

INDUSTRIAL OPTIMISATION SOLUTIONS BASED ON OPENFOAM®¹ TECHNOLOGY

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Abstract. *This paper presents a fast gradient-based optimisation method for automotive flow design using the open-source toolbox OpenFOAM® as the development environment. The usability and flexibility of OpenFOAM® in the prediction of aerodynamic forces and detailed flow structures of passenger vehicles has been validated and demonstrated.*

A deterministic optimisation method is developed and implemented in the aerodynamic design of an automotive vehicle. The proposed methodology is based on a RANS flow solver, while the required gradients are calculated using the continuous Adjoint technique.. The conjugate gradients method has been used to drive the calculated gradients to zero and update the design parameters. Optimisation is performed by means of drag coefficient (C_D) minimisation while the modification of the vehicle geometry is carried out using a localised surface deformation technique. The theory underlying the computation of the Adjoint sensitivities is briefly discussed as well as the implementation of the optimisation and surface deformation methodologies into the open-source toolbox OpenFOAM®. Results are presented as proof-of-concept for the drag reduction of an automotive vehicle showing that significant benefits can be gained by the use of the developed method.

1 INTRODUCTION

Computational Fluid Dynamics (CFD) methods have matured to a stage, where it is possible to gain substantial insight into fluid flow processes of engineering relevance.

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However, the motives of fluid dynamics engineers typically go beyond improved understanding to the definitive aim of improving the performance of the engineering systems in consideration. It is in recognition of circumstances that the present paper investigates the use of automated design optimisation methodologies in order to boost the power of CFD for engineering design purposes.

Optimum design problems require the merit or performance of designs to be measured explicitly in terms of an objective function. At the same time, it may be required that one or more constraints should be satisfied. To describe allowable variations in design, mesh-morphing is introduced for the model shape to be modified with no need for parameterisation of the CAD model or automatic mesh generation. The method can however be disadvantaged by having a negative impact on the quality of the modified mesh. The existing mesh is deformed based on predefined actions, such as stretching or contraction of nodes, thus saving computational time during each optimisation loop. The allowed freedom of the shape is defined via three control points that can move in all xyz-directions, thus 9 design parameters/degrees of freedom.

The optimisation method described in this paper is a continuous Adjoint gradient-based method. There is a long history of the use of the Adjoint technique in CFD shape optimisation with the major contributors being Jameson [1], Giles [2], Anderson [3] and others. During the past few years many investigators used and extended the Adjoint method mainly for aerodynamic design focused on the aerodynamics of airfoils, which involve very simple boundary conditions as well as simple parameterisations [4]. An example of a more complicated application of Adjoint CFD optimisation is presented in [5] where shape optimisation has been performed on diesel fuel injectors in terms of cavitation control.

In the automotive industry experiment is still the main designing tool. Nevertheless, it's not at all likely that repeated trial in an interactive design and analysis procedure can lead to a truly optimum design. Using an automated optimisation method, not only designs can be rapidly evaluated but directions of improvement can be identified as well. Possession of techniques which result in a faster design cycle gives a crucial advantage in a competitive environment. Steps towards this direction are addressed in the present paper, using the Adjoint method. This study is a parallel work of an optimisation performed on the same vehicle using traditional stochastic methods such as genetic algorithms [6].

The Adjoint method has a number of advantages relative to other gradient-based methods, for example finite differences. Apart from its rapid convergence, it provides the gradients of the cost function in a way that the computational effort required for this calculation is independent of the number of the design variables. Of course the possibility of getting trapped into local minima exists as in every gradient-based method. In the Adjoint method the governing flow equations are treated as constraints by adding them to the cost function through Lagrange multipliers providing the augmented form of the cost functional. By taking the variation of the augmented cost function and the consequent limitation of the flow field variations, the Adjoint variables' variations as well as the sensitivity derivatives of the cost function with respect to the design variables are obtained. The gradient of the cost function at each location of the design space is dependent on the flow field and the co-state variables distribution along the wall to be designed. So, the efficient solution of the flow and the

Adjoint equations may lead to the calculation of the exact values of the sensitivity derivatives.

The problem setup and the solution procedure in OpenFOAM is depicted in the following sections. Results of the aerodynamic optimisation of an automotive vehicle are presented and discussion about the method and the possibility of improvement follow. Conclusions drawn from the results indicate the necessity and benefits of further development.

2 ADJOINT EQUATIONS

In this section, the Adjoint equations are described, together with the derivation of the sensitivities for the specific problem considered in this paper. For the sake of generality during the analysis an arbitrary cost function is defined and noted I_C .

The incompressible Navier-Stokes flow equations, to be noted as $R(U)$, reads:

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0, \\ \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} - \mathbf{T}) &= \rho \mathbf{g}, \end{aligned} \quad (0.1)$$

$$\text{where, } \mathbf{T} = -p\mathbf{I} + \mu \left[\nabla \otimes \mathbf{u} + (\nabla \otimes \mathbf{u})^T \right]$$

These are integrated and introduced as constraints to the optimisation problem. In this way it is ensured that the state variables are uniquely determined for a given set of parameters in the domain of interest. The analysis of [7] has been followed for the extraction of the Adjoint equations and their boundary conditions. The considered cost function I_C is augmented to the weak form of the constraints $R(U)$, through the Lagrange multiplier Ψ to give the augmented cost function I_{aug} :

$$\begin{aligned} I_{aug} &= I_C + \int_V \Psi \cdot R dV = I_C + \int_V \Psi_p \cdot \nabla \cdot \mathbf{u} dV + \int_V \Psi_u \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} - \mathbf{T}) dV = \\ & I_C + \int_{\partial V} \Psi_p \cdot \mathbf{u} \vec{n} dA + \int_{\partial V} \Psi_u \cdot (\rho \mathbf{u} \otimes \mathbf{u} - \mathbf{T}) \vec{n} dA - \int_V \nabla \Psi_p \cdot \mathbf{u} dV + \int_V (\nabla \otimes \Psi_u) \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} - \mathbf{T}) dV \end{aligned} \quad (0.2)$$

where, $\Psi = (\Psi_u, \Psi_p)^T$, $\Psi_u = (\Psi_1, \Psi_2, \Psi_3)$ is the vector of the co-state variables, V is the computational domain. The second equality results by application of the Green-Gauss theorem. ∂V is the boundary around the domain V , dA is the infinitesimal area and $\vec{n} = (n_x, n_y, n_z)$ is the outward normal vector along ∂V .

The augmented cost function I_{aug} is a functional of the flow variables U , the co-state or Adjoint variables Ψ and the vector of design variables D . An optimal point of the minimisation problem should meet the above necessary conditions, reads:

$$R(U) = 0$$

$$\frac{\partial I_{aug}}{\partial U} = 0 \quad (0.3)$$

$$\frac{\partial I_{aug}}{\partial D} = 0$$

The first condition is satisfied by the solution of the flow equations. The derivation of the Adjoint equations results from the second condition. The design variables D are considered fixed while solving these equations from which the vector of co-state variables Ψ is obtained. Having solved the Adjoint equations and obtained the co-state variables their values can be substituted to the third condition giving the Adjoint gradients with respect to the design variables D . The design parameters D can be updated using the conjugate gradient method [8] and the whole process is then repeated. A more detailed analysis of the extraction of the Adjoint equations can be found [5, 9]. The final form Adjoint equations read:

$$\begin{aligned} -\nabla \cdot \Psi_{\mathbf{u}} &= 0 \\ -\rho \mathbf{u} \left(\nabla \otimes \Psi_{\mathbf{u}} + (\nabla \otimes \Psi_{\mathbf{u}})^T \right) - \nabla \cdot \mathbf{T}_{adj} &= 0, \end{aligned} \quad (0.4)$$

$$\text{where } \mathbf{T}_{adj} = -\rho \Psi_p I + \mu \left(\nabla \otimes \Psi_{\mathbf{u}} + (\nabla \otimes \Psi_{\mathbf{u}})^T \right).$$

The above expressions are very similar to the Navier-Stokes equations and can be characterised as the co-state or Adjoint continuity and momentum equations without having the corresponding physical meaning.

The scope of this paper is the aerodynamic improvement of an automotive vehicle. As a result, the cost function can be defined in terms of minimising the drag coefficient $I_c = C_D$. A multi-objective test case involving other objectives is possible but for a first approach was considered out of the scope of this paper.

From the analysis [9], the following boundary conditions are derived for the specific cost function:

$$\Psi_{\mathbf{u}} = -\vec{e}_i \quad \text{on the moving boundaries/objective} \quad (0.5)$$

$$\nabla_i \Psi_{\mathbf{u}} = \mathbf{0} \quad \text{on the non-moving boundaries/non-objective} \quad (0.6)$$

where \vec{e}_i is the direction of the flow. The Adjoint velocities ($\Psi_{\mathbf{u}}$) can be considered equal to zero at the inlet and exit since $\Psi_{\mathbf{u}}$ becomes negligible towards the farfield. For stability reasons inbound and outbound flow is interchangeable during the computation. At the non-moving boundaries, $\Psi_{\mathbf{u}}$ is treated as a ‘‘slip’’ condition (eq. (0.6)). For the Adjoint pressure Ψ_p Neumann condition is applied for the whole domain:

$$\nabla \Psi_p = 0 \quad \text{on the wall boundaries} \quad (0.7)$$

As in the case of Ψ_u , for the Adjoint pressure as well inbound and outbound flow is interchangeable during the calculation. This condition at the inlets and outlets is considered to ensure stability in the Adjoint flow. The reason is that the Adjoint velocities are generated from the moving surface towards the domain and are not corresponding to the physical inlets and outlets.

Once the Adjoint system of equations is solved and the Adjoint variables are calculated the sensitivity derivatives can be computed and driven to zero as implied by the 3rd condition of equation (0.8). In the general case the gradients can be estimated according to [5, 10] as:

$$\delta I_{aug} = \frac{\partial I_C}{\partial D} \delta D + \iint_W p \Psi_u \delta(\bar{n}dA) + \iint_W \bar{n} \mu \left[\nabla \otimes \Psi_u + (\nabla \otimes \Psi_u)^T \right] \delta \mathbf{u} \quad (0.9)$$

By accounting for the boundary conditions of the specific case of this paper the Adjoint gradients reduce to the 3rd term of equation (0.9). This term is actually resulting through partial differentiation of the diffusion part of the Adjoint equations. Following the analysis proposed by Anderson [3], it can be expressed in terms of design variables. Expressing the velocities on the new surface in a Taylor series and noting that the velocities on the old and new surface are both zero, the variation of the velocity components can be written in the following manner thus contribute to the sensitivity derivatives:

$$\delta \mathbf{u} = - \frac{\Psi_{\mathbf{u}}}{\Psi_x} \delta x - \frac{\Psi_{\mathbf{u}}}{\Psi_y} \delta y - \frac{\Psi_{\mathbf{u}}}{\Psi_z} \delta z \quad (0.10)$$

Considering the design points to be D_i where $i = 1, \dots, n$, the variations of the geometrical quantities in δI_{aug} read:

$$\delta(x, y, z) = \hat{\mathbf{a}} \begin{matrix} \circ \\ \circ \\ \circ \end{matrix} \sum_{i=1}^n \frac{\Psi(x, y, z)}{\Psi_{D_i}} \delta D_i, \quad (0.11)$$

The final form of the sensitivity derivatives with respect to the design variables is obtained using the shape parameterisation and the consequence derivation of the variations of the above geometrical entities. The variations of the geometric entities are calculated using a central finite difference scheme around a small perturbation ε , for example for δx we have:

$$\delta x = \frac{x(\delta D_{\varepsilon}) - x(\delta D_{-\varepsilon})}{\varepsilon} \quad (0.12)$$

The optimisation approach chosen in this study is the conjugate gradients method [8], because it is more efficient and stable than the steepest descent method for cases with many design parameters. There are methods that converge faster than conjugate

gradients but require second derivatives which are very costly to calculate. The Adjoint sensitivities are normalised so that the step-size used is of the same magnitude as the design points' displacement.

3 SOLVER IMPLEMENTATION

The first page must contain the Title, Author(s), Affiliation(s), Key words and the Abstract. The second page must begin with the Introduction. The first line of the title is located 3 cm from the top of the printing box.

OpenFOAM (Open Field Operation And Manipulation) was used for developing the method and performing the optimisation procedure. OpenFOAM is an open source (GNU General Public License – GPL) CFD toolbox that can be used to simulate a broad range of physical problems due to its high level symbolic application programming interface (API). The flexibility of this interface allows for a straight forward implementation of the continuous Adjoint and the shape morpher, using previously validated components that make up the other applications in the toolbox.

The solver uses a segregated approach and a SIMPLE-type algorithm to couple the Adjoint velocities and pressure. The perturbation of turbulent viscosity $\delta\mu$ is considered negligible, through each geometry modification, so that the primal turbulent viscosity can be re-used for the Adjoint diffusion term. This is a convenient assumption from the numerical point of view and quite realistic considering the fact that the geometry changes slightly in every optimisation cycle. In the case of considering turbulent perturbation another Adjoint equation for the turbulence model will appear. This complication is not handled in the present study but the reader can refer to Anderson's work [11] for more details on how to derive the Adjoint equations for the turbulent viscosity μ .

More details about the implementation of the Adjoint solver in FOAM can be found in previous work by the authors [12] where the application was topology optimisation using an Adjoint-based solver. For the topology optimisation methodology, the porosity is just an auxiliary variable to describe a continuous transition from fluid to solid. In the case of [12] the porosity is treated as a source term in the Adjoint equations. Thus, by eliminating this source term we reduce the equation to the desired form for the shape optimisation case.

The optimisation process works in three stages. First the primal is solved along with the turbulence equations. Then the calculated velocity and turbulent viscosity are used for the solution of the Adjoint equations where the Adjoint variables are computed. The third step is the calculation of the sensitivity derivatives with respect to the design variable and the update of the design variables using the conjugate gradients method.

The shape modification is performed using morphing boxes. The design variables are the displacement of the morphing box's control points. The generated mesh can be seen in Figure 1 and consists of approximately 730 thousand primarily hexahedral cells. Lower order than hex elements are found on some surfaces due to projection of the mesh to the surface to produce surface conforming boundaries.

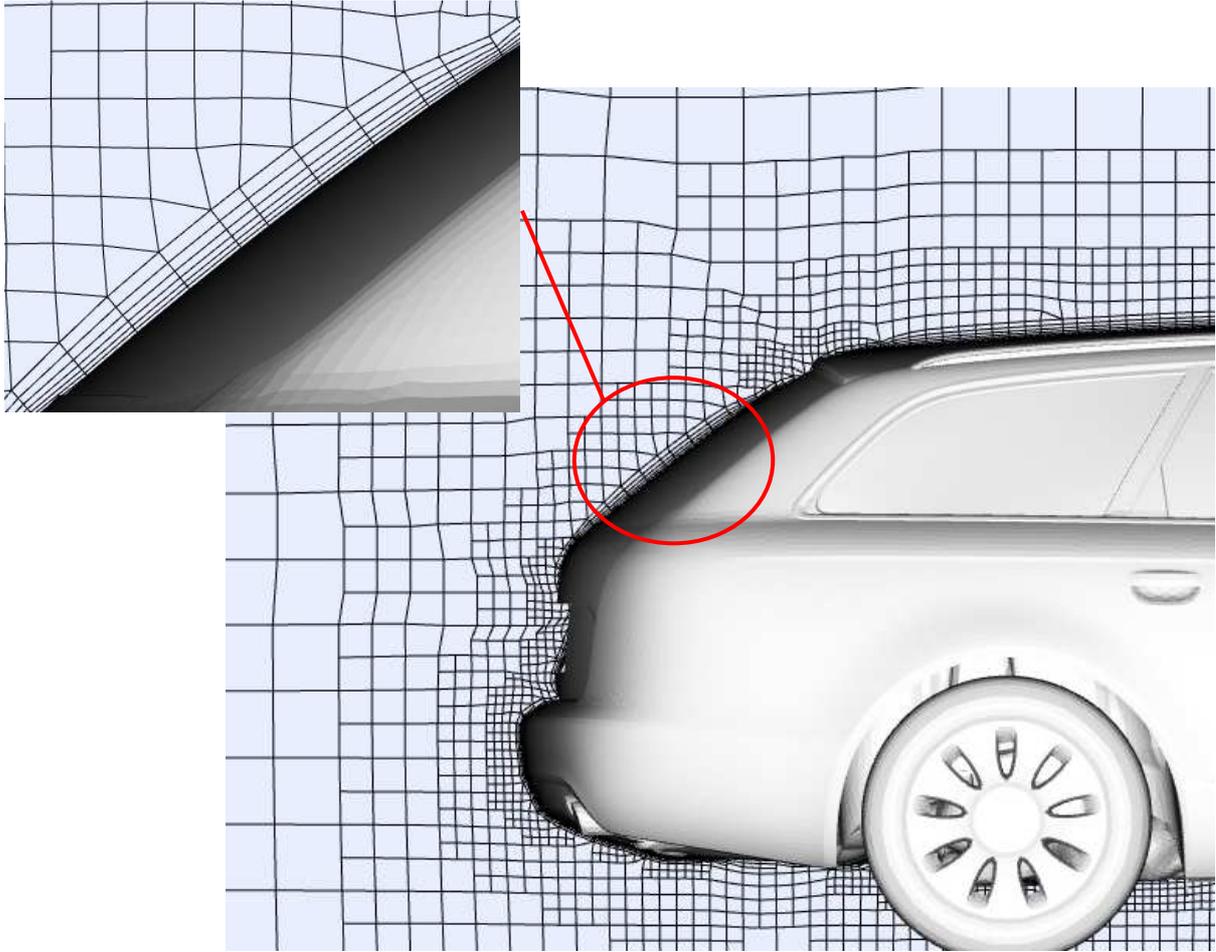


Figure 1. Computational mesh around the vehicle and detail of the layers.

After the mesh was built, a morphing box was created and fitted exactly onto the rear part of the vehicle, as shown in Figure 2. The box allows precise control of morphing operations to examine various parametric shapes. The geometry that is subject to modification is contained by the box. Morphing parameters were specified in predefined degrees of freedom so that the shape of the back of the vehicle could be altered without the under-body being very affected. A total of three control points were set to influence the shape of the rear of the vehicle each of which has a mirror image point on the other side of the vehicle and degrees of freedom in the x y and z directions. In Figure 2 the control points are also depicted in red along with their directions of movement. The control points on the right act as mirror image of those on the left. This results in a total of nine design parameters that affect the shape of the vehicle in a symmetric way.

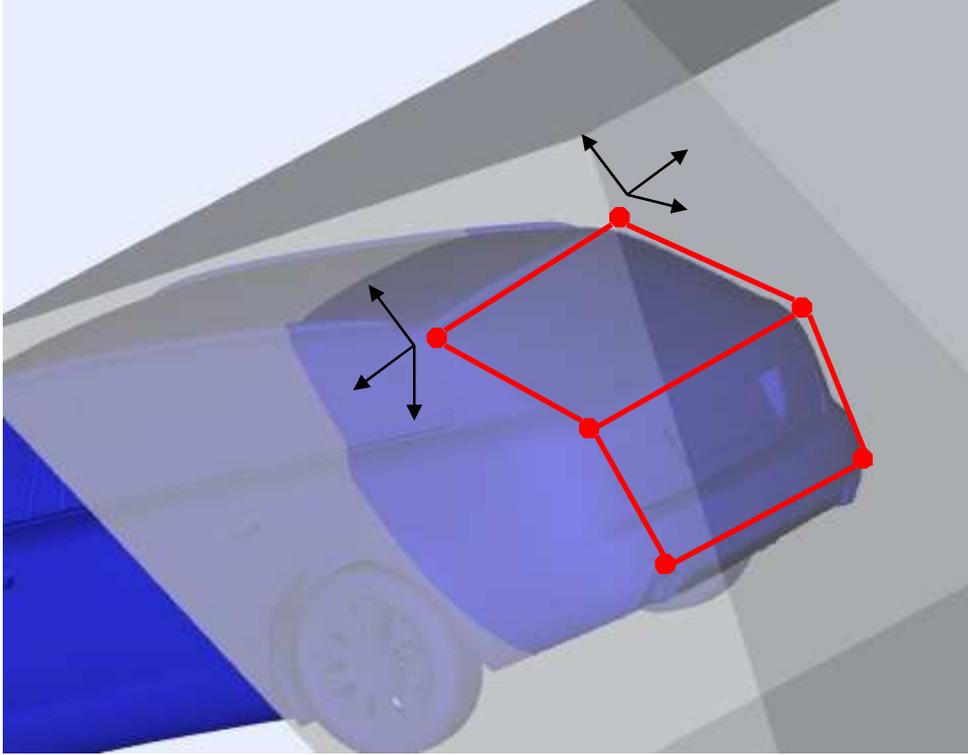


Figure 2. Morphing box's representation. (The geometry under modification is included in the side box).

4 TEST CASE

The optimisation case serves as proof-of-concept to the described methodology. The example focuses on the external aerodynamics of an automotive vehicle (see Audi A6 Avant shown in Figure 3). The main objective of the simulations presented here was to find the optimal aerodynamic shape for the rear part of the vehicle body. The optimisation problem was therefore defined by means of the minimisation of the drag coefficient. The optimisation procedure consisted of generating a parametric mesh morphing model of the vehicle geometry performing a CFD and Adjoint analysis for the calculation of the sensitivities that drive the deterministic optimisation algorithm towards the optimal design.

The air flow was computed as an incompressible-subsonic turbulent gas (i.e. constant density). The SIMPLE solution procedure for pressure-velocity coupling was employed in the calculations with the GAMG solver. A normal inlet velocity boundary condition was specified at the entry of the tunnel with a value of 38.89 m/s (or 140 kph driving speed). The flow is assumed to be incompressible and isothermal with physical properties derived from air at 293 K. A hybrid formulation of the Spalart-Allmaras turbulence model, specifically intended for aerodynamic calculations, was applied in every simulation. Constant inlet properties are set using a turbulent length scale of 0.015 m and intensity based on the inlet velocity of 5%. Pressure boundary conditions are zero-gradient everywhere except on the outlets, where a fixed relative pressure of 0 is enforced. For the Adjoint equations the boundary conditions were set according to the boundary equations of chapter 2. To ensure stability, it was found that first-order

upwind discretisation had to be employed for convection terms. The flow is assumed to be steady state and advanced using standard under-relaxation for all solution variables.



Figure 3. Audi A6 Avant (courtesy of AUDI, www.audi.com – AUDI AG © 2007)

The solver is run initially without sensitivity updates to obtain a steady solution for both the primal and the Adjoint (~1500 iterations each). Figure 4 depicts results on the symmetry plane for the primal and Adjoint velocities.

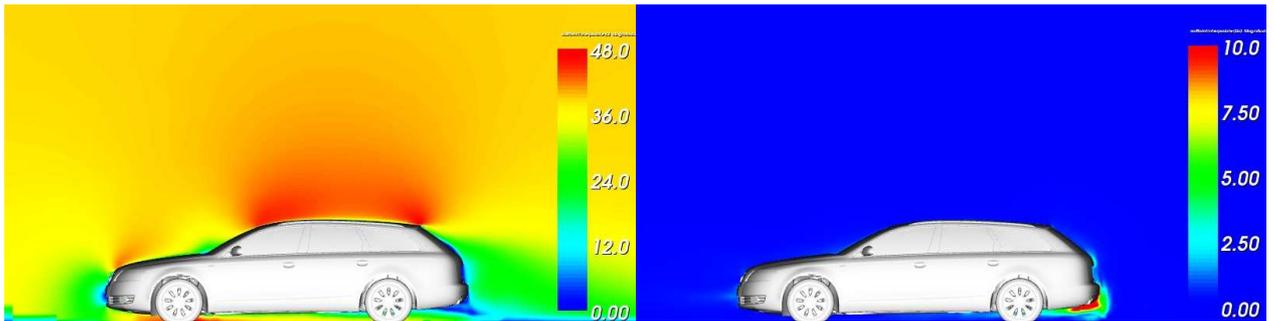


Figure 4. Primal (left) and Adjoint (right) velocity fields for the baseline design.

It is obvious that the main impact on the drag coefficient magnitude is concentrated in the rear of the vehicle geometry where higher values of the Adjoint velocities appear. Therefore, concentrating the shape modification in the rear area does not compromise significantly the overall result.

The optimisation procedure converged in 14 iterations which correspond to 2x30x14 flow iterations giving a 2.5% reduction in the drag coefficient. The computation time corresponds to less than a complete primal calculation. So adding the initialization of the Adjoint and primal fields the optimisation time was equivalent to ~2.5 primal calculations. The convergence history is presented in Figure 5.

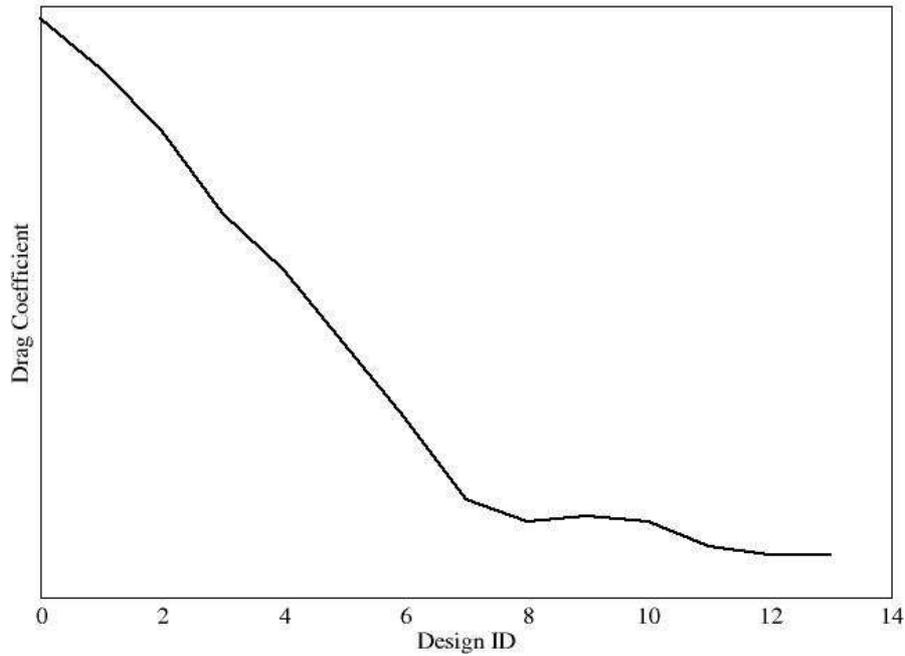


Figure 5. Convergence history of the drag coefficient.

A deeper convergence could be achieved by ensuring convexity in the cost function. Nevertheless, the drag reduction was quite significant compared to traditional optimisation methods. The fast convergence of the present method is the most important benefit gained from the use of gradient-based optimisation for cases of this type.

A cross section of the baseline compared to the optimised design is depicted in Figure 6. The morphing methodology was restricting (9 degrees of freedom) the development of the optimisation shape and compromising the mesh quality as well as the exploration of the design space. Nevertheless, for this exploratory case it was considered adequate to investigate the benefits of the optimisation method.

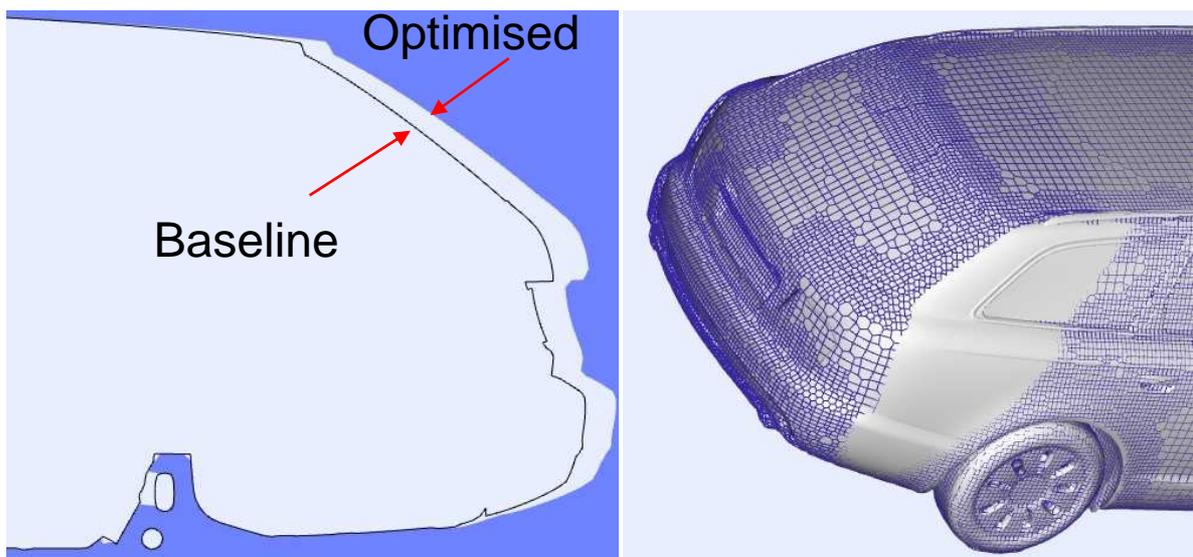


Figure 6. Comparison of baseline and optimised geometries

5 CONCLUSIONS

The theory underlying the computation of Adjoint shape sensitivities with respect to the design variables and its implementation into the CFD environment OpenFOAM was presented. The application of the developed code to the minimisation of the drag coefficient of an automotive vehicle investigated the potential of this methodology. The solutions presented above are relevant to the accuracy of the CFD methods employed and restricted by the flexibility of the parameterisation. The results obtained in this proof-of-concept can be considered promising, although additional work is clearly required. Further work will be focused on improving the mesh morphing capabilities to give more generic shapes with more degrees of freedom. In addition, extension of the code to other objective functions and handling of multi-objective problems is planned. Such implementations only involve modification of the Adjoint boundary conditions. Adaptations of this nature to the Adjoint solver are quite straight forward due to the flexible high level symbolic API of OpenFOAM.

6 ACKNOWLEDGEMENTS

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REFERENCES

1. Jameson, A., *Aerodynamic Design via Control Theory*, in *ICASE Rep. no. 88-64*, 1988.
2. Giles, M.B. and N.A. Pierce, *Adjoint Equations in CFD: Duality, Boundary Conditions, and Solution Behaviour*, in *AIAA Report 97-1850*, 1997.
3. Anderson, W.K. and V. Venkatakrishnan, *Aerodynamic Design Optimisations on Unstructured Grids with a Continuous Adjoint Formulation*. AIAA Paper 97-0643, 1997.
4. Castro, C., C. Lozano, F. Palacios, and E. Zuazua, *A Systematic Continuous Adjoint Approach to Viscous Aerodynamic Design on Unstructured Grids*, in *AIAA paper 2006-51*, 2006.
5. Petropoulou, S., M. Gavaises, and A. Theodorakakos, *An Adjoint Method for Hole Cavitating Control Through Inverse Nozzle Design*. SAE Paper 06P-162, 2006.
6. Campos, F., P. Geremia, and E. Skaperdas, *Automatic Optimisation of Automotive Designs Using Mesh Morphing and CFD*, in *EACC European Automotive CFD Conference: Frankfurt*, 2007.
7. Soto, O. and R. Löhner, *A Mixed Adjoint Formulation for Incompressible RANS Problems*. AIAA-02-0451 2002.
8. Shewchuk, J.R., *An Introduction to the Conjugate Gradient Method Without the Agonizing Pain*, 1994.
9. Petropoulou, S., *Adjoint-Based Geometry Optimisation with Applications to Automotive Fuel Injector Nozzles*. City University London, 2006.

10. Petropoulou, S., M. Gavaises, and A. Theodorakakos, *An Adjoint Method for Controlled Cavitation Inverse Nozzle Design*. International Journal of Automotive Technology, submitted 2006.
11. Anderson, W.K. and D.L. Bonhaus, *Aerodynamic Design on Unstructured Grids or Turbulent Flows*. NASA Technical Memorandum No. 112876, 1997.
12. Othmer, C., E. de Villiers, and H.G. Weller, *Implementation of a Continuous Adjoint for Topology Optimisation of Ducted Flows*, in *18th AIAA CFD Conference: Miami, 2007*.