Aerodynamic Shape Optimization Using the Adjoint-based Truncated Newton Method

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Abstract This paper presents the development and application of the truncated Newton (TN) method in aerodynamic shape optimization problems. The development is presented for problems governed by the laminar flow equations of incompressible fluids. The method was developed in OpenFOAM[©] with the aim to stress its advantages over standard gradient-based optimization algorithms. The Newton equations are solved using the conjugate gradient (CG) method which requires the computation of the product of the Hessian of the objective function and a vector, escaping thus the need for computing the Hessian matrix itself. The latter would have a computational cost that scales with the number of design variables and, thus, becomes unaffordable in large-scale problems with many design variables. A combination of the continuous adjoint method and the direct differentiation of the flow and adjoint PDEs is used to compute all Hessian-vector products. A grid displacement PDE (Laplace equation) is also used to compute the necessary derivatives of grid displacements w.r.t. the design variables. The programmed method is used to optimize the sidewall shapes of 2*D* ducts for minimum total pressure losses.

1 Introduction to the Truncated Newton Method

An unconstrained optimization problem, in which the target is to minimize the objective function F by controlling the design variables b_i , i = 1, ..., N can be solved by means of the Newton method, according to which the design variables are updated as follows

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$$b_i^{n+1} = b_i^n + \delta b_i \tag{1a}$$

$$\frac{\delta^2 F}{\delta b_i \delta b_j}^n \delta b_j = -\frac{\delta F}{\delta b_i}^n \tag{1b}$$

where *n* is the Newton iteration counter, to be omitted hereafter. The direct solution of eq. 1b requires the computation of the Hessian of *F*, with computational cost that scales with N [3].

Considering eq. 1b as a linear system of equations of the form Ax = q, a possible way to solve it is through the Conjugate Gradient (CG) method, which is schematically given in Algorithm 1.

Algorithm	1:	The	CG	Method	for	the	Solution	of A	Ax =	q
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 $m \leftarrow 0$ $x \leftarrow \text{init}()$ $r^{m} \leftarrow Ax - q; \ s \leftarrow -r^{m}$ while $|r^{m}| < \varepsilon$, (CG Iterations) do $\eta \leftarrow \frac{(r^{m})^{T} r^{m}}{s^{T} As}$ $x \leftarrow x + \eta s$ $r^{m+1} \leftarrow r^{m} + \eta As$ $\beta \leftarrow \frac{(r^{m+1})^{T} r^{m+1}}{(r^{m})^{T} r^{m}}$ $s \leftarrow -r^{m+1} + \beta s$ $m \leftarrow m + 1$ end while

Based on Algorithm 1, the cost of each CG iteration is dominated by the cost of computing the matrix-vector product (*As*). In its truncated variant (Truncated Newton, TN, [4]), the stopping criterion in Algorithm 1 becomes $m \leq M_{CG}$, where M_{CG} is a user-defined small integer (to be used instead of $|r^m| < \varepsilon$). Regarding eq. 1b, since the Hessian matrix stands for *A*, the use of the TN method in aerodynamic shape optimization problems means that the Hessian matrix itself is no more needed and only its product with a vector must be computed. On the other hand, the gradient of *F* must be available and the (continuous) adjoint method, [5], is the less expensive way to compute it, at a CPU cost which is independent of *N*.

2 The Continuous Adjoint Method for the Computation of $\frac{\delta F}{\delta h}$

The continuous adjoint method, [5], starts by differentiating the objective function F augmented by the field integral of the flow equations multiplied by the so-called adjoint fields, in order to derive the adjoint PDEs. The latter are, then, discretized and numerically solved to compute the adjoint fields. The gradient of F is expressed

in the form of field or boundary integrals of quantities involving the previously computed flow and adjoint fields.

Let us assume a 2D laminar flow of an incompressible fluid governed by the continuity $(R^p = 0)$ and the momentum $(R^v_i = 0)$ equations, where

$$R^{p} = -\frac{\partial v_{j}}{\partial x_{j}} \tag{2}$$

$$R_i^{\nu} = \nu_j \frac{\partial \nu_i}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial p}{\partial x_i} , \quad i = 1, 2$$
(3)

Here, v_i are the velocity components, p the static pressure divided by the constant density, $\tau_{ij} = v \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)$ the stress tensor and v the constant viscosity. Dealing with internal aerodynamics, we assume that the objective function F to

Dealing with internal aerodynamics, we assume that the objective function F to be minimized is the volume-averaged total pressure losses (for the flow inside a duct) which is written as

$$F = \int_{S_{I,O}} F_{S,i} n_i dS \quad , \qquad F_{S,i} = -\left(p + \frac{1}{2}v_k^2\right) v_i \tag{4}$$

where $S = S_I \cup S_O \cup S_W$ is the domain boundary with S_I being the inlet, S_O the outlet, S_W the wall boundary and **n** the outward unit normal vector to the surface. Recall that, for any flow quantity Φ , the total derivative $\delta \Phi / \delta b_n$, which represents the total change in Φ caused by variations in b_n , is

$$\frac{\delta\Phi}{\delta b_n} = \frac{\partial\Phi}{\partial b_n} + \frac{\partial\Phi}{\partial x_k} \frac{\delta x_k}{\delta b_n}$$
(5)

In eq. 5, the partial derivative $\partial \Phi / \partial b_n$ represents only the variation in Φ caused due to changes in the design variables, without considering space deformations.

The development of the augmented objective function

$$F_{aug} = F + \int_{\Omega} u_i R_i^{\nu} d\Omega + \int_{\Omega} q R^p d\Omega$$
(6)

leads to the adjoint continuity $(R^q = 0)$ and adjoint momentum $(R^u_i = 0)$ equations,

$$R^q = -\frac{\partial u_j}{\partial x_j} \tag{7}$$

$$R_{i}^{u} = u_{j} \frac{\partial v_{j}}{\partial x_{i}} - \frac{\partial (u_{i}v_{j})}{\partial x_{j}} - \frac{\partial \tau_{ij}^{a}}{\partial x_{j}} + \frac{\partial q}{\partial x_{i}}, \ i = 1, 2$$
(8)

where $\tau_{ij}^a = v \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ are the components of the adjoint stress tensor. By satisfying eqs. 7 and 8, all field integrals in $\delta F_{aug}/\delta b_n$ which depend on $\delta v_i/\delta b_n$ and $\delta p/\delta b_n$ are eliminated. The adjoint boundary conditions are derived by eliminating the total derivatives of the flow variables along the boundaries, while also con-

sidering the flow boundary conditions. In this paper, we will refrain from further developing the adjoint boundary conditions, see [5].

After satisfying the adjoint PDEs, eqs. 7 and 8, the expression for the gradient of F (i.e. the rhs term in eq. 1b)is

$$\frac{\delta F}{\delta b_n} = \int_{\Omega} A_{jk} \frac{\partial}{\partial x_j} \left(\frac{\delta x_k}{\delta b_n} \right) d\Omega \tag{9}$$

where

$$A_{jk} = -u_i v_j \frac{\partial v_i}{\partial x_k} - u_j \frac{\partial p}{\partial x_k} - \tau^a_{ij} \frac{\partial v_i}{\partial x_k} + u_i \frac{\partial \tau_{ij}}{\partial x_k} + q \frac{\partial v_j}{\partial x_k}$$
(10)

3 Computation of Hessian(F)–Vector Products

As explained in Section 1, the TN method requires the computation of $\frac{\delta^2 F}{\delta b_n \delta b_m} s_m$, where s_m might be the components of any vector.

Let us use overbar to denote the product of the total gradient $\frac{\delta \Phi}{\delta b_m}$ of any quantity Φ and s_m , namely

$$\overline{\Phi} = \frac{\delta \Phi}{\delta b_m} s_m \tag{11}$$

It can be proved that

$$\overline{\frac{\partial \Phi}{\partial x_j}} = \frac{\delta}{\delta b_m} \left(\frac{\partial \Phi}{\partial x_j} \right) s_m = \frac{\partial \overline{\Phi}}{\partial x_j} - \frac{\partial \Phi}{\partial x_k} \frac{\partial \overline{x_k}}{\partial x_j}$$
(12)

Also, for any pair of Φ and Ψ ,

$$\frac{\delta}{\delta b_m} \left(\Psi \frac{\partial \Phi}{\partial x_j} \right) s_m = \overline{\Psi} \frac{\partial \Phi}{\partial x_j} + \Psi \frac{\partial \overline{\Phi}}{\partial x_j} - \Psi \frac{\partial \Phi}{\partial x_k} \frac{\partial \overline{x_k}}{\partial x_j}$$
(13)

Based on the above, it is a matter of mathematical development to show that

$$\frac{\delta^2 F}{\delta b_n \delta b_m} s_m = \int_{\Omega} \overline{A_{jk}} \frac{\partial}{\partial x_j} \left(\frac{\delta x_k}{\delta b_n} \right) d\Omega + \int_{\Omega} A_{jk} \frac{\delta}{\delta b_m} \left[\frac{\partial}{\partial x_j} \left(\frac{\delta x_k}{\delta b_n} \right) \right] s_m d\Omega + \int_{\Omega} A_{jk} \frac{\partial}{\partial x_j} \left(\frac{\delta x_k}{\delta b_n} \right) s_m \frac{\delta(d\Omega)}{\delta b_m}$$
(14)

where

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$$\overline{A_{jk}} = -\overline{u_i}v_j\frac{\partial v_i}{\partial x_k} - u_i\overline{v_j}\frac{\partial v_i}{\partial x_k} - u_iv_j\frac{\partial \overline{v_i}}{\partial x_k} + u_iv_j\frac{\partial v_i}{\partial x_\lambda}\frac{\partial \overline{x_\lambda}}{\partial x_k} - \overline{u_j}\frac{\partial p}{\partial x_k} - u_j\frac{\partial \overline{p}}{\partial x_k} \\
+ u_j\frac{\partial p}{\partial x_\lambda}\frac{\partial \overline{x_\lambda}}{\partial x_k} - v\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right)\frac{\partial v_i}{\partial x_k} + v\left(\frac{\partial u_i}{\partial x_\lambda}\frac{\partial \overline{x_\lambda}}{\partial x_j} + \frac{\partial u_j}{\partial x_\lambda}\frac{\partial \overline{x_\lambda}}{\partial x_i}\right)\frac{\partial v_i}{\partial x_k} \\
- v\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\frac{\partial \overline{v_i}}{\partial x_k} + v\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_\lambda}\right)\frac{\partial v_i}{\partial x_\lambda}\frac{\partial \overline{x_\lambda}}{\partial x_k} \\
+ \overline{u_i}\frac{\partial}{\partial x_k}\left[v\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right] + u_i\frac{\partial}{\partial x_k}\left[v\left(\frac{\partial \overline{v_i}}{\partial x_j} + \frac{\partial \overline{v_j}}{\partial x_i}\right)\right] \\
- u_i\frac{\partial}{\partial x_k}\left[v\left(\frac{\partial v_i}{\partial x_\lambda}\frac{\partial \overline{x_\lambda}}{\partial x_j} + \frac{\partial v_j}{\partial x_\lambda}\frac{\partial \overline{x_\lambda}}{\partial x_i}\right)\right] - u_i\frac{\partial}{\partial x_k}\left[v\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right]\frac{\partial \overline{x_\lambda}}{\partial x_k} \\
+ \overline{q}\frac{\partial v_j}{\partial x_k} + q\frac{\partial \overline{v_j}}{\partial x_k} - q\frac{\partial v_j}{\partial x_\lambda}\frac{\partial \overline{x_\lambda}}{\partial x_k}\right] \tag{15}$$

and, [2],

$$\frac{\delta(d\Omega)}{\delta b_m} s_m = \frac{\partial}{\partial x_\lambda} \left(\frac{\delta x_\lambda}{\delta b_m} s_m \right) d\Omega = \frac{\partial \overline{x_\lambda}}{\partial x_\lambda} d\Omega \tag{16}$$

since $\overline{x_{\lambda}} = \frac{\delta x_{\lambda}}{\delta b_m}$. By denoting

$$\overline{\overline{x_{k,n}}} = \frac{\delta^2 x_k}{\delta b_n \delta b_m} s_n \tag{17}$$

it can be proved that

$$\int_{\Omega} A_{jk} \frac{\delta}{\delta b_m} \left[\frac{\partial}{\partial x_j} \left(\frac{\delta x_k}{\delta b_n} \right) \right] s_m d\Omega = \int_{\Omega} A_{jk} \frac{\partial \overline{\overline{x_{k,n}}}}{\partial x_j} d\Omega - \int_{\Omega} A_{jk} \frac{\partial}{\partial x_\lambda} \left(\frac{\delta x_k}{\delta b_n} \right) \frac{\partial \overline{x_\lambda}}{\partial x_j} d\Omega$$
(18)

4 Computation of $\overline{v_i}$ and \overline{p}

Computing $\overline{v_i}$ and \overline{p} is straightforward and can be done by formulating the product of the direct differentiation (DD, i.e. derivation w.r.t. b_n) of the flow equations and s_m . It is

$$\overline{R^{p}} = \frac{\delta R^{p}}{\delta b_{m}} s_{m} = 0 \quad , \qquad \overline{R_{i}^{v}} = \frac{\delta R_{i}^{v}}{\delta b_{m}} s_{m} = 0 \tag{19}$$

where

$$\overline{R^{p}} = \frac{\partial \overline{v_{j}}}{\partial x_{j}} - \frac{\partial v_{j}}{\partial x_{k}} \frac{\partial \overline{x_{k}}}{\partial x_{j}}$$
(20)

and

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$$\overline{R_{i}^{v}} = \frac{\partial(\overline{v_{i}}v_{j})}{\partial x_{j}} + \frac{\partial(v_{i}\overline{v_{j}})}{\partial x_{j}} - \frac{\partial}{\partial x_{j}} \left[\mathbf{v} \left(\frac{\partial\overline{v_{i}}}{\partial x_{j}} + \frac{\partial\overline{v_{j}}}{\partial x_{i}} \right) \right] + \frac{\partial\overline{p}}{\partial x_{i}} \\ - \frac{\partial(v_{i}v_{j})}{\partial x_{k}} \frac{\partial\overline{x_{k}}}{\partial x_{j}} + \frac{\partial}{\partial x_{j}} \left[\mathbf{v} \left(\frac{\partial v_{i}}{\partial x_{k}} \frac{\partial\overline{x_{k}}}{\partial x_{j}} + \frac{\partial v_{j}}{\partial x_{k}} \frac{\partial\overline{x_{k}}}{\partial x_{i}} \right) \right] \\ + \frac{\partial}{\partial x_{k}} \left[\mathbf{v} \left(\frac{\partial v_{i}}{\partial x_{j}} + \frac{\partial v_{j}}{\partial x_{i}} \right) \right] \frac{\partial\overline{x_{k}}}{\partial x_{j}} - \frac{\partial p}{\partial x_{k}} \frac{\partial\overline{x_{k}}}{\partial x_{i}}$$
(21)

5 Computation of $\overline{u_i}$ and \overline{q}

Similarly, the product of the DD of the adjoint equations and s_m yields

$$\overline{R^{q}} = \frac{\delta R^{q}}{\delta b_{m}} s_{m} = 0 \quad , \qquad \overline{R_{i}^{u}} = \frac{\delta R_{i}^{u}}{\delta b_{m}} s_{m} = 0 \tag{22}$$

where

$$\overline{R^{q}} = \frac{\partial \overline{u_{j}}}{\partial x_{j}} - \frac{\partial u_{j}}{\partial x_{k}} \frac{\partial \overline{x_{k}}}{\partial x_{j}}$$
(23)

and

$$\overline{R_{i}^{u}} = \overline{u_{j}} \frac{\partial v_{j}}{\partial x_{i}} + u_{j} \frac{\partial \overline{v_{j}}}{\partial x_{i}} - \frac{\partial (\overline{u_{i}}v_{j})}{\partial x_{j}} - \frac{\partial (u_{i}\overline{v_{j}})}{\partial x_{j}} \\
- \frac{\partial}{\partial x_{j}} \left[v \left(\frac{\partial \overline{u_{i}}}{\partial x_{j}} + \frac{\partial \overline{u_{j}}}{\partial x_{i}} \right) \right] + \frac{\partial \overline{q}}{\partial x_{i}} - u_{j} \frac{\partial v_{j}}{\partial x_{k}} \frac{\partial \overline{x_{k}}}{\partial x_{i}} \\
+ \frac{\partial (v_{j}u_{i})}{\partial x_{k}} \frac{\partial \overline{x_{k}}}{\partial x_{j}} + \frac{\partial}{\partial x_{j}} \left[v \left(\frac{\partial u_{i}}{\partial x_{k}} \frac{\partial \overline{x_{k}}}{\partial x_{j}} + \frac{\partial u_{j}}{\partial x_{k}} \frac{\partial \overline{x_{k}}}{\partial x_{i}} \right) \right] \\
+ \frac{\partial}{\partial x_{k}} \left[v \left(\frac{\partial u_{i}}{\partial x_{j}} + \frac{\partial u_{j}}{\partial x_{i}} \right) \right] \frac{\partial \overline{x_{k}}}{\partial x_{j}} - \frac{\partial q}{\partial x_{k}} \frac{\partial \overline{x_{k}}}{\partial x_{i}} \right]$$
(24)

6 Computation of $\overline{x_k}$ and $\overline{\overline{x_{k,n}}}$

In aerodynamic shape optimization problems, a widely used grid displacement model, i.e. a mathematical model that propagates known displacements of the boundary grid nodes to the internal nodes, is based on the Laplace equation with Dirichlet boundary conditions. Written for the derivatives of the grid coordinates x_K w.r.t. the design variables, it takes the form

$$R_i^x = \frac{\partial^2}{\partial x_j^2} \left(\frac{\delta x_k}{\delta b_n} \right) = 0 \tag{25}$$

from which it can readily be deduced that

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$$\frac{\partial^2 \overline{x_k}}{\partial x_i^2} = 0 \tag{26}$$

It can also be proved that

$$\frac{\partial^2 \overline{\overline{x_{k,n}}}}{\partial x_j^2} = 2 \frac{\partial^2}{\partial x_j \partial x_\lambda} \left(\frac{\delta x_k}{\delta b_m}\right) \frac{\partial \overline{x_\lambda}}{\partial x_j}$$
(27)

which can numerically be solved to compute $\overline{x_{k,n}}$ with appropriate boundary conditions depending also on the adopted parameterization model.

7 The TN Algorithm – Comments on the CPU Cost

Using eqs. 16 to 18, eq. 14 can be written as

$$\frac{\delta^2 F}{\delta b_n \delta b_m} s_m = \int_{\Omega} \left[\overline{A_{jk}} + A_{jk} \frac{\partial \overline{x_\lambda}}{\partial x_\lambda} - A_{\lambda k} \frac{\partial \overline{x_j}}{\partial x_\lambda} \right] \frac{\partial}{\partial x_j} \left(\frac{\delta x_k}{\delta b_n} \right) d\Omega + \int_{\Omega} A_{jk} \frac{\partial \overline{\overline{x_{k,n}}}}{\partial x_j} d\Omega$$
(28)

where $\overline{A_{jk}}$ is given by eq. 15. To compute $\overline{A_{jk}}$, apart from the flow and adjoint fields, the "overbar" fields $(\overline{v_i}, \overline{u_i}, \overline{p}, \overline{q})$, as well as $\overline{x_i}$ and their spatial derivatives must be available.

So, in each Newton cycle, the numerical solution of $R^p = 0$ and $R_i^v = 0$ (where R^p and R_i^v are given by eqs. 2 and 3) yields the flow fields (p, v_i) . The solution of $R^q = 0$ and $R_i^u = 0$ (where R^q and R_i^u are given by eqs. 7 and 8) yields the adjoint fields (q, u_i) . So, far, the computational cost is approximately equal to that of twice solving the flow equations or 2 EFS (EFS stands for an Equivalent Flow Solution, i.e. the cost for solving the flow equations).

Before solving for \overline{p} and $\overline{v_i}$, $\overline{x_k}$ must be computed by solving eq. 26 at the cost of 1 GDS (GDS stands for Grid Displacement Solutions, i.e. the cost of solving the grid displacement PDE or any of the PDEs that result from its differentiation). It should be mentioned that 1 GDS is significantly cheaper than 1 EFS. Eq. 26 has to be solved once per CG iteration, contributing a total cost of M_{CG} GDS per optimization cycle.

Computing \overline{p} and $\overline{v_i}$ requires the numerical solution of equations 19 (considering also eqs. 20 and 21). Similarly, to compute \overline{q} and $\overline{u_i}$ requires the numerical solution of equations 22 (considering also eqs. 23 and 24). Both systems of equations should be solved within the CG loop (i.e. M_{CG} times) and contribute $2M_{CG}$ EFS to the overall cost of a Newton iteration or cycle.

Within each CG iteration, the computation of $\overline{A_{jk}}$ also requires the availability of the $\delta x_k/\delta b_n$ and $\overline{\overline{x_{k,n}}}$ fields. To this end, eqs. 25 and 27 must be solved for $n \in [1, N]$. This results to $2M_{CG}N$ GDS per optimization cycle.

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Based on the above, the overall CPU cost per Newton iteration is equal to $2+2M_{CG}$ EFS and $(1+2N)M_{CG}$ GDS. However, since the cost of a GDS is significantly lower than that of an EFS, the GDS part can be considered negligible for a moderate number of design variables. This leads to a cost per Newton cycle that is, practically, independent of the number of design variables *N*.

8 Applications

In this section, two applications of the developed TN optimization algorithm are presented.

The first one deals with the shape optimization of an S-bend duct. The flow is laminar with a Reynolds number of Re = 785 based on the inlet height and a mesh consisting of 27500 quadrilaterals is used. Each of the upper and lower sides are parameterized using 9 Bézier–Bernstein control points, fig. 1. The first and last two control points per side are kept fixed while the x and y coordinates of the rest are allowed to vary, giving rise to a total of 20 design variables. In fig. 2, the convergence history of the developed TN algorithm is compared to those of steepest descent (SD) and the Fletcher-Rives Conjugate Gradient (CG), [1], method. Comparisons are presented twice, in terms of the cycles required to reach the minimum and the corresponding EFS. In addition, an investigation of the effect of the M_{CG} number can be seen in the same figures. It can be observed that TN outperforms SD and CG, since it computes the optimized duct shape using less optimization cycles and, especially, by requiring less EFS. In addition, it can be seen that, even though increasing M_{CG} reduces the number of optimization cycles required to reach the minimum, there is no obvious gain from the EFS point of view. In fig. 3, the flow velocity magnitude in the initial and optimized ducts is presented.

The second case is concerned with the optimization of a divergent duct. The flow Reynolds number is Re=475 and a mesh consisting of 20000 quadrilaterals is used. The initial and optimized geometries along with the Bézier–Bernstein control points used to parameterize the duct shape are depicted in fig. 4. In fig. 5, the flow velocity magnitude in the initial and optimized ducts is presented. In fig. 6, the convergence history of the TN, SD and CG are illustrated. In this case as well, TN outperforms SD and CG from the optimization cycles point of view; regarding EFS, TN and CG compute the optimal solution almost at the same cost. Increasing M_{CG} has the same effect as in the first case, i.e. the optimized geometry is computed in less optimization cycles but without a significant advantage in CPU cost. This seems to indicate that, at least for the cases studied, a low M_{CG} number should be chosen.



Fig. 1 S-bend duct optimization: dust shape and the Bézier–Bernstein control points parameterizing it. Axes not in scale. Control points depicted with a dark cycle remain fixed during the optimization.

9 Conclusions

A Truncated Newton method for computing an approximation to the second-order correction of the design variables by iteratively solving Newton's equation using Conjugate Gradient was presented. The method built on previous work of the authors for Euler flows and extended the mathematical background for incompressible, laminar flows. The proposed Truncated Newton method computes the required Hessian-vector products by utilizing a combination of (continuous) adjoint and direct differentiation. The cost per optimization cycle is approximately equal to $2 + 2M_{CG}$ equivalent flow solutions, where M_{CG} is the number of CG iterations used to approximate the solution of Newton's equation; this cost is practically independent of the design variables number. In contrast to previous work, the new formulation is solving for the projected total derivatives of the flow quantities $(\frac{\delta \Phi}{\delta b_m} s_m)$ instead of the partial ones $(\frac{\partial \Phi}{\partial b_m} s_m)$ by also involving a grid displacement model and its differentiation. In the two applications presented, each with a moderate number of design variables, it was shown that Truncated Newton outperforms other optimization methods in terms of optimization cycles and is, at least, as fast as Conjugate Gradient in terms of CPU cost. A parametric study for M_{CG} has also shown that its value should remain as low as possible. On going research on further improving the Truncated Newton method speed-up is performed.



Fig. 2 S-bend duct optimization: Convergence of the steepest descent (SD), Conjugate Gradient (CG) and Truncated Newton (TN) optimization algorithms, w.r.t. optimization cycles (a) and EFS (b). As explained in the text, the part of the CPU cost which is due to GDS is neglected.

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Fig. 3 S-bend duct optimization: Velocity magnitude for the initial (a) and optimized (b) geometries.



Fig. 4 Divergent duct optimization: initial (continuous line) and optimized (dashed line) dust shapes and the Bézier–Bernstein control points parameterizing them. Axes not in scale. Control points depicted with dark marks remain fixed during the optimization.

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Fig. 5 Divergent duct optimization: Velocity magnitude for the initial (a) and optimized (b) geometries.

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Fig. 6 Divergent duct optimization: Convergence of the steepest descent (SD), Conjugate Gradient (CG) and Truncated Newton (TN) optimization algorithms, w.r.t. optimization cycles (a) and EFS (b).