is straight. It should be also observed that the shape derivatives computed here are given in their raw form without any smoothing. Before these derivatives can be used in any gradient based optimisation algorithm, a smoothing procedure should be applied in order to control the roughness of the resulting new shape. However, this was not the subject of the current work.

CONCLUSIONS

Shape derivative based on topological arguments was derived in this paper. The newly proposed way of computing shape derivatives results in a simple expression involving only the primal and adjoint fields. It was also shown that topological derivative is consistent with the definition of the shape derivatives when source terms in momentum equation are infinitesimally close to the boundary of the domain in the limit of vanishing source term intensity. An example of the computation of shape derivatives using topological arguments demonstrates consistency with the classical formulation of shape derivatives.

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Figure 7: Sensitivity Vectors.