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Adjoint-Based Sensitivity Analysis for Buoyancy-Driven Incompressible Navier-Stokes Equations with Heat Transfer

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Abstract

This paper presents the adjoint-based sensitivity equation and the adjoint buoyancydriven, steady-state Navier-Stokes-Fourier equations for a perfect gas. Related applications are of relevance for the optimisation of fluids-engineering devices where the temperature distribution is crucial, *e.g.* in thermal comfort studies. Starting from the weakly compressible, buoyancy-driven, Reynolds-averaged Navier-Stokes-Fourier (RANS-F) equations, the coupled adjoint equations and the resulting sensitivity equation are derived. Attention is confined to shape design for temperature-wake optimisation using a continuous adjoint approach. The example included refers to a laminar, two-dimensional (2D) ducted flow around a heated ellipsoid, for which the predicted sensitivity is verified against results obtained from a direct differentiation approach. Results convey that the predicted sensitivity generally mimics the gradient of the cost function.

Keywords: sensitivity analysis, heat transfer, adjoint Navier-Stokes-Fourier equations, shape optimisation, Boussinesq approximation, finite volume method.

1 Introduction

The adjoint sensitivity analysis has become an established technique for shape optimisation when many degrees of freedom are present [1, 2, 3]. Using weakly compressible, segregated computational procedures based upon pressure correction or pressure projection techniques, which are widely employed in industrial computational fluid dynamics (CFD), the continuous adjoint approach is of advantage [4, 5, 6]. The approach is based on an augmented cost function \tilde{J} which inheres the primal governing equations (here the RANS-F equations) as constraints which have to be satisfied in the computational domain. Accordingly, the primal RANS-F equations are augmented with Lagrange multipliers and added to the thermo-fluid dynamic cost function. For shape optimisation, the variational formulation of the augmented cost function indicates the behaviour of the cost function with the variation of the shape. The ansatz is restricted to small variations in surface-normal direction as the variation is linearised. Permitting arbitrary variations of the flow field variables (pressure, temperature, velocity), the adjoint RANS-F equations and the sensitivity equation, which displays the gradient of the cost function, are derived. Subsequently, a simple, gradient-based, *steepest descent* optimisation technique might guide the morphing process of the shape in order to obtain an improved cost function. Contrary to other optimisation strategies, the adjoint approach only needs one flow simulation for both, the primal and the adjoint system, no matter how many design parameters are present.

The paper will focus upon coupled momentum-energy-transport systems in an virtually incompressible fluid environment. The buoyancy term is approximated by a Boussinesq ansatz [7], which supplies an additional source term to the primal momentum equation. Starting from the primal RANS-F equations [8], the adjoint (dual) equations and the sensitivity equations are derived along a route described by other recent publications [9, 10, 11]. The study is confined to the sensitivity of the temperature wake behind a heated, 2D ellipsoid that is centrally mounted in a channel. Steadystate simulations are performed with the open source finite volume solver open field operation and manipulation (OpenFOAM) [12]. The comparison between the gradient obtained from the direct differentiation and the adjoint approach reveals that the sensitivity generally predicts the gradient of the cost function with fair accuracy.

2 Theory

2.1 Primal Momentum-Heat Transport System

We consider steady-state systems for virtually incompressible fluids where buoyancy is a driving force in the momentum equation. Using the Boussinesq-ansatz [7] for modeling the buoyancy influence, the momentum equation obtains a supplementary temperature dependent term. The system is closed by the energy equation for perfect gas, given by Equation (1)

$$\frac{\partial}{\partial x_j} u_i u_j = -\frac{\partial p^*}{\partial x_i} + \frac{\partial}{\partial x_j} \left(2\nu_g S_{ij} \right) + \left(1 - \beta (T - T_0) \right) \cdot g_i ,$$

$$\frac{\partial u_i}{\partial x_i} = 0 ,$$

$$u_j \frac{\partial T}{\partial x_j} = \frac{\partial}{\partial x_j} \left(k_{eff} \frac{\partial T}{\partial x_j} \right) + 2 \frac{\nu_g}{c_v} S_{ij} \frac{\partial u_i}{\partial x_j} ,$$
(1)

where $p^* = \frac{p + \frac{2}{3}k\rho}{\rho}$ is the modified pressure (enhanced by isotropic contributions of the turbulence model), ρ is related to the density, $\nu_g = \nu + \nu_t$ is the effective kine-

matic viscosity as sum of kinematic turbulent and molecular viscosity, β is the volume expansion coefficient, g_i the gravity acceleration vector, c_v the specific heat capacity, $\kappa_{eff} := \frac{\kappa}{c_v \rho} + \frac{\kappa_t}{c_v \rho}$ is the sum of turbulent and laminar heat conductivity scaled with $\frac{1}{c_v \cdot \rho}$ and $2S_{ij} := \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ is the symmetric rate-of-strain tensor. Mind that the gravity vector acts in negative z/x_3 -direction.

2.2 Derivation of Adjoint System

The subsection presents the derivation of the adjoint energy, momentum and continuity equations. The residual form of the RANS-F equations is denoted in Equation (2)

These primal equations are augmented with Lagrange multipliers $(\hat{T}, \hat{u}, \hat{p})$ and added to the cost function J. This leads to an augmented cost function \tilde{J} . The linearised variation $\delta^{lc}\tilde{J}$ of the augmented cost function consists of convective and local variations. The local variation describes the variation of the flow on the original location. The convective variation describes the variation of the (old) flow due to a change of location by δn . As the primal residual equations are fulfilled everywhere, the convective variation of the RANS-F with respect to the operator $\delta^c \equiv \frac{\partial}{\partial n} \delta n$ vanishes. Typical cost functions of the present study involve the definition of Γ_{obj} , the boundary where the cost function is evaluated, along the inlet and outlet, whereas Γ_{dsg} , the surface which is enabled for shape variations, is chosen to be a wall boundary of the heated ellipsoid. Therefore $\Gamma_{dsg} \cap \Gamma_{obj} = \emptyset$ and no convective variations of the cost function exist. The variation of the augmented cost function is denoted by Equation (3)

$$\delta^{lc}\tilde{J} = \delta^{lc}J + \int \left(\hat{u}_i\delta^l R_i + \hat{p}\delta^l Q + \hat{T}\delta^l H\right)d\Omega .$$
(3)

Integration by parts leads to a formulation where variations of primal flow variables can be factored out. Using the frozen-turbulence assumption [5] ($\delta^{lc}\mu_g \equiv 0$), we finally arrive at the adjoint volume equations for the adjoint momentum (\hat{u}_i), continuity (\hat{p}) and temperature (\hat{T}), given by Equation (4)

$$-2u_{j}\hat{S}_{ij} + \frac{\partial\hat{p}}{\partial x_{i}} - \frac{\partial}{\partial x_{j}}\left(2\nu_{g}\hat{S}_{ij}\right) + \hat{T}\frac{\partial T}{\partial x_{i}} + \frac{\partial}{\partial x_{j}}\left(2\frac{\nu_{g}}{c_{v}}\hat{T}S_{ij}\right) = 0,$$

$$\frac{\partial\hat{u}_{i}}{\partial x_{i}} = 0, \qquad (4)$$

$$-u_{j}\frac{\partial\hat{T}}{\partial x_{j}} - \frac{\partial}{\partial x_{j}}\left(k_{eff}\frac{\partial\hat{T}}{\partial x_{j}}\right) + \hat{u}_{j} \cdot g_{j} \cdot \beta = 0,$$

where $2\hat{S}_{ij} = \left(\frac{\partial \hat{u}_i}{\partial x_j} + \frac{\partial \hat{u}_i}{\partial x_j}\right)$. The system is closed by appropriate boundary conditions, given in Equation (5) and Equation (6).

Adjoint boundary conditions for inlet and wall

$$\hat{T} = 0,
\hat{u}_t = 0,
\hat{u}_n = -\frac{\partial j_{\Gamma}}{\partial p},
\frac{\partial \hat{p}}{\partial n} = 0.$$
(5)

Adjoint boundary conditions for outlet

$$u_{i}\hat{u}_{i} + u_{n}\hat{u}_{n} + \nu_{g}\frac{\partial\hat{u}_{n}}{\partial n} + \frac{\partial j_{\Gamma}}{\partial u_{n}} = \hat{p} ,$$

$$\hat{u}_{t}u_{n} + \nu_{g}\frac{\partial\hat{u}_{t}}{\partial n} + \frac{\partial j_{\Gamma}}{\partial u_{t}} = 0 ,$$

$$\hat{T}u_{n} + \kappa_{eff}\frac{\partial\hat{T}}{\partial n} + \frac{\partial j_{\Gamma}}{\partial T} = 0 .$$
(6)

We assume prescribed velocity and fixed pressure gradient at wall and inlet, fixed velocity gradient and prescribed pressure at the outlet. Note that the Boussinesq term is now settled at the right-hand side of the temperature equation, whereas terms involving the adjoint temperature have been transferred to the right-hand side of the momentum equation.

2.3 Derivation of sensitivity equation

Having solved the adjoint RANS-F equations, the remaining non-zero part of the augmented cost function variation, defined at a wall boundary is given in Equation (7)

$$\delta \tilde{J} \equiv \delta^l \tilde{J} = -\oint \kappa_{eff} \delta n \frac{\partial T}{\partial n} \frac{\partial \hat{T}}{\partial n} d\Gamma - \oint \nu_g \delta n \frac{\partial u_t}{\partial n} \frac{\partial \hat{u}_t}{\partial n} d\Gamma .$$
⁽⁷⁾

From this we compute the adjoint sensitivity, i.e. the gradient of the cost function with respect to a normal variation of the boundary, along the design surface and obtain

$$\frac{\partial \tilde{J}}{\partial n} \approx -\oint_{\Gamma_{dsg}} \kappa_{eff} \frac{\partial T}{\partial n} \frac{\partial \hat{T}}{\partial n} d\Gamma - \oint_{\Gamma_{dsg}} \nu_g \frac{\partial u_t}{\partial n} \frac{\partial \hat{u}_t}{\partial n} d\Gamma .$$
(8)

2.4 Optimisation with steepest descent

The steepest descent method is perhaps the most simple optimisation approach which steps in the negative direction of the gradient. It can readily be coupled to the result of a sensitivity analysis along Γ_{dsg} . Using mesh morphing tools like in the automatic netgeneration for structural analysis (ANSA) [13], the computational grid is optimised, by moving each surface cell of Γ_{dsg} in the direction of the negative gradient multiplied by an arbitrary (unique) step size α . This paper will however only focus on the comparison between the gradients obtained from an efficient adjoint technique and a direct sensitivity analysis of design-surface perturbations.

3 Verification

The adjoint equations are similar to the primal equations. Therefore a great portion of the primal solver can be re-used to solve the adjoint equations. In conjunction with the present study, a semi-implicit pressure linked equation solver (SIMPLE) is used within the open source CFD environment OpenFOAM.

The adjoint sensitivity displays the gradient of the cost function with respect to a normal displacement of the design surface. For verification purposes we compare the adjoint sensitivity to the gradient of the cost function obtained from a direct differentiation method. The latter is based upon shifting each discrete boundary element of Γ_{dsg} by a small distance in normal direction and evaluate the related change of cost function. Note that the comparison deliberately ignores non-linear interactions and is thus confined to small variations.

3.1 Heated Ellipsoid

For the verification study we simulate the laminar flow over a 2D heated ellipsoid which is centrally mounted in a channel. The computational domain covers $10^{-2}m$ x $2 \times 10^{-3}m$. The ellipsoid has a height of $2 \times 10^{-4}m$. Only half of the symmetric configuration is computed. The mesh consists of 24 000 hexahedral control volumes and features hanging nodes. Figure 1 displays the computational grid.



Figure 1: Computational Grid

The inlet velocity is assigned to $1.5 \times 10^{-1} \frac{m}{s}$. The Reynolds number based on the height of the channel $(h = 2 \times 10^{-3}m)$ is $Re_h = 20$. The mean temperature is set to T = 290K. The ellipsoid is heated with a temperature of T = 291K. The related Grashof number is $Gr = \frac{g \cdot \beta \cdot \Delta T h^3}{\nu^2} = 1$, with acceleration force component $g = 9.81 \frac{m^2}{s}$ and $\beta = 3 \times 10^{-3}/K$.

The upper and lower domain boundaries were assigned to symmetry boundary conditions. For inlet and outlet we employ typical boundary conditions, i.e. prescribed velocity and temperature as well as zero pressure gradient at inlet and zero gradient for temperature and velocity as well as prescribed pressure at the outlet. A no-slip wall is applied along the ellipsoid (design surface). The temperatures are set to 290Kalong the lower and upper boundaries and T = 291K along the design surface. For the simulation we use the buoyant SIMPLE solver *buoyantBoussinesqSimpleFoam.C* of OpenFOAM and its adjoint analogue. The verification study employs a *uniformity of temperature* cost function at the outlet as an example for the adjoint sensitivity analysis. The cost function J is defined as

$$J = \int_{\Gamma_{out}} j_{\Gamma} d\Gamma := \int_{\Gamma_{out}} \frac{1}{2} \left(T - T_d \right)^2 d\Gamma , \qquad (9)$$

where T_d denotes a desired temperature, which in this case refers to $T_d = 291K$. The cost function is associated to a contribution to the adjoint boundary condition (6) defined in Equation (10)

$$\frac{\partial j_{\Gamma}}{\partial T} = (T - T_d) \quad . \tag{10}$$

As the chosen cost function only depends on the temperature, all other boundary contributions of the cost function vanish.

3.2 Results

All simulations were iterated over 25 000 iterations to guarantee a fair level of convergence. In Figure 2, Figure 3 and Figure 4 the results for the primal velocity and density are presented.



Figure 2: Predicted primal magnitude of the velocity



Figure 4: Predicted primal density field

Due to the influence of heating, small density variations occur in the vicinity of the ellipsoid $(0.997\frac{g}{m})$ which are convected downstream. The temperature has its maximum at the ellipsoid and also features a plume downstream of the heated obstacle. Since the Re-number is fairly low, a significant amount of diffusion distributes the density and temperature plume along the complete outlet cross section. The displacement of the velocity field towards the upper boundary induced by the obstacle is supported by buoyancy terms downstream of the ellipsoid.

Figure 5 and 6 depict the results for the adjoint velocities, temperature and pressure.



Figure 5: Adjoint x-velocity (left) and y-velocity (right)



Figure 6: Adjoint temperature (left) and pressure (right)

Note that the adjoint solution usually runs "backward" but has no strict physical meaning, therefore the plausibility of the results is usually hard to judge. The main criterion on judging the quality of the results is the sensitivity. The sensitivity is computed from the primal and adjoint flow field in a postprocessing step, according to Equation (8). The normal gradients of the primal and adjoint velocity are computed with the Open-FOAM function *snGrad* and projected into the tangential direction. Results of the discrete adjoint sensitivity analysis are outlined in Figure 7 including a diagram for the sensitivity plotted on the surface of the ellipsoid. The diagram shows the 410 discrete design surface elements along the abscissa and their sensitivity values on the ordinate.



Figure 7: Contour plot (left) and diagram (right) of adjoint sensitivity for test case Heated Ellipsoid

Large improvements are obtained at the ends of the ellipsoid, smaller ones along the crest. Note that the sensitivity displays the gradient of the cost function with respect to an outward movement of the surface, i.e. with respect to increasing the fluid volume.

We will now compare the gradient of the cost function obtained from the adjoint solution with the gradient of the cost function obtained from a direct differentiation approach using (first-order) finite differences. We thus approximate the gradient of the cost function for each node on the surface Γ_{dsg} from a first-order accurate differencing scheme, according to Equation (11)

$$\frac{\partial J}{\partial n} \approx \frac{J_{new} - J_{old}}{\delta n} \quad . \tag{11}$$

Note that this approximation is only valid for perturbations, which are small enough to neglect non-linearities, but prone to numerical errors for very small perturbations. The generation of the required 400 computational meshes has been scripted to minimise mesh-quality influences on the approximated cost function gradient and a normal perturbation of $\delta n = 2 \times 10^{-7} m$ has been used in the present study. Figure 8 shows the sensitivities along the axis of the ellipsoid obtained from the direct differentiation approach.



Figure 8: Sensitivity obtained from a direct differentiation

Figure 9 shows the comparison of the adjoint sensitivity and the gradient of the direct differentiation approach.



Figure 9: Sensitivity from direct differentiation plotted on ellipsoid

The adjoint sensitivity displays a satisfactory agreement with the result of the direct differentiation analysis. The agreement deteriorates at the respective ends of the obstacle due to pronounced local non-linearities of the primal flow field (i.e. flow reversal). The trend – or sign of the gradient – however always agrees between the two gradient evaluation techniques.

4 Conclusion

The adjoint buoyancy-driven Navier-Stokes-Fourier equations have been derived from the primal equations along the line of the continuous adjoint approach. A Boussinesq approximation has been used to model buoyancy influences. The adjoint system has been exemplified for the case of a temperature related objective function, located away from the design surface at the outlet. A verification study at low Re-number reveals a fair predictive agreement between the adjoint sensitivity and the gradient obtained from the direct differentiation. Related deviations can primarily be attributed to nonlinearities. Inconsistencies between the discrete primal and dual approach might also have a small influence, but are deemed negligible due to the dominance of the selfadjoint diffusion mechanisms. Future work is devoted to more complex thermo-fluid dynamic applications.

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