Airfoil Optimization for Unsteady Flows with Application to High-Lift Noise Reduction

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Abstract

AIRFOIL OPTIMIZATION FOR UNSTEADY FLOWS

WITH APPLICATION TO HIGH-LIFT NOISE REDUCTION

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The use of steady-state aerodynamic optimization methods in the computational fluid dynamic (CFD) community is fairly well established. In particular, the use of adjoint methods has proven to be very beneficial because their cost is independent of the number of design variables. The application of numerical optimization to airframe-generated noise, however, has not received as much attention, but with the significant quieting of modern engines, airframe noise now competes with engine noise. Optimal control techniques for unsteady flows are needed in order to be able to reduce airframe-generated noise.

In this thesis, a general framework is formulated to calculate the gradient of a cost function in a nonlinear unsteady flow environment via the discrete adjoint method. The unsteady optimization algorithm developed in this work utilizes a Newton-Krylov approach since the gradient-based optimizer uses the quasi-Newton method BFGS, Newton's method is applied to the nonlinear flow problem, GMRES is used to solve the resulting linear problem inexactly, and last but not least the linear adjoint problem is solved using Bi-CGSTAB. The flow is governed by the unsteady two-dimensional compressible Navier-Stokes equations in conjunction with a one-equation turbulence model, which are discretized using structured grids and a finite difference approach. The effectiveness of the unsteady optimization algorithm is demonstrated by applying it to several problems of interest including shocktubes, pulses in converging-diverging nozzles, rotating cylinders, transonic buffeting, and an unsteady trailing-edge flow.

In order to address radiated far-field noise, an acoustic wave propagation program based on the Ffowcs Williams and Hawkings (FW-H) formulation is implemented and validated. The general framework is then used to derive the adjoint equations for a novel hybrid URANS/FW-H optimization algorithm in order to be able to optimize the shape of airfoils based on their calculated far-field pressure fluctuations. Validation and application results for this novel hybrid URANS/FW-H optimization algorithm show that it is possible to optimize the shape of an airfoil in an unsteady flow environment to minimize its radiated far-field noise while maintaining good aerodynamic performance.

Acknowledgements

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LIST OF SYMBOLS

Alphanumeric Symbols

A	wing area
a	speed of sound
$\mathcal{A}^n$	unsteady flow Jacobian at time step n
c	chord length of airfoil
C_j	constraint equations
C_L, C_D	lift and drag coefficients
e	total energy
E, F	inviscid flux vectors in x- and y-directions
E_v, F_v	viscous flux vectors in x- and y-directions
$\mathbb{F}[\,]$	Fourier transform
$\mathcal{F}_j$	dipole term
H	stagnation enthalpy
h	height above ground
$H()$	Heaviside step function
$h(x_j)$	airfoil thickness at location x_j
I	identity matrix
$I(W/m^2)$	noise intensity at ground level
I^n	objective function at time step n
J	Jacobian matrix of coordinate transformation
$\mathcal{J}$	penalized objective function
k	level of fill for ILU(k)
$\mathcal{L}$	Lagrangian
M	Mach number
m	number of GMRES search directions
$\mathcal{M}$	Preconditioner
N	total number of time steps

N_B	number of grid blocks
N_c	number of coarse time steps
N_con	number of constraint equations
$N(dB)$	overall sound pressure level
N_F	number of flow variables
$\mathcal{O}$	objective function
p	pressure
Q	conserved flow variables
Q^n	flow variables at time step n
Q_k^n	flow variables at time step n and stage k
$\mathcal{Q}$	Monopole term
R	flow solver residual
R_1, R_2	Riemann invariants
$\mathcal{R}^n$	unsteady flow solver residual at time step n
$\mathcal{R}_k^n$	unsteady flow solver residual at time step n and stage k
$\mathcal{R}e$	Reynolds number
$\hat{S}$	viscous flux vector for thin-layer approximation
T	final time
t	time
T_∞	free-stream temperature
T_P	period
T_{jk}	Lighthill stress tensor
U, V	ξ- and η-components of contravariant velocity
u, v	x- and y-components of velocity
V_∞	flyover speed
V_n, V_t	normal and tangential velocity
w_T	weight for thickness constraint
W_{up}	all-up weight
x, y	Cartesian coordinates

Y	vector of design variables

Greek Symbols

α	angle of attack
Δt	time discretization step
Δt_c	coarse time discretization step
$\delta()$	Dirac delta function
δ_{ij}	Kronecker delta
$\epsilon^{(2)}$	second-order artificial dissipation coefficient
$\epsilon^{(4)}$	fourth-order artificial dissipation coefficient
γ	specific heat ratio
μ	dynamic laminar viscosity
μ_t	turbulent eddy viscosity
ψ^n	vector of Lagrange multipliers (adjoint variables) at time step n
ρ	density
σ	spectral radius of the flux Jacobian
τ_{ij}	viscous stress tensor
$\tilde{\nu}$	turbulence model working variable
Υ	pressure switch
ξ, η	curvilinear coordinates

Superscripts

$\bar{}$	time average
$\hat{}$	transformation to curvilinear space
$\tilde{}$	dimensional variable
$'$	perturbation from the mean
$*$	target value
T	transpose

Subscripts

$\nabla_b R$	partial differentiation of R with respect to b carried out with all other variables held constant

∞	free-stream quantity
M	associated with mean flow
T	associated with turbulence model
j,k	ξ- and η-direction nodal indices

Abbreviations

BDF	Backwards Difference Formula
BFGS	Broyden-Fletcher-Goldfarb-Shanno
Bi-CGSTAB	Bi-Conjugate Gradient STABilized
CFD	Computational Fluid Dynamics
DES	Detached-Eddy Simulation
ESDIRK	Explicit first stage, Single diagonal coefficient, Diagonally Implicit Runge-Kutta
FFT	Fast Fourier Transform
FW-H	Ffowcs Williams and Hawkings
GMRES	Generalized Minimal RESidual
ILU	Incomplete Lower-Upper
LES	Large Eddy Simulation
OΔE's	Ordinary Difference Equations
OASPL	OverAll Sound Pressure Level
ODE's	Ordinary Differential Equations
PDE's	Partial Differential Equations
SQP	Sequential Quadratic Programming
URANS	Unsteady Reynolds-Averaged Navier-Stokes

Chapter 1

INTRODUCTION

Increased computer capabilities have enabled exceptional growth in the field of Computational Fluid Dynamics (CFD) such that numerical simulation and optimization of unsteady turbulent flow conditions are now feasible. In this chapter, background information about aerodynamic design optimization is given in Section 1.1, and a brief introduction to aircraft noise is presented in Section 1.2. Finally, the objectives of this thesis and a document outline can be found in Section 1.3.

1.1 Aerodynamic Design using Numerical Optimization

The goal of all aerodynamic design methods, be they experimental, analytical or computational, is to find a shape which improves an aerodynamic measure of interest, such as lift or drag, while adhering to appropriate constraints, for example structural integrity, fuel tank volume, etc. Since computational aerodynamic design methods tend to increase the level of automation during the design process, they enjoy great popularity [68, 73]. Although automation may reduce design processing time as well as the dependence of the result on the expertise of the designer, its success depends heavily on the reliability and accuracy of the computational methods and on how well the designer has set the goals.

The natural choice for solving design problems computationally is the use of numerical optimization methods. Thus, the designer has to cast the given aerodynamic design problem into a well-posed optimization problem. This includes the definition of an objective function which is to be minimized, design variables which describe the aerodynamic shape, and possibly constraints which confine the feasible shapes. The numerical optimization method can then determine, in an iterative, automated, and systematic approach, design variable values within the feasible region of the design space which improve and eventually minimize the objective function. The objective function value is calculated using a suitable flow analysis

tool, the so-called flow solver. The flow solver has a significant influence on the efficiency of the numerical optimization method since the iterative process requires repeated evaluations of the objective function. Furthermore, the accuracy of the objective function evaluations, and hence the accuracy of the flow solver, also ultimately determines the overall accuracy of the computational aerodynamic design method.

Numerical optimization methods that are available include direct search methods, stochastic methods, and gradient-based methods [25, 44, 103]. Gradient-based methods are likely the most effective for aerodynamic design problems, since significant design improvements can be obtained in comparatively few evaluations of the objective function. However, gradient-based methods require a relatively smooth design space and usually converge only to a local optimum, which is certainly an improvement of the initial design but not necessarily the best obtainable design. The main challenge for the implementation of gradient-based methods is an accurate and efficient computation of the gradient. The use of an adjoint method [108] for this purpose, which has been pioneered by Jameson [64] for steady-state aerodynamic design optimization, has proved to be accurate and very efficient since its cost is independent of the number of design variables [109]. For more details about all the aforementioned concepts see Chapter 3.

The use of steady-state aerodynamic optimization methods in the CFD community is fairly well established [1, 2, 32, 33, 65, 72, 104]. In particular, Nemec and Zingg [97, 101, 102] successfully used a Newton-Krylov approach to two-dimensional steady optimization using the Reynolds-Averaged Navier-Stokes (RANS) equations which lays the groundwork for this thesis. However, a much smaller amount of work has been done on applying optimization methods to unsteady aerodynamic problems even though many devices of interest, such as helicopter rotors, turbomachinery blades and high-lift components, operate in unsteady flow environments. Yee *et al.* [152] attempted aerodynamic shape optimization of rotor airfoils in an unsteady viscous flow, and He *et al.* [52] applied active control and drag optimization to unsteady flow past a cylinder. The optimal control of a vortex trapped by an airfoil with a cavity was investigated by Iollo and Zannetti [62], and Duta *et al.* [30, 31] used a harmonic adjoint approach to turbomachinery design. Marsden *et al.* [82, 83, 84] applied a surrogate management framework to an aerodynamic noise reduction problem involving laminar and turbulent trailing-edge flow. Nadarajah and Jameson [89, 90] designed airfoils undergoing a pitching oscillation using a discrete adjoint approach to reduce the time-averaged drag

coefficient while maintaining the time-averaged lift coefficient. Lastly, Mani and Mavriplis applied a discrete adjoint formulation for flow problems on dynamically deforming unstructured meshes for the Euler equations in two dimensions [79, 81] and the Navier-Stokes equations in three dimensions [85] using the second-order accurate backward difference formula temporal discretization. They also used the adjoint for time-step adaptation and error reduction in unsteady flow problems [80]. The work for this thesis was developed in parallel and is distinguished from their work in several important respects, as the present work is using a more general framework to derive the adjoint equations (Section 3.3) which allows the use of higher-order time marching methods (Section 2.3), remote objective functions (Section 5.6), and the coupling with a wave propagation program (Chapter 4). In the context of unsteady flows, frequency domain methods which allow for reduced computational expense, particularly for problems with strong periodic behaviour, have also been used for unsteady optimization by various authors [93, 94, 136]. However, most unsteady problems have no dominant periodic behavior and therefore frequency domain methods should be viewed as complementary to time-domain methods [85].

1.2 Introduction to Aircraft Noise

In all branches of engineering and technology, power requirements to overcome resistance are reduced by decreasing the resistance of each component constituting the overall resistance. Most people would agree that reducing power requirements by fifty percent is a major advancement in engineering. However, a human listener would perceive an acoustic power reduction of fifty percent as small since it amounts to just $3\,dB$ on the logarithmic decibel scale. In order for a human listener to realize that a noise has been subjectively halved, a noise reduction of about $10\,dB$, corresponding to a drop in acoustic power of ninety percent, is necessary (compare with Figure 1.1).

Aircraft noise is defined as the noise intensity, $I(W/m^2)$, as measured by an observer at ground level directly below the aircraft, which corresponds to $\theta = 90°$, where θ is the angle measured in the longitudinal flight plane from downstream. The OverAll Sound Pressure Level (OASPL) radiated from this aircraft is then given by [76]

$$N(dB) = 120 + 10\log_{10} I(W/m^2). \tag{1.1}$$

Figure 1.1: Common environmental sound levels [135].

Aircraft noise sources are typically divided into two main sources; the engine and the airframe, which themselves are composed of many different noise sources. The three primary noise sources of a turbofan engine are the fan, the fan jet, and the primary jet. Airframe noise is generated by the air flowing over the airplane's fuselage, wing, landing gear, and high-lift devices such as the leading-edge slats and trailing-edge flaps. All these different noise sources combine in a complicated fashion that can make it very difficult to achieve large reductions in the OASPL. For example, a human observer clearly hears the noise of a dominant source, but sources that are about $10\,dB$ less than this dominant source are not heard. Thus, the elimination of the dominant source would achieve a significant $10\,dB$ reduction in noise. On

the other hand, noise reductions made to the other noise sources would lead to little or no reduction of the OASPL. In contrast, two sources of equal intensity produce a combined noise that is $3\,dB$ louder than either noise source alone. Thus, the elimination of one of the sources would only result in an insignificant $3\,dB$ reduction in noise.

The dominant source of aircraft noise in the past has been the engine. However, the changeover from the turbojet engines to the high-bypass ratio turbofan engines has produced a large reduction in engine noise and has concurrently resulted in a reduction in fuel burn, implying economical and environmental benefits [76]. As a result, the noise produced by individual aircraft has been reduced dramatically since the beginning of the jet age. Over a period of thirty years from the mid 1960s to the 1990s, aircraft noise at a given thrust level was reduced by $20\,dB$ [113]. To the human listener, this is heard subjectively as a fourfold reduction in noise as the acoustic power has been reduced by a factor of one hundred. Nowadays during aircraft approach and landing, when engines operate at reduced thrust and high-lift devices and undercarriage are in the deployed state, the noise from the airframe is only marginally lower than the engine noise [69, 125, 149]. In some modern aircraft the engine noise is even lower than the airframe noise [113] as shown in Figure 1.2.

1. Typical 1992-level aircraft, data taken from [149]   2. Typical 2002-level aircraft (A340-300) [113]

Figure 1.2: Breakdown of noise components during approach for two different aircraft and decades.

The importance of individual airframe noise sources is configuration dependent, but typically noise due to the high-lift system dominates for medium-sized aircraft, whereas undercarriage noise is more important for larger aircraft [15]. Aircraft high-lift systems consist of many sharp edges and corners, such as trailing edges, the cusps of the slats and the side edges of the flaps. In general, the deployment of any high-lift component (slat or flap) increases the far-field noise level, and the larger the deployment angle, the higher the noise. The changes in noise levels with the high-lift system components are, however, frequency dependent. Increasing flap deployment angles affects almost the entire mid- and high-frequency domain with the most significant effects at high frequencies. The noise predominantly comes from the flow in the vicinity of the flap side edges, associated with flow separation in the flap cross-flow [17]. When the flap angle increases, for example, from $0°$ to $50°$, the increase in noise level can be as high as $10\,dB$ at high frequencies [49]. On the other hand, the deployment of slats mainly increases noise in the low- to mid-frequency domain, probably associated with flow separation in the slat cove [47]. When, for example, the slats are deployed from the retracted position to $20°$, the noise level is increased by up to about $4\,dB$ within the frequency band from 0.1 to 2.5 kHz [49]. In this case the flow can be approximated as two-dimensional, leading to noise source distributions along the spanwise direction of the slats.

The fact that the slat deployment can be treated two-dimensionally and affects mostly the low- and mid-frequency domain makes this an ideal test case for high-lift noise reduction, since both conditions make the computational size of the problem viable. Significant acoustic phenomena are intrinsically three-dimensional; however, the flow structures responsible for generating noise can be quasi-two-dimensional like the flow separation in the slat cove. Singer *et al.* [125] found that two-dimensional simulations can be used in this case to find the correct features of the radiated sound, even though the amplitudes are overpredicted. For more details see Chapter 4.

Noise from automobiles and aircraft is a significant problem around the world. In Europe, for example, it is estimated that roughly twenty per cent of the European Union's population (close to 80 million people) are exposed to noise levels that are considered unacceptable [34]. It is well known that the noise from air traffic can be a source of irritation and annoyance, but a study carried out as part of the HYpertension and Exposure to Noise near Airports (HYENA) project [50] (a four-year study exploring the health effects associated with exposure to aircraft noise) found that it can also be damaging to people's health. The study

showed that night-time noise from aircraft, traffic or even a partner snoring can increase a person's blood pressure even if it does not wake them. The increase in blood pressure was related to the loudness of the noise, such that a greater increase in blood pressure could be seen where the noise level was higher. People with high blood pressure (hypertension) have an increased risk of developing heart disease, stroke, kidney disease and dementia [50]. A similar study [114] found that people who have been living for at least five years under a flight path near an international airport, have a greater risk of developing high blood pressure than people living in quieter areas. It showed that an increase in night-time aircraft noise of $10\,dB$ increased the risk of high blood pressure by fourteen per cent in both men and women.

Because of the projected growth in air travel and the increase in population density near airports, it is clear that measures need to be taken to reduce noise levels from aircraft, in particular during night-time, in order to protect the health of people living near airports. Current Federal Aviation Administration (FAA) and European noise regulations do exactly this and require future civil aircraft to be substantially quieter than current ones [128]. In state of the art aircraft, multiple sources are producing noise at similar intensities (see Figure 1.2), thus all of these sources must be reduced by commensurate levels to achieve any significant overall noise reduction.

The noise intensity at ground level for an aircraft in straight and level flight at some flyover speed, V_∞, in the "clean" configuration (flaps, slat and undercarriage stowed) and with the engine cut back, varies approximately as V_∞^5 for a wide range of aircraft [10, 40, 59]. Here, the atmospheric sound absorption at higher frequencies is ignored due to the relatively low heights involved in flyover experiments. This proportionality can be inferred from a simple formula which can be derived by assuming that the turbulent boundary layer noise scattered by the wing trailing edge is the dominant noise source [76]. Using the average lift coefficient, $\bar{C}_L$, the free-stream Mach number, M_∞, the speed of sound, a_∞, the height above ground, h, and the all-up weight, $W_{up} = 0.5\rho_\infty V_\infty^2 A \bar{C}_L$, where A is the wing area and ρ_∞ the free-stream density, the noise intensity at ground level is given by

$$I(W/m^2) = K \left(\frac{W_{up} V_\infty M_\infty^2}{\bar{C}_L h^2} \right) = K \left(\frac{0.5\rho_\infty A V_\infty^5}{a_\infty^2 h^2} \right), \tag{1.2}$$

where $K \approx 7 \cdot 10^{-7}$ for larger aircraft. Although the coefficient K varies with the Reynolds number ranging from gliders, light aircraft, to large jumbo-jets, one can find that this formula

fits the experimental data collected from ground noise measurements for all aircraft over the past twenty-five years remarkably well [76], thereby covering an enormous range of weights from about $10\,N$ to $4 \cdot 10^6\,N$. As an example for a larger aircraft in the "clean" configuration with $W_{up} = 2 \cdot 10^6\,N$, $\bar{C}_L = 0.5$, $V_\infty = 125\,m/s$ implying $M_\infty = 0.38$ and $h = 120\,m$, the resulting OASPL at the ground level is $N = 95.4\,dB$. For other angles θ in the longitudinal flight plane the noise directivity follows the $\sin^2(\theta/2)$ law [76].

It should be noted that Eq. (1.2) is not sufficient for accurate predictions or even noise certification requirements. However, it gives some insight into the dominant noise characteristics generated by "clean" aircraft. It also provides information on the lower bound of airframe noise for present-day aircraft if it were possible to entirely eliminate all extra noise arising from the "dirty" configuration (high-lift system and undercarriage deployed). For aircraft flying in the "dirty" configuration, the radiated noise is highly geometry dependent but it still remains proportional to about V_∞^5 [76].

By investigating Eq. (1.2) one can immediately think about a few operational measures to reduce the airframe noise on approach. These include the use of lighter aircraft and steeper approaches, as well as later high-lift system and undercarriage deployment. A reduction in approach speed, which is typically about 1.3 times the aircraft stalling speed [76], would also reduce noise significantly. All such measures would have implications for the design of future high-lift systems and undercarriages and the challenge will be to aerodynamically dissipate the large amounts of energy produced during approach with significantly less noise than nowadays or to create the unavoidable noise at less obtrusive frequencies.

1.3 Objectives and Outline

When an aircraft is landing and the flaps and slats are deployed, the airflow around this high-lift airfoil becomes unsteady and very complex, involving phenomena such as flow separation and shear-layer instability both in the slat region and near the side edges of the flaps. These complex flow features cause pressure fluctuations that can escape to the ground level as noise, as described in the previous section and Chapter 4. The task of this research project is to simulate this situation using a two-dimensional CFD simulation and a wave propagation program, which enable the use of gradient-based numerical optimization, in order to change the shape of the high-lift airfoil to minimize its radiated noise while maintaining good flight performance.

In more detail, the objectives of this thesis are two-fold:

1. Develop an efficient unsteady aerodynamic optimization algorithm based on a Newton-Krylov and adjoint approach, where the underlying physical model is the Unsteady Reynolds-Averaged Navier-Stokes (URANS) equations. Tasks which have to be accomplished in order to achieve this objective include

    (a) Extend the two-dimensional steady turbulent Newton-Krylov based group codes PROBE [111] (single-block) and TORNADO [97] (multi-block) to handle unsteady turbulent flows using the URANS equations and the one-equation Spalart-Allmaras turbulence model while maintaining the efficiency of the steady flow solvers.

    (b) Develop a general framework to derive the adjoint equations for the unsteady turbulent flow solver.

    (c) Apply the unsteady aerodynamic optimization algorithm to several problems of interest in order to validate and test it. Factors under consideration are the accuracy and efficiency of the gradient computation and the overall efficiency of the unsteady optimization procedure.

2. Extend the unsteady optimization algorithm to be able to perform far-field noise minimizations by coupling the URANS solver with a wave propagation program. The associated tasks include

    (a) Evaluate available wave propagation programs, implement one, and validate it by using model problems with analytical solutions and by directly comparing the wave propagation program output with a URANS simulation.

    (b) Use the developed framework to derive the adjoint equations for this hybrid acoustic prediction code. Validate the resulting hybrid acoustic prediction optimization algorithm using remote inverse shape designs and apply it to airframe-generated noise reduction problems.

Chapters 2 and 3 address tasks 1(a) and (b), as the underlying equations and numerical algorithm of the flow solver and a description of all the components of the gradient based unsteady aerodynamic optimization algorithm are presented, respectively. Chapter 4

is concerned with task 2(a) since an overview of available wave propagation programs and details about the implementation of the chosen two-dimensional Ffowcs Williams and Hawkings (FW-H) equation in the frequency domain are given and results of validation cases are shown. Chapter 5 presents the validation and evaluation of the unsteady aerodynamic optimization algorithm as well as the hybrid acoustic prediction optimization algorithm based on a wide spectrum of applications, therby covering tasks 1(c) and 2(b). Finally, Chapter 6 concludes this thesis, highlights the contributions, and outlines some potential future research directions. The development and application of this unsteady aerodynamic optimization algorithm and the hybrid acoustic prediction optimization algorithm is also presented in Rumpfkeil and Zingg [115, 116, 117, 118, 119, 120].

Chapter 2

GOVERNING FLOW EQUATIONS

This chapter discusses the underlying equations and numerical algorithm of the flow solver. In Section 2.1, the unsteady thin-layer Reynolds-averaged Navier-Stokes equations are presented in conjunction with the one-equation Spalart-Allmaras turbulence model. Sections 2.2 and 2.3 discuss the spatial and temporal discretization of the governing flow equations, respectively. Section 2.4 then describes how the nonlinear system of the discretized equations is solved using an inexact Newton-Krylov algorithm.

2.1 Navier-Stokes Equations

The Navier-Stokes equations operate on the non-dimensional conservative variables

$$
Q = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix},
\tag{2.1}
$$

where the dimensional Cartesian coordinates $\tilde{x}$ and $\tilde{y}$, density $\tilde{\rho}$, velocities $\tilde{u}$ and $\tilde{v}$, total energy $\tilde{e}$, and time $\tilde{t}$ are scaled as

$$
x = \frac{\tilde{x}}{c}, \quad y = \frac{\tilde{y}}{c}, \quad \rho = \frac{\tilde{\rho}}{\tilde{\rho}_\infty}, \quad u = \frac{\tilde{u}}{\tilde{a}_\infty}, \quad v = \frac{\tilde{v}}{\tilde{a}_\infty}, \quad e = \frac{\tilde{e}}{\tilde{\rho}_\infty a_\infty^2}, \quad t = \frac{\tilde{t} a_\infty}{c}.
\tag{2.2}
$$

Here the ∞ subscript indicates free-stream quantities, c is the airfoil chord, $a = \sqrt{\gamma p / \rho}$ is the speed of sound with $\gamma = 1.4$ for air and the pressure, p, is related to the flow variables via the equation of state for an ideal gas where $p = (\gamma - 1)\left(e - \frac{1}{2}\rho(u^2 + v^2)\right)$.

The unsteady two-dimensional Reynolds-averaged Navier-Stokes equations in Cartesian coordinates are given by

$$
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = \frac{1}{\mathcal{R}e}\left(\frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y}\right),
\tag{2.3}
$$

with the inviscid fluxes

$$E = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (e + p)u \end{bmatrix}, \quad F = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (e + p)v \end{bmatrix}, \tag{2.4}$$

and the viscous fluxes

$$E_v = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \phi_1 \end{bmatrix}, \quad F_v = \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \phi_2 \end{bmatrix}, \tag{2.5}$$

where

$$\begin{aligned}
\tau_{xx} &= (\mu + \mu_t)(4u_x - 2v_y)/3 \\
\tau_{xy} &= (\mu + \mu_t)(u_y + v_x)/3 \\
\tau_{yy} &= (\mu + \mu_t)(-2u_x + 4v_y)/3 \\
\phi_1 &= u\tau_{xx} + v\tau_{xy} + (\mu \mathcal{P}r^{-1} + \mu_t \mathcal{P}r_t^{-1})(\gamma - 1)^{-1}\partial_x(a^2) \\
\phi_2 &= u\tau_{xy} + v\tau_{yy} + (\mu \mathcal{P}r^{-1} + \mu_t \mathcal{P}r_t^{-1})(\gamma - 1)^{-1}\partial_y(a^2).
\end{aligned} \tag{2.6}$$

Here μ and μ_t are the dynamic and turbulent eddy viscosities, respectively. The dynamic eddy viscosity is related to the free-stream temperature, $T_\infty \equiv 460°R$, and the constant $S^* = 198.6°R$ via Sutherland's law

$$\mu = \frac{\tilde{\mu}}{\mu_\infty} = \frac{a^3(1 + S^*/T_\infty)}{a^2 + S^*/T_\infty}. \tag{2.7}$$

The Reynolds number, $\mathcal{R}e$, is defined as

$$\mathcal{R}e = \frac{\rho_\infty \, c \, a_\infty}{\mu_\infty}, \tag{2.8}$$

which is not based on u_∞ like experimentally given Reynolds numbers, which are therefore scaled by the free-stream Mach number $M_\infty = u_\infty/a_\infty$ in the code. The laminar and turbulent Prandtl numbers $\mathcal{P}r \equiv 0.72$ and $\mathcal{P}r_t \equiv 0.90$ are assumed to be constant.

2.1.1 Turbulence Model

> *"When I meet God, I am going to ask him two questions:*
> *Why relativity? And why turbulence?*
> *I really believe he will have an answer for the first."*
>
> Werner Heisenberg (1901-1976)

A turbulence model is needed for the Navier-Stokes equations to calculate the turbulent eddy viscosity μ_t. The one-equation Spalart-Allmaras [131] turbulence model is used, which is optimized for aerodynamic applications, particularly for flows past a wing. The non-dimensional dependent variable is $\tilde{\nu}$, with the transport equation given by

$$
\begin{aligned}
\frac{\partial \tilde{\nu}}{\partial t} + u\frac{\partial \tilde{\nu}}{\partial x} + v\frac{\partial \tilde{\nu}}{\partial y} \;=\;& \frac{c_{b1}}{\mathcal{R}e}[1 - f_{t2}]\tilde{S}\tilde{\nu} - \frac{1}{\mathcal{R}e}\left[c_{w1}f_w - \frac{c_{b1}}{\kappa^2}f_{t2}\right]\left(\frac{\tilde{\nu}}{d_w}\right)^2 \\
& +\; \frac{1+c_{b2}}{\sigma \mathcal{R}e}\nabla \cdot [(\nu + \tilde{\nu})\nabla\tilde{\nu}] - \frac{c_{b2}}{\sigma \mathcal{R}e}(\nu + \tilde{\nu})\nabla^2\tilde{\nu} + \mathcal{R}e f_{t1}\Delta U^2.
\end{aligned}
\tag{2.9}
$$

The first term on the right hand side is the production term, the second is the destruction, the third and fourth are diffusion terms, and the fifth is the trip, or transition, term. The turbulent eddy viscosity μ_t is found from $\tilde{\nu}$ by

$$
\mu_t = \rho\tilde{\nu}f_{v1},
\tag{2.10}
$$

where

$$
f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}, \quad \chi = \frac{\tilde{\nu}}{\nu} \quad \text{and} \quad \nu = \rho\mu.
\tag{2.11}
$$

The modified vorticity, $\tilde{S}$ is given by

$$
\tilde{S} = S\mathcal{R}e + \frac{\tilde{\nu}}{\kappa^2 d_w^2}f_{v2},
\tag{2.12}
$$

where $S = \left|\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right|$ is the magnitude of the vorticity, d_w is the distance to the closest wall, and

$$
f_{v2} = 1 - \frac{\chi}{1 + \chi f_{v1}}.
\tag{2.13}
$$

The destruction function f_w is

$$
f_w = g\left[\frac{1 + c_{w3}^3}{g^6 + c_{w3}^6}\right]^{\frac{1}{6}},
\tag{2.14}
$$

with

$$g = r + c_{w2}(r^6 - r) \quad \text{and} \quad r = \frac{\tilde{\nu}}{\tilde{S}\kappa^2 d_w^2}. \tag{2.15}$$

Transition can be enforced using the two functions f_{t1} and f_{t2} [131]. They are set to zero in this work. The remaining parameters are the following constants

$$
\begin{array}{rclrcl}
c_{b1} & = & 0.1355 & c_{b2} & = & 0.622 \\
c_{w1} & = & c_{b1}/\kappa^2 + (1 + c_{b2})/\sigma & \kappa & = & 0.41 \\
c_{w2} & = & 0.3 & c_{w3} & = & 2.0 \\
c_{v1} & = & 7.1 & \sigma & = & \frac{2}{3}.
\end{array}
\tag{2.16}
$$

Ashford [3] proposed the following changes to Eqs. (2.12) and (2.13) to keep $\tilde{S}$ positive

$$\tilde{S} = S f_{v3} \mathcal{R}e + \frac{\tilde{\nu}}{\kappa^2 d_w^2} f_{v2}, \tag{2.17}$$

with $c_{v2} = 5.0$ in

$$f_{v2} = \left(1 + \frac{\chi}{c_{v2}}\right)^{-3} \quad \text{and} \quad f_{v3} = \frac{(1 + \chi f_{v1})(1 - f_{v2})}{\chi}, \tag{2.18}$$

which are incorporated in this work.

2.1.2 Thin-Layer Approximation and Coordinate Transformation

The Navier-Stokes equations can be simplified using the thin-layer approximation in which the viscous effects resulting from the derivatives in the streamwise direction are assumed to be small enough to be neglected. This assumption does not hold for low Reynolds numbers or highly separated flows.

Structured grids are used to discretize the physical domain. All grids are generated with the multi-block grid-generation tool AMBER2D [96]. For single-element airfoils or cylinders, single-block C- or O-topology grids are used, while for airfoils with blunt trailing edges or multi-element airfoils, multi-block C- or H-topology grids are used. A curvilinear coordinate transformation is applied to map the curved grid in physical coordinates (x, y) to a unit square grid in curvilinear computational coordinates (ξ, η) [112]

$$\xi = \xi(x, y), \quad \eta = \eta(x, y). \tag{2.19}$$

The two-dimensional thin-layer Navier-Stokes equations in curvilinear coordinates are given by

$$\frac{\partial \hat{Q}_M}{\partial t} + \frac{\partial \hat{E}}{\partial \xi} + \frac{\partial \hat{F}}{\partial \eta} = \frac{1}{\mathcal{R}e}\left(\frac{\partial \hat{S}}{\partial \eta}\right), \tag{2.20}$$

and they operate on the conservative mean flow variables

$$\hat{Q}_M = J^{-1}\begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{bmatrix}, \tag{2.21}$$

where the metric Jacobian of the transformation J is

$$J^{-1} = (x_\xi y_\eta - x_\eta y_\xi). \tag{2.22}$$

The inviscid flux vectors become

$$\hat{E} = J^{-1}\begin{bmatrix} \rho U \\ \rho U u + \xi_x p \\ \rho U v + \xi_y p \\ (e+p)U \end{bmatrix}, \quad \hat{F} = J^{-1}\begin{bmatrix} \rho V \\ \rho V u + \eta_x p \\ \rho V v + \eta_y p \\ (e+p)V \end{bmatrix}, \tag{2.23}$$

where U and V are the contravariant velocities

$$U = \xi_x u + \xi_y v, \quad V = \eta_x u + \eta_y v. \tag{2.24}$$

The modified viscous flux vector is

$$\hat{S} = J^{-1}\begin{bmatrix} 0 \\ \eta_x m_1 + \eta_y m_2 \\ \eta_x m_2 + \eta_y m_3 \\ \eta_x(um_1 + vm_2 + m_4) + \eta_y(um_2 + vm_3 + m_5) \end{bmatrix}, \tag{2.25}$$

with

$$\begin{aligned}
m_1 &= (\mu + \mu_t)(4\eta_x u_\eta - 2\eta_y v_\eta)/3 \\
m_2 &= (\mu + \mu_t)(\eta_y u_\eta + \eta_x v_\eta) \\
m_3 &= (\mu + \mu_t)(-2\eta_x u_\eta + 4\eta_y v_\eta)/3 \\
m_4 &= (\mu \mathcal{P}r^{-1} + \mu_t \mathcal{P}r_t^{-1})(\gamma - 1)^{-1}\eta_x \partial_\eta(a^2) \\
m_5 &= (\mu \mathcal{P}r^{-1} + \mu_t \mathcal{P}r_t^{-1})(\gamma - 1)^{-1}\eta_y \partial_\eta(a^2).
\end{aligned} \tag{2.26}$$

Finally, the Spalart-Allmaras turbulence model without transition terms in curvilinear co-ordinates is given in the thin-layer approximation by neglecting all mixed derivatives as follows

$$\frac{\partial \tilde{\nu}}{\partial t} + U \frac{\partial \tilde{\nu}}{\partial \xi} + V \frac{\partial \tilde{\nu}}{\partial \eta} - \frac{1}{\mathcal{R}e} \left[c_{b1} \tilde{S} \tilde{\nu} - c_{w1} f_w \left(\frac{\tilde{\nu}}{d_w} \right)^2 + \frac{1 + c_{b2}}{\sigma} T_1 - \frac{c_{b2}}{\sigma} T_2 \right] = 0, \qquad (2.27)$$

where

$$\begin{aligned} T_1 &= \xi_x \frac{\partial}{\partial \xi} \left[(\nu + \tilde{\nu}) \xi_x \frac{\partial \tilde{\nu}}{\partial \xi} \right] + \eta_x \frac{\partial}{\partial \eta} \left[(\nu + \tilde{\nu}) \eta_x \frac{\partial \tilde{\nu}}{\partial \eta} \right] \\ &+ \xi_y \frac{\partial}{\partial \xi} \left[(\nu + \tilde{\nu}) \xi_y \frac{\partial \tilde{\nu}}{\partial \xi} \right] + \eta_y \frac{\partial}{\partial \eta} \left[(\nu + \tilde{\nu}) \eta_y \frac{\partial \tilde{\nu}}{\partial \eta} \right], \end{aligned} \qquad (2.28)$$

and

$$T_2 = (\nu + \tilde{\nu}) \left[\xi_x \frac{\partial}{\partial \xi} \left(\xi_x \frac{\partial \tilde{\nu}}{\partial \xi} \right) + \eta_x \frac{\partial}{\partial \eta} \left(\eta_x \frac{\partial \tilde{\nu}}{\partial \eta} \right) + \xi_y \frac{\partial}{\partial \xi} \left(\xi_y \frac{\partial \tilde{\nu}}{\partial \xi} \right) + \eta_y \frac{\partial}{\partial \eta} \left(\eta_y \frac{\partial \tilde{\nu}}{\partial \eta} \right) \right]. \qquad (2.29)$$

2.2 Spatial Discretization

The spatial discretization scheme of the thin-layer Navier-Stokes equations (2.20) is the one used in ARC2D [112] for C- or O-topology grids and TORNADO [96] for H-topology grids. The discretization for the inviscid fluxes uses a second-order centered-difference operator with second- and fourth-order scalar artificial dissipation [66] in every node (j,k):

$$\left(\frac{\partial \hat{E}}{\partial \xi} \right)_{j,k} \approx \frac{\hat{E}_{j+1,k} - \hat{E}_{j-1,k}}{2} - \nabla_\xi d_{j+\frac{1}{2},k} \quad \text{and} \quad \left(\frac{\partial \hat{F}}{\partial \eta} \right)_{j,k} \approx \frac{\hat{F}_{j,k+1} - \hat{F}_{j,k-1}}{2} - \nabla_\eta d_{j,k+\frac{1}{2}}. \qquad (2.30)$$

The artificial dissipation term in the ξ-direction is given by

$$d_{j+\frac{1}{2},k} = \sigma_{j+\frac{1}{2},k} J^{-1}_{j+\frac{1}{2},k} \left(\epsilon^{(2)}_{j+\frac{1}{2},k} \Delta_\xi (J \hat{Q}_M)_{j,k} - \epsilon^{(4)}_{j+\frac{1}{2},k} \Delta_\xi \nabla_\xi \Delta_\xi (J \hat{Q}_M)_{j,k} \right), \qquad (2.31)$$

where the combinations of operators acting on $J \hat{Q}_M$ are adjusted near the boundaries and

$$\begin{aligned} \Upsilon_{j,k} &= \frac{|p_{j+1,k} - 2p_{j,k} + p_{j-1,k}|}{|p_{j+1,k} + 2p_{j,k} + p_{j-1,k}|} \qquad &(2.32) \\ \Upsilon^*_{j,k} &= \max(\Upsilon_{j+1,k}, \Upsilon_{j,k}, \Upsilon_{j-1,k}) \qquad &(2.33) \\ \epsilon^{(2)}_{j,k} &= \kappa_2 (\frac{1}{4} \Upsilon^*_{j+1,k} + \frac{1}{2} \Upsilon^*_{j,k} + \frac{1}{4} \Upsilon^*_{j-1,k}) \qquad &(2.34) \\ \epsilon^{(4)}_{j,k} &= \max(0, \kappa_4 - \epsilon^{(2)}_{j,k}). \qquad &(2.35) \end{aligned}$$

The spectral radius of the flux Jacobian matrix is $\sigma_{j,k} = (|U| + a\sqrt{\xi_x^2 + \xi_y^2})_{j,k}$, and the dissipation constants have typical values of $\kappa_4 = 0.01$ and $\kappa_2 = 0$ for subsonic flows, such that the pressure switch Υ to control first-order dissipation near shocks is disabled; $\kappa_2 = 1.0$ for transonic flows. Lastly, Δ_ξ and ∇_ξ are the first-order forward and backward difference operators

$$\Delta_\xi(\cdot)_{j,k} = (\cdot)_{j+1,k} - (\cdot)_{j,k} \quad \text{and} \quad \nabla_\xi(\cdot)_{j,k} = (\cdot)_{j,k} - (\cdot)_{j-1,k}, \tag{2.36}$$

and values at the half nodes are computed by averaging, for example

$$(\cdot)_{j+\frac{1}{2},k} = \frac{(\cdot)_{j+1,k} + (\cdot)_{j,k}}{2}. \tag{2.37}$$

Analogous terms are used for the artificial dissipation in the η-direction. The viscous fluxes are of the form

$$\partial_\eta(\alpha_{j,k}\partial_\eta\beta_{j,k}), \tag{2.38}$$

and the discretization of this term uses the following conservative three-point stencil

$$\nabla_\eta\left(\alpha_{j,k+\frac{1}{2}}\,\Delta_\eta\beta_{j,k}\right) = \alpha_{j,k+\frac{1}{2}}(\beta_{j,k+1} - \beta_{j,k}) - \alpha_{j,k-\frac{1}{2}}(\beta_{j,k} - \beta_{j,k-1}). \tag{2.39}$$

The Spalart-Allmaras turbulence model (2.27) is discretized as described in [97, 131]. A first-order upwind discretization is used for the convective term in the ξ-direction

$$U\frac{\partial\tilde{\nu}}{\partial\xi} \approx \frac{1}{2}(U_{j,k} + |U_{j,k}|)(\tilde{\nu}_{j,k} - \tilde{\nu}_{j-1,k}) + \frac{1}{2}(U_{j,k} - |U_{j,k}|)(\tilde{\nu}_{j+1,k} - \tilde{\nu}_{j,k}) \tag{2.40}$$

and an analogous term is used for the η direction. The diffusion term has the same form as the viscous terms, Eq. (2.38), and thus the same discretization is applied. The magnitude of the vorticity is discretized as follows

$$S \approx \frac{1}{2}\left|\xi_x(v_{j+1,k} - v_{j-1,k}) + \eta_x(v_{j,k+1} - v_{j,k-1}) - \xi_y(u_{j+1,k} - u_{j-1,k}) - \eta_y(u_{j,k+1} - u_{j,k-1})\right|. \tag{2.41}$$

2.2.1 Boundary Conditions

Boundary conditions need to be applied since the physical domain is bounded. A brief overview is given here; for more details see Hirsch [55] and Nemec [97].

Solid Wall

For inviscid flows, tangency is required at solid walls, which implies that $V_n = 0$. The tangential velocity V_t and pressure are extrapolated from the interior and the stagnation enthalpy, $H = (e + p)/\rho$, is set to the free-stream value, H_∞.

For viscous flows, the no-slip condition $u = v = 0$ is used, and the wall is considered to be adiabatic. Furthermore, the pressure gradient is set to zero, which in conjunction with the adiabatic condition and the perfect gas law, results in a zero density gradient as well.

Far-field

Two locally one-dimensional Riemann invariants

$$R_1 = V_n + \frac{2a}{\gamma - 1} \quad \text{and} \quad R_2 = V_n - \frac{2a}{\gamma - 1}, \tag{2.42}$$

as well as the entropy function $S = \rho^\gamma / p$ and the tangential velocity V_t are used to define the far-field boundary conditions. Here, V_n is the velocity normal to the boundary and $V_n < 0$ is considered an inflow situation. In the subsonic inflow case, R_2 is extrapolated from the interior and R_1, V_t, and S are set to free-stream conditions. In the subsonic outflow case, R_1 is extrapolated from the interior, while the remaining three variables are set to free-stream values. Zero-order extrapolation is used in all cases.

For viscous flows downstream of the body, this approach is not appropriate due to effects resulting from the wake crossing the outflow boundary, and a simple zeroth-order extrapolation of ρ, ρu, ρv, and p is used instead.

Wake-cut and Block Interface

For H-topology grids and wake-cuts ρ, ρu, ρv, p and the turbulence variable $\tilde{\nu}$ are averaged at block interfaces in the normal direction. Block interfaces in the streamwise direction, on the other hand, are overlapped using an appropriate number of halo or ghost points.

Turbulence Model

The boundary conditions used for the Spalart-Allmaras turbulence model are straightforward. At solid walls $\tilde{\nu}$ is set to zero. At inflow far-field boundaries $\tilde{\nu}$ is set to its free-stream

value, $\tilde{\nu}_\infty = 0.001$, and at outflow far-field boundaries, a zeroth-order extrapolation from the interior is used.

2.3 Temporal Discretization

"The only reason for time is so that everything doesn't happen at once."

Albert Einstein (1879-1955)

After the spatial discretization and the application of boundary equations, the thin-layer Navier-Stokes equations (2.20) can be written as a coupled system of nonlinear Ordinary Differential Equations (ODE's):

$$\frac{\mathrm{d}\hat{Q}}{\mathrm{d}t} + R(\hat{Q}) = 0, \tag{2.43}$$

where $R(\hat{Q})$ contains the spatially discretized convective and viscous fluxes as well as the boundary conditions. For turbulent flows it also contains the spatially discretized one-equation Spalart-Allmaras turbulence model (2.27) and its boundary conditions. Note that the term $\frac{\mathrm{d}\hat{Q}}{\mathrm{d}t}$ is only added to interior or time dependent boundary nodes. $\hat{Q}$ denotes the discrete flow variable vector with dimension N_F for the remainder of this thesis. For a grid with N_B blocks, the total number of flow variables is given by $N_\mathrm{F} = n_\mathrm{max} \cdot \sum_{i=1}^{N_\mathrm{B}} (j_{\mathrm{max}_i} \cdot k_{\mathrm{max}_i})$, where $n_\mathrm{max} = 5$ for turbulent and $n_\mathrm{max} = 4$ for laminar flows. At each node (j, k)

$$\hat{Q}_{j,k} = \begin{bmatrix} \hat{Q}_M \\ \hat{Q}_T \end{bmatrix}_{j,k} = J_{j,k}^{-1} \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \tilde{\nu} \end{bmatrix}_{j,k}, \tag{2.44}$$

where $\hat{Q}_T$ denotes the turbulence model variable, which is scaled with the metric Jacobian and ignored for laminar flows.

The time-marching methods used in this work for temporal discretization are the second-order Backward Difference Formula (BDF) and the Explicit first stage, Single diagonal coefficient, Diagonally Implicit Runge-Kutta (ESDIRK) scheme of fourth-order. For all temporal discretization methods one has to choose a suitable time discretization step Δt to compromise between accuracy on the one hand and computational time on the other hand, while maintaining stability.

BDF2

Applying the BDF2 time-marching method to Eq. (2.43) leads to the following coupled system of Ordinary Difference Equations (OΔE's):

$$\mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, \hat{Q}^{n-2}) := \frac{3\hat{Q}^n - 4\hat{Q}^{n-1} + \hat{Q}^{n-2}}{2\Delta t} + R(\hat{Q}^n) = 0. \qquad (2.45)$$

These nonlinear OΔE's implicitly define the solution at the next time step $\hat{Q}^n$, given the solutions at the previous two time steps $\hat{Q}^{n-1}$ and $\hat{Q}^{n-2}$.

ESDIRK4

The ESDIRK scheme was developed by Bijl, Carpenter and Vatsa [6]. A fourth-order accurate scheme for Eq. (2.43) using six stages is given by the following coupled system of OΔE's:

$$\mathcal{R}_k^n(\hat{Q}_k^n, \ldots, \hat{Q}_1^n, \hat{Q}^{n-1}) := \frac{\hat{Q}_k^n - \hat{Q}^{n-1}}{\Delta t} + \sum_{j=1}^{k} a_{kj} R(\hat{Q}_j^n) = 0 \quad \text{for } k = 1, \ldots, 6. \qquad (2.46)$$

Here, $\hat{Q}_k^n$ is the solution for the next time step n at stage k, given the solutions at the previous time level $\hat{Q}^{n-1}$ and previous stages $\hat{Q}_j^n$ with $j = 1, \ldots, k-1$. The sixth and last stage gives the solution at the new time level, that is $\hat{Q}^n := \hat{Q}_6^n$. The terms a_{kj} are the Butcher coefficients for the scheme, which are given in Table 2.1. The c_k's indicate the point

$c_1=0$	$a_{11}=0$	0	0	0	0	0
$c_2=\frac{1}{2}$	$a_{21}=\frac{1}{4}$	$a_{22}=\frac{1}{4}$	0	0	0	0
$c_3=\frac{83}{250}$	$a_{31}=\frac{8611}{62500}$	$a_{32}=\frac{-1743}{31250}$	$a_{33}=\frac{1}{4}$	0	0	0
$c_4=\frac{31}{50}$	$a_{41}=\frac{5012029}{34652500}$	$a_{42}=\frac{-654441}{2922500}$	$a_{43}=\frac{174375}{388108}$	$a_{44}=\frac{1}{4}$	0	0
$c_5=\frac{17}{20}$	$a_{51}=\frac{15267082809}{155376265600}$	$a_{52}=\frac{-71443401}{120774400}$	$a_{53}=\frac{730878875}{902184768}$	$a_{54}=\frac{2285395}{8070912}$	$a_{55}=\frac{1}{4}$	0
$c_6=1$	$a_{61}=\frac{82889}{524892}$	$a_{62}=0$	$a_{63}=\frac{15625}{83664}$	$a_{64}=\frac{69875}{102672}$	$a_{65}=\frac{-2260}{8211}$	$a_{66}=\frac{1}{4}$

Table 2.1: Butcher table for a six-stage ESDIRK scheme.

in time $t + c_k \Delta t$, which is represented by the solution at stage k[1]. One can also infer the

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[1] This is only relevant for time dependent boundary conditions

explicit first stage update since $a_{11} = 0$ which implies that $\hat{Q}_1^n := \hat{Q}^{n-1}$. Because of this trivial first stage, the actual implementation in the code is only a five-stage process [63]:

$$\mathcal{R}_k^n(\hat{Q}_k^n, \ldots, \hat{Q}_2^n, \hat{Q}^{n-1}) := \frac{\hat{Q}_k^n - \hat{Q}^{n-1}}{a_{kk}\Delta t} + R(\hat{Q}_k^n) + \frac{1}{a_{kk}} \sum_{j=1}^{k-1} a_{kj} R(\hat{Q}_j^n) = 0 \quad \text{for } k = 2, \ldots, 6.$$

(2.47)

The presented ESDIRK scheme is L-stable, and each stage is at least second-order accurate (see Bijl, Carpenter and Vatsa [6] for more details). In order to achieve fourth-order accuracy in time, the nonlinear OΔE's (2.47) at each stage of ESDIRK must be solved to an appropriately small error [63].

2.4 Solving the Nonlinear System

The spatial and temporal discretization of the thin-layer Navier-Stokes equations (2.20) leads to the nonlinear systems of OΔE's (2.45) and (2.47), respectively. These equations describe a classical root finding problem, and Newton's method is a well known and fast method for solving this problem. This section gives a brief overview of the inexact Newton-Krylov algorithm incorporated in this work using the OΔE's (2.45) as an example (the OΔE's (2.47) stemming from the ESDIRK4 temporal discretization are solved in an analogous manner). For a more thorough description see Pueyo [110] and Chisholm [14].

Leaving $\hat{Q}^{n-1}$ and $\hat{Q}^{n-2}$ fixed while expanding Eq. (2.45) in a Taylor series around the current iterate for the next time step $\hat{Q}^p$ yields the following implicit definition of the next iterate $\hat{Q}^{p+1}$

$$\mathcal{R}^n(\hat{Q}^{p+1}, \hat{Q}^{n-1}, \hat{Q}^{n-2}) = \mathcal{R}^n(\hat{Q}^p, \hat{Q}^{n-1}, \hat{Q}^{n-2}) + \mathcal{A}^p \Delta \hat{Q}^p + \ldots = 0, \tag{2.48}$$

where $\Delta \hat{Q}^p = \hat{Q}^{p+1} - \hat{Q}^p$, and $\mathcal{A}^p$ is the Jacobian of $\mathcal{R}^n(\hat{Q}^p, \hat{Q}^{n-1}, \hat{Q}^{n-2})$ given by

$$\mathcal{A}^p = \nabla_{\hat{Q}^p} \mathcal{R}^n(\hat{Q}^p, \hat{Q}^{n-1}, \hat{Q}^{n-2}) = \frac{3}{2\Delta t} I + \frac{\partial R(\hat{Q}^p)}{\partial \hat{Q}^p}, \tag{2.49}$$

which is a large sparse non-symmetric matrix with dimensions $N_{\mathrm{F}} \times N_{\mathrm{F}}$. Ignoring higher-order terms leads to the following linear system

$$\mathcal{A}^p \Delta \hat{Q}^p = -\mathcal{R}^n(\hat{Q}^p, \hat{Q}^{n-1}, \hat{Q}^{n-2}), \tag{2.50}$$

which has to be solved for each Newton update ("outer iteration" or "subiteration")

$$\hat{Q}^{p+1} = \hat{Q}^p + \Delta\hat{Q}^p. \tag{2.51}$$

Once converged, i.e. $\mathcal{R}^n(\hat{Q}^{p+1}, \hat{Q}^{n-1}, \hat{Q}^{n-2}) \approx 0$, $\hat{Q}^n := \hat{Q}^{p+1}$, and the next time step can be calculated, if desired. A typical absolute convergence tolerance for the unsteady residual $\mathcal{R}^n$ used in this work is 10^{-10} to avoid error propagation. The initial guess $\hat{Q}^p_M$ is calculated through linear extrapolation from the previous two time steps for BDF2 and through constant extrapolation from the previous stage for ESDIRK4, whereas both methods use constant extrapolation for $\hat{Q}^p_T$. The term inexact stems from the fact that an exact solution of the linear system (2.50) is not required for fast convergence of Newton's method [24], and computational resources are saved by lowering the degree of convergence of the iterative linear solver [110]. Typically, for turbulent flows the linear residual is dropped by two to three orders of magnitude, whereas for laminar flows one order of magnitude is already sufficient.

For start-up strategies, such as adding a local time step which is slowly phased out and clipping negative $\tilde{\nu}$ values, that are used in this work to solve the nonlinear system of ODE's (2.43) for steady state situations, see Chisholm [14].

2.4.1 The Linear Problem

The inexact solution of Eq. (2.50) is obtained using the matrix-free version of the Generalized Minimal RESidual (GMRES(m)) Krylov subspace method [122, 123], where m represents the number of search directions. Usually, forty search directions are sufficient to decrease the GMRES residual by three orders of magnitude for turbulent and one order of magnitude for laminar flow problems, and no restart is performed. Since GMRES only needs matrix vector products of the form $\mathcal{A}^p\mathbf{v}$, the flow Jacobian matrix does not need to be formed explicitly (although an approximate form is still required for the preconditioner). Instead a forward-difference approximation, which requires only one additional residual evaluation, can be used

$$\mathcal{A}^p\mathbf{v} \approx \frac{\mathcal{R}^n(\hat{Q}^p + \epsilon\mathbf{v}, \hat{Q}^{n-1}, \hat{Q}^{n-2}) - \mathcal{R}^n(\hat{Q}^p, \hat{Q}^{n-1}, \hat{Q}^{n-2})}{\epsilon}, \tag{2.52}$$

where $\epsilon = \sqrt{\epsilon_m} / ||\mathbf{v}||_2$, and $\epsilon_m = 2.2 \cdot 10^{-16}$ is the approximate value of machine zero.

Preconditioning, Scaling and Reordering

Preconditioning of the flow Jacobian is required in order to cluster its eigenvalue spectrum around unity, which significantly improves the efficiency of GMRES. The preconditioning matrix $\mathcal{M}$ is applied from the right side, so that the residual of the linear system is not affected by it, and Eq. (2.50) becomes

$$\mathcal{A}^p \mathcal{M}^{-1} \mathcal{M} \Delta \hat{Q}^p = -\mathcal{R}^n(\hat{Q}^p, \hat{Q}^{n-1}, \hat{Q}^{n-2}). \tag{2.53}$$

Pueyo [110] found that using an approximate flow Jacobian to determine the preconditioner leads to more rapid convergence of the GMRES algorithm than using the true flow Jacobian with its lack of diagonal dominance. Thus, the preconditioner is based on the flow Jacobian matrix $\mathcal{A}^p$, except that it is only formed with second-order dissipation, and the fourth-order dissipation is approximated by adding extra second-order dissipation

$$\epsilon_p^{(2)} = \epsilon_r^{(2)} + \phi \, \epsilon_r^{(4)}, \tag{2.54}$$

where the subscript r denotes the contribution from the residual, and the subscript p denotes the resulting value for the artificial-dissipation coefficient used in the preconditioner. The coefficient ϕ is assumed to be constant with respect to the flow variables, and a value of 6.0 was found to work the best [97, 110].

The preconditioning matrix is then decomposed using Incomplete Lower-Upper factorization [87] (ILU(k)) with a level of fill k. Higher fill levels allow more non-zero entries during the Gaussian elimination process, resulting in a better approximation of the lower and upper factorization matrices. However, this gain in accuracy is counteracted by an increase in computational cost. For a more detailed overview, see Saad [122]. The level of fill used for most cases in this work is $k = 2$, but more complex flow problems require $k = 4$. In summary, the preconditioning matrix is an incomplete factorization of a first-order flow Jacobian with a reduced stencil size and an improved diagonal dominance compared to the true flow Jacobian as a result of Eq. (2.54), leading to a reduction in the computational effort and storage requirements for the ILU(k) factorization. The preconditioner is also frozen after the first outer iteration of every time step, saving even more computational time.

In addition, all the entries within the flow Jacobian that correspond to boundary conditions are pivoted and scaled since they are not of the same order of magnitude as the entries

for the interior nodes, which can lead to poor convergence of GMRES. Lastly, the reverse Cuthill-McKee reordering [20] of grid nodes based on an initial double-bandwidth ordering for single-block and a reverse ordering for multi-block grids [97, 110] is used, leading to a significant reduction of the bandwidth of the preconditioning matrix and therefore even more savings in computational cost.

Chapter 3

UNSTEADY OPTIMIZATION

"But, Mr. Fogg, eighty days are only the estimate of the least possible time in which the journey can be made."

"A well-used minimum suffices for everything."

In *Around the World in Eighty Days* by Jules Verne (1828-1905)

This chapter provides a description of all of the components of the gradient-based optimization algorithm for unsteady flows used in this work. The formulation of the discrete time-dependent optimal control problem is presented in Section 3.1. A description of the design variables and grid-perturbation strategies is given in Section 3.2, and the derivation of the discrete gradient using a Lagrangian approach can be found in Section 3.3. Finally, the optimizer, which is based on a quasi-Newton method, is discussed in Section 3.4.

3.1 Formulation of the Discrete Time-dependent Optimal Control Problem

The control of an unsteady flow in the time interval $[0, T]$ is considered. The time-dependent optimal control problem consists of determining values of design variables, Y, such that an objective or cost function $\mathcal{O}$ is minimized:

$$\min_Y \ \mathcal{O}(Q^1, \ldots, Q^N, Y) = \sum_{n=1}^{N} I^n(Q^n, Y) \tag{3.1}$$

subject to constraint equations C_j

$$C_j(Q^1, \ldots, Q^N, Y) \leq 0 \qquad j = 1, \ldots, N_{\text{con}}, \tag{3.2}$$

where the function $I^n = I^n(Q^n, Y)$ depends on the time-dependent flow solution Q^n and design variables Y for $n = 1, \ldots, N$. The number of time steps, N, can be calculated from

the relation $T = N\Delta t$, where Δt is the chosen constant time discretization step, and N_{con} denotes the number of constraint equations.

The optimization problem defined by Eqs. (3.1) and (3.2) can now be cast into an unconstrained problem by including the constraint equations (3.2) into the objective function $\mathcal{O}$ defined by Eq. (3.1), leading to the penalized objective function

$$\mathcal{J}(Q^1, \ldots, Q^N, Y) = \mathcal{O} + w_T \sum_{j=1}^{N_{\text{con}}} C_j = \sum_{n=1}^{N} I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\text{con}}} C_j \tag{3.3}$$

where w_T is a user specified weight. The constraint equations (3.2) usually represent airfoil thickness constraints that prevent the occurrence of infeasible shapes, for example airfoil surface cross-overs, and to enforce structural requirements, such as minimum airfoil thicknesses. In that case, the constraints C_j are a function of the design variables only and are expressed as a quadratic external penalty term as follows

$$C_j = \begin{cases} [1 - h(x_j)/h^*(x_j)]^2 & \text{if } h(x_j) < h^*(x_j) \\ 0 & \text{otherwise} \end{cases}, \tag{3.4}$$

where $h^*(x_j)$ represents the minimum thickness allowed at location x_j, and $h(x_j)$ represents the current airfoil thickness.

The flow variables Q^n have to satisfy the governing flow equations (2.45) using BDF2 or (2.47) using ESDIRK4 within a feasible region of the design space Ω. Here, the definitions are extended to include the design variables Y in the unsteady flow residuals

$$\begin{aligned} \mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, \hat{Q}^{n-2}, Y) &= 0 \quad \forall Y \in \Omega \text{ and } n = 1, \ldots, N \\ &\text{or} \\ \mathcal{R}_k^n(\hat{Q}_k^n, \ldots, \hat{Q}_2^n, \hat{Q}^{n-1}, Y) &= 0 \quad \forall Y \in \Omega \text{ and } k = 2, \ldots, 6 \text{ and } n = 1, \ldots, N. \end{aligned} \tag{3.5}$$

These equations implicitly define $\hat{Q}^n = J^{-1} Q^n$ and $\hat{Q}^n = J^{-1} Q_6^n$ respectively for $n = 1, \ldots, N$ with J^{-1} the inverse of the metric Jacobian of the coordinate transformation, which is a diagonal matrix of dimension $N_\text{F} \times N_\text{F}$.

At each step of the optimization procedure, a gradient-based optimizer requires the value of the objective function $\mathcal{J}$, which is provided by the solution of the flow equations (3.5), as well as the objective function gradient $\frac{\partial \mathcal{J}}{\partial Y}$. Thus, for a certain number of optimization iterations (one objective function and gradient evaluation), the overall efficiency of the optimization algorithm is dominated by the time required to solve the flow equations (see

Section 2.4) and to compute the gradient. The calculation of the gradient of time-dependent problems is generally a computationally expensive task since one needs to solve the adjoint equations in reverse time from a final solution (see Section 3.3). Thus one has to store the entire flow history (potentially huge memory requirements) and then to integrate the adjoint equations backwards in time (equally huge processor requirements).

3.2 Design Variables and Grid-Perturbation Strategies

The vector of design variables, Y, usually contains parameters that control the shape of an airfoil. Depending on the problem of interest, other design variables may include the angle of attack, the horizontal and vertical translations which control the position of slats and flaps in multi-element configurations (relative deflection angles within a configuration are kept constant), the angular velocity of a rotating cylinder, or the strength of a pulse in the outflow pressure of a nozzle.

Cubic B-splines are used to parametrize the airfoil shape [22, 58], and the coordinates of the B-spline control points are used as design variables. Only vertical displacements are allowed and the control points associated with the leading and trailing edges remain fixed (for more details see Nemec [97]).

As the shape of airfoils or the positions of slats and flaps change during the optimization process, the location of the grid nodes has to be adjusted accordingly. This could be accomplished by simply generating a new grid for each new geometry using a grid-generation tool. However, this is computationally expensive due to the need for elliptic grid smoothers and very difficult to automate, especially for complex geometries. A better strategy is to use a high-quality grid as a baseline for all other grids and to just perturb this base grid into a new grid for the desired geometry. Note that a new grid should not be obtained by perturbing the most recently used grid instead of perturbing the base grid since this results in an objective function that is path-dependent, and thus non-unique and non-differentiable.

A simple algebraic grid perturbation technique for structured grids is to perturb each grid line running from the airfoil surface to the outer boundary individually. Burgreen *et al.* [12] computed the perturbation of each node on these grid lines by interpolating the perturbation between the airfoil and the far-field based on the arc length along the line. Nemec [97] modified this method for multi-block grids, where grid lines may not touch the airfoil or

the far-field boundary, and he used trigonometric functions to preserve orthogonality for 2D multi-element airfoils. These methods are very fast, but they can generate poor quality or tangled grids for large perturbations.

A more physically meaningful alternative to the algebraic grid perturbation is to treat the entire grid as an elastic medium. The interior deforms like a block of rubber according to the equations of linear elasticity, when the geometry changes. Tezduyar *et al.* [134] used a finite element method to compute the interior deformation by relating the stiffness of each element to the inverse of its size. This makes the grid stiffer near the airfoil and causes the deformations to propagate further towards the outer boundary. This linear elasticity approach can also break down for large deformations; however, Bar-Yoseph *et al.* [5] proposed a quasi-linear approach to avoid this. They deformed the geometry through a series of linear increments and at each increment they locally increased the stiffness in highly strained areas. This results in a quasi-linear elasticity grid perturbation method, that is very robust, even with large geometry changes, but is also relatively computationally expensive (on the order of one steady flow solve). It has been implemented by Truong [138, 139, 140] and is applied in this work if the algebraic grid perturbation technique produces poor quality grids or fails entirely. This only happened in the unsteady laminar trailing-edge flow test case presented in Section 5.5.

3.3　The Discrete Adjoint Approach for the Gradient Calculation

Historically, there are two different adjoint approaches: the discrete approach, in which one works with the algebraic equations that come from the discretization of the original fluid dynamic equations, and the continuous approach, in which the adjoint equations are analytically formulated and then discretized [43]. For an explanation of the advantages and disadvantages of both methods see Appendix A. Since the fully-discrete adjoint method is conceptually more straightforward and the full flow Jacobian is already implemented [97], this is the method of choice in this work.

For the discrete adjoint method the time discretization scheme for the governing equations (3.5) must be chosen at the beginning of the derivation. The framework is demon-

strated here using the implicit Euler time-marching method. It is straightforward to modify the equations to use any other time-marching method (e.g. see Appendix B for BDF2 and Appendix E for ESDIRK4).

The initial flow solution $\hat{Q}^0$ at $t = 0$ is known, and for the implicit Euler method the time-dependent flow solution $Q^n = J\hat{Q}^n$ for $n = 1, \ldots, N$ is implicitly defined via

$$\mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, Y) := \frac{d\hat{Q}^n}{dt} + R(\hat{Q}^n, Y) = \frac{\hat{Q}^n - \hat{Q}^{n-1}}{\Delta t} + R(\hat{Q}^n, Y) = 0, \tag{3.6}$$

where $R = R(\hat{Q}^n, Y)$ contains the spatially discretized convective and viscous fluxes as well as the boundary conditions and turbulence model.

The inexact Newton-Krylov strategy described in Section 2.4 can be used to drive $\mathcal{R}^n = \mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, Y)$ in Eq. (3.6) to zero. However, it does not matter how one solves Eq. (3.6) as long as $\mathcal{R}^n = 0$ for all n, since this is a requirement for the following derivation.

The task of minimizing the cost function $\mathcal{J}$ subject to $\mathcal{R}^n = 0$ for all n can now be written as an unconstrained optimization problem of minimizing the Lagrangian function

$$\mathcal{L}(\hat{Q}^1, \ldots, \hat{Q}^N, \psi^1, \ldots, \psi^N, Y) = \sum_{n=1}^{N} I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\text{con}}} C_j(Y) + \sum_{n=1}^{N} (\psi^n)^T \mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, Y) \tag{3.7}$$

with respect to $\hat{Q}^1, \ldots, \hat{Q}^N, \psi^1, \ldots, \psi^N$ and Y, where $\psi^1, \ldots, \psi^N$ are the N vectors of Lagrange multipliers. Note that the flow Jacobian $\nabla_{\hat{Q}^n} \mathcal{R}^n$ in Eq. (2.49) and in the actual code is given in terms of variables in the curvilinear space, and thus it is more convenient to derive the adjoint equations in the same space, i.e., to take derivatives with respect to $\hat{Q}^n$ rather than Q^n. This is easily accomplished for functions that depend on Q^n, such as $I^n(Q^n, Y)$, as follows

$$\nabla_{\hat{Q}^n} I^n = \frac{\partial I^n}{\partial Q^n} \frac{\partial Q^n}{\partial \hat{Q}^n} = \nabla_{Q^n} I^n \cdot J. \tag{3.8}$$

A necessary condition for an extremal is that the gradient of $\mathcal{L}$ with respect to $\hat{Q}^1, \ldots, \hat{Q}^N$, $\psi^1, \ldots, \psi^N$ and Y should vanish. Since the states $\hat{Q}^1, \ldots, \hat{Q}^N$ are calculated starting from $\hat{Q}^0$ using the residuals given by Eq. (3.6), it is automatically guaranteed that $\nabla_{\psi^n} \mathcal{L} = 0$ for $n = 1, \ldots, N$.

The Lagrange multipliers ψ^n must now be chosen such that $\nabla_{\hat{Q}^n} \mathcal{L} = 0$ for $n = 1, \ldots, N$,

which leads to

$$0 = \nabla_{\hat{Q}^n} I^n + (\psi^n)^T \nabla_{\hat{Q}^n} \mathcal{R}^n + (\psi^{n+1})^T \nabla_{\hat{Q}^n} \mathcal{R}^{n+1}$$

$$\text{for} \quad n = 1, \ldots, N{-}1 \tag{3.9}$$

$$0 = \nabla_{\hat{Q}^N} I^N + (\psi^N)^T \nabla_{\hat{Q}^N} \mathcal{R}^N. \tag{3.10}$$

This can equivalently be written as

$$\psi^N = -\left((\nabla_{\hat{Q}^N} \mathcal{R}^N)^T \right)^{-1} (\nabla_{\hat{Q}^N} I^N)^T \tag{3.11}$$

$$\psi^n = -\left((\nabla_{\hat{Q}^n} \mathcal{R}^n)^T \right)^{-1} \left[(\nabla_{\hat{Q}^n} I^n)^T + (\nabla_{\hat{Q}^n} \mathcal{R}^{n+1})^T \psi^{n+1} \right]$$

$$\text{for} \quad n = N{-}1, \ldots, 1. \tag{3.12}$$

Since $\hat{Q}^1, \ldots, \hat{Q}^N$ have been calculated with the current iterate of Y, the vectors of Lagrange multipliers ψ^n can be calculated recursively backwards from the final flow solution (3.11) using (3.12). The system of equations (3.11) and (3.12) is known as the system of adjoint equations for the model (3.6), or as the adjoint model. In this context, the Lagrange multipliers are also known as the adjoint variables. Calculating the adjoint variables in this manner ensures that $\nabla_{\hat{Q}^n} \mathcal{L} = 0$ for $n = 1, \ldots, N$.

Finally, one can evaluate the gradient of the objective function $\mathcal{J}$ with respect to the design variables Y, as follows

$$\frac{\partial \mathcal{J}}{\partial Y} = \frac{\partial \mathcal{L}}{\partial Y}\bigg|_{\frac{\partial \mathcal{L}}{\partial \hat{Q}^n} = \frac{\partial \mathcal{L}}{\partial \psi^n} = 0} = \sum_{n=1}^{N} \nabla_Y I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\text{con}}} \nabla_Y C_j(Y) + \sum_{n=1}^{N} (\psi^n)^T \nabla_Y R(\hat{Q}^n, Y). \tag{3.13}$$

Note that $\frac{\partial \mathcal{L}}{\partial Y}$ is evaluated given that $\frac{\partial \mathcal{L}}{\partial \hat{Q}^n} = \frac{\partial \mathcal{L}}{\partial \psi^n} = 0$ for $n = 1, \ldots, N$ is already satisfied, which implies that $\mathcal{R}^n = 0$ for $n = 1, \ldots, N$ and thus $\mathcal{J} = \mathcal{L}|_{\frac{\partial \mathcal{L}}{\partial \hat{Q}^n} = \frac{\partial \mathcal{L}}{\partial \psi^n} = 0}$ which yields Eq. (3.13). Thus, the gradient of $\mathcal{J}$ is entirely determined by the solution of the adjoint equations in reverse time from the final flow solution and the partial derivatives of the objective function, the constraints and the residuals with respect to the design variables (while $\hat{Q}^n$ is held constant).

In summary, the approach taken here is to delegate the majority of the computation to specialized solvers, instead of attempting to minimize the Lagrangian (3.7) for all variables simultaneously. For a given Y, the grid perturbation code and flow solver can be used to solve the flow equations (3.6) and yield $\hat{Q}^n$. The linear adjoint systems in Eqs. (3.11) and (3.12)

can then be solved to give ψ^n. Finally, Eq. (3.13) can be evaluated to yield a value for the gradient $\frac{\partial \mathcal{J}}{\partial Y}$ which is then used by a gradient-based optimization algorithm (see Section 3.4) to update Y. This process is repeated until a value of Y is found which gives $\frac{\partial \mathcal{J}}{\partial Y} \approx 0$.

In order to solve the linear problem arising from the flow equations, the matrix-free version of GMRES(m) is used with a forward-difference approximation to the matrix-vector products (see Subsection 2.4.1). In addition to memory savings, the matrix-free approach is much easier to implement, and a fairly accurate differentiation of the lengthy flow residual equations is "automatically" provided. However, due to the transpose of the unsteady flow Jacobian $\nabla_{\hat{Q}^n} \mathcal{R}^n$ in the adjoint equations, the matrix-free approach cannot be used here, and the matrices are formed and stored explicitly, as are the terms $\nabla_{\hat{Q}^n} I^n$. The Bi-Conjugate Gradient STABilized (Bi-CGSTAB) algorithm [145] is used to solve the linear systems in the unsteady adjoint equations, since it is up to fifty percent faster than GMRES(m). However, for a steady-state adjoint problem Bi-CGSTAB works not nearly as well and GMRES(m) is used instead. The reason for this is most likely accounted for by the fact that $(\nabla_{\hat{Q}^n} \mathcal{R}^n)^T$ is more diagonally dominant than the transpose of the steady flow Jacobian $(\nabla_{\hat{Q}} R)^T$ due to the extra terms on the diagonal, which makes this matrix more suited for the use of Bi-CGSTAB. Unfortunately, there are no computational savings by using Bi-CGSTAB for the unsteady flow solves, and therefore GMRES(m) is used as mentioned in Subsection 2.4.1. This is puzzling since the unsteady flow Jacobian and its transpose have the same eigenvalues, and thus the iterative linear solvers are expected to show similar behaviour for the forward and backward linear problems. However, there are also a few important differences in the linear problems which may account for the different behaviour:

- The scaling of the adjoint solution is much worse, leading to solutions that span several orders of magnitude as opposed to the flow solution which is on the order of unity.

- The linear adjoint problem must be converged further than the nonlinear problem in the flow solve, presumably due to the large variations in the adjoint variables and the associated residual vector.

- The nonlinear unsteady flow solve problem has a very good initial guess by using the flow solutions from the previous time steps; the linear unsteady adjoint problem on the other hand has a bad initial guess since the adjoint solution varies much more from time step to time step.

- Only a few linear iterations are used per nonlinear (outer) iteration in the forward problem.

The remaining terms, namely the objective function sensitivities $\nabla_Y I^n(Q^n, Y)$, the constraint sensitivities $\nabla_Y C_j(Y)$, and the residual sensitivities $\nabla_Y R(\hat{Q}^n, Y)$, are evaluated using fourth-order centered finite differences which are not computationally expensive for the few design variables typically used and yield accurate results. Even the employment of the more expensive quasi-linear elasticity grid perturbation method does not increase the overall computational costs dramatically since the flow and adjoint solvers are so much more expensive for typical time horizons used in this work. Overall the computational costs of unsteady optimization problems are directly proportional to the desired number of time steps and (almost) independent of the number of design variables.

3.4 Optimizer

The optimizer used to solve the optimization problem can have a significant impact on the efficiency of the optimization procedure [67]. In this research L-BFGS-B [13, 153], a limited-memory quasi-Newton code for large-scale bound-constrained or unconstrained optimization, is used. Note that by using the quadratic penalty method (3.4) to incorporate constraints, the optimization problems in this work are cast into unconstrained problems; however it is still desirable to have lower and upper bounds on some or all of the design variables in order to prevent too drastic changes and thus flow solver convergence problems.

L-BFGS-B has been developed at the Optimization Technology Center, a joint venture of Argonne National Laboratory and Northwestern University and is described in detail in Byrd *et al.* [13]. It is programmed in FORTRAN 77, uses reverse communication, does not scale any of the design variables, and proceeds roughly as follows. At each optimization iteration, a limited-memory BFGS [11, 42, 45, 124] approximation to the Hessian is updated. This limited-memory matrix is used to define a quadratic model of the objective function. A search direction is then computed using a two-stage approach. First, the gradient projection method [13] is used to identify a set of active design variables, i.e. variables that will be held at their bounds. In the second stage, the quadratic model is approximately minimized with respect to the free design variables. The search direction is defined to be the vector

leading from the current iterate to this approximate minimizer, and a line search is performed along the search direction. The step length is determined by a routine [88] that enforces a sufficient decrease and curvature condition. For unconstrained optimization problems, such as the ones dealt with in this work, the well-known necessary condition for an optimum is that the gradient of the objective function $\mathcal{J}$ is equal to zero, thus the optimizer has converged when the maximum norm of the gradient vector is below a user specified absolute tolerance (typically taken to be 10^{-6}).

Chapter 4

NOISE PREDICTION TECHNIQUE

"NOISE, n. A stench in the ear. Undomesticated music. The chief product and authenticating sign of civilization."

Ambrose Bierce (1842-1914)

A computational obstacle that immediately arises in problems concerning noise is that accurate propagation of the pressure signatures over a large number of wavelengths can only be obtained with very small computational mesh spacings. This makes all high-lift noise reduction problems, where the computational domain has to cover tens or hundreds of chord lengths, infeasible for even today's largest parallel computers. A typical approach to tackle high-lift noise reduction problems nonetheless is to represent the CFD solution on a reasonable computational mesh that does not extend too far from the aircraft. The location of a fixed near-field plane within the computational mesh can then be specified as shown in Figure 4.1.

Figure 4.1: Schematic of the propagation of the aircraft pressure signature.

This near-field plane or surface serves as an interface between the CFD solution and a wave propagation program based on principles of geometrical acoustics and nonlinear wave propagation [78, 129]. Such a program is able to model the wave propagation and to calculate the pressure fluctuations at a user specified ground plane which can then be used as a measure of the airframe-generated noise. In Section 4.1, the merits and drawbacks of two different wave propagation formulations, namely the Kirchhoff and Ffowcs Williams and Hawkings formulations, are discussed. Section 4.2 derives the two-dimensional Ffowcs Williams and Hawkings equation in the frequency-domain, which is the wave propagation formulation of choice in this work, and subsequently, the entire solution process is outlined. Finally, Section 4.3 presents results of validation cases for the implemented wave propagation formulation.

4.1 Acoustic Wave Propagation Modelling

Several prediction methodologies for far-field signals based on near-field inputs with a solid physical and mathematical basis are currently available. The most popular among them are the formulations based on the Lighthill acoustic analogy [75]: the Kirchhoff approach [37, 38] and the Ffowcs Williams and Hawkings (FW-H) approach [41].

The Kirchhoff approach is based on an inhomogeneous wave equation which is derived by assuming that the required acoustic pressure fluctuation ($p' = p - p_\infty$) and its time and normal derivatives are probed on a near-field surface which is located within the linear flow region. However, the beginning of the linear flow region is not very well defined and thus the placement of the Kirchhoff near-field surface has to be a judicious compromise between being far enough from the source to be in the linear flow region, yet close enough to be within the well resolved region of the grid. Despite this ambiguity, the Kirchhoff approach has been used successfully by many authors [8, 9, 37, 38, 4, 106, 151].

The FW-H approach [41], on the other hand, is an exact rearrangement of the continuity and momentum equations. The time histories of all flow variables on the near-field surface are required, but their temporal or spatial derivatives are not needed. Di Francescantonio [26] demonstrated that the FW-H approach - just like the Kirchhoff approach - can be applied using a fictitious near-field surface that does not coincide with the surface of the solid body. Singer *et al.* [126, 127] have shown that the FW-H approach produces correct results for the

far-field signal when this fictitious surface is placed in the non-linear near-field, whereas the Kirchhoff method, using the same surface, produces erroneous results. More applications of the FW-H approach and comparisons between the FW-H and Kirchhoff approaches can be found in the literature [107, 9, 8].

For three-dimensional flows, Farassat and Succi [39] developed the so-called formulation 1A of the FW-H approach, which is the best formulation because all significant acoustic phenomena are three-dimensional. However, the computational cost to compute sufficiently resolved three-dimensional data on the near-field surface is in most cases still prohibitively large. Furthermore, the flow structures responsible for generating noise can be pseudo-two-dimensional, with a finite correlation length in the third direction [77]. Singer *et al.* [125] compared two- and three-dimensional solutions for slat noise and demonstrated the usefulness of the two-dimensional results, which gave the correct features of the radiated sound, but overpredicted the amplitude. This implies that two-dimensional simulations can be used to find trends, even though they do not represent all of the underlying physics exactly. This motivates the implementation of a two-dimensional wave propagation program based on the FW-H approach for this work, which will be described in detail in the next section.

4.2 The 2D FW-H Equation in the Frequency-Domain

The FW-H equation [41] is the most general form of the Lighthill acoustic analogy [75] and is currently the most accurate method available for calculating the far-field pressure fluctuations caused by bodies in arbitrary motion and by non-linear flow regions. The differential form of the FW-H equation, which is an exact rearrangement of the continuity and momentum equations into the form of an inhomogeneous wave equation, is given by

$$\left\{\frac{1}{a_\infty^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x_i^2}\right\}[a_\infty^2\rho'H(f)] = \frac{\partial}{\partial t}[\mathcal{Q}\delta(f)] - \frac{\partial}{\partial x_i}[\mathcal{F}_i\delta(f)] + \frac{\partial^2}{\partial x_i\partial x_j}[T_{ij}H(f)], \qquad (4.1)$$

where T_{ij} is the so-called Lighthill stress tensor, and the monopole term $\mathcal{Q}$ and dipole terms $\mathcal{F}_i$ are defined as

$$\mathcal{Q} = [\rho(u_j - v_j) + \rho_\infty v_j]\frac{\partial f}{\partial x_j}, \qquad (4.2)$$

$$\mathcal{F}_i = [\rho u_i(u_j - v_j) + p\delta_{ij} - \tau_{ij}]\frac{\partial f}{\partial x_j}. \qquad (4.3)$$

Here, $\rho = \rho_\infty + \rho'$, $u_i = U_i + u_i'$ and $p = p_\infty + p'$ are the total density, velocity and pressure, respectively. Free-stream quantities are indicated by the subscript ∞, U_i are the components of the uniform mean velocity, and a prime denotes a perturbation from the mean. The Cartesian coordinates and time are x_i and t respectively, δ_{ij} is the Kronecker delta, τ_{ij} is the viscous stress tensor which is zero for inviscid flows, and repeated indices follow the usual Einstein summation convention. The function $f(x_i, t) = 0$ defines the near-field surface, which always surrounds the moving source region such that $f > 0$ outside this source region, and $\frac{\partial f}{\partial x_i} = n_i$, where n_i is the unit normal vector that points into the fluid. The velocities of the surface $f = 0$ are represented by v_i, and $H(f)$ is the Heaviside function. For more details and a derivation of Eq. (4.1), see Appendix C.

The right-hand side of Eq. (4.1) consists of three inhomogeneous acoustic source terms with clear physical meanings. The monopole source term $\mathcal{Q}$, which is also known as the thickness source term, accounts for the displacement of the fluid by the moving body, and is completely determined by the geometry and kinematics of the body. The dipole or loading source term $\mathcal{F}_i$ is generated by the force that acts on the fluid as a result of the presence of the body. The last term, which is called the quadrupole source term, is a volume distribution of sources and accounts for nonlinear effects, such as noise generated by shocks, vorticity, and turbulence in the flowfield, and variations in the local sound speed or refraction of waves by shear layers and wakes [35, 36]. As long as the integration surface is placed outside of all regions where the quadrupole source term is large, its contribution is included in the two surface source terms and hence it can be neglected. However, in some problems, such as jets, the shear layers are nearly semi-infinite, and it is not possible to place the surface in such a way as to neglect the computationally expensive volume integration of the quadrupole contribution. Nonetheless, in many other cases, for example low-speed flows as encountered in high-lift noise reduction problems, the quadrupole source distribution is only significant near the body and thus the quadrupole contribution can be neglected, if the integration surface is placed around all regions of high shear.

Although Eq. (4.1) is a three-dimensional equation, one can interpret the equation as being two dimensional by running the indices only over 1 and 2. The main difficulty in solving this equation in two dimensions is the semi-infinite time integral that arises when using the appropriate two-dimensional Green function in the time-domain. This "tail effect" requires an infinitely long time to account for all contributions of the sources and is thus

infeasible. There is no such problem for the solution in three dimensions since the appropriate three-dimensional Green function includes a delta function that makes the time integral finite.

To avoid this costly or infeasible time integration in the two-dimensional time-domain, the problem can be transformed into the frequency-domain [48, 77]. However, a direct application of a Fourier transform to Eq. (4.1) is not useful because it is very difficult to simplify the resulting spatial integrals. Thus, Lockard [77] assumes a uniform rectilinear motion of the control surface $f = f(x_i + U_i t)$, where U_i is the constant velocity of the surface. His derivation, which is outlined in the following, continues with the application of a Galilean transformation of Eq. (4.1) from the Cartesian coordinates (x_i, t) to $(y_i, \bar{t})$, with

$$y_i = x_i + U_i t \quad, \qquad \bar{t} = t, \tag{4.4}$$

$$\frac{\partial}{\partial x_i} = \frac{\partial}{\partial y_i} \quad, \qquad \frac{\partial}{\partial t} = \frac{\partial}{\partial \bar{t}} + U_i \frac{\partial}{\partial y_i}, \tag{4.5}$$

which yields

$$\left\{ \frac{\partial^2}{\partial t^2} + U_i U_j \frac{\partial^2}{\partial y_i \partial y_j} + 2U_j \frac{\partial^2}{\partial y_j \partial t} - a_\infty^2 \frac{\partial^2}{\partial y_i^2} \right\} [\rho' H(f)]$$

$$= \frac{\partial}{\partial t} [\mathcal{Q} \delta(f)] - \frac{\partial}{\partial y_i} [\mathcal{F}_i \delta(f)] + \frac{\partial^2}{\partial y_i \partial y_j} [T_{ij} H(f)]. \tag{4.6}$$

The surface velocity v_i has been replaced by $-U_i$, which can be inferred from $f(x_i + U_i t) = 0$. Note that this implies that the mean flow is in the positive direction (or equivalently that the surface moves in the negative direction) when $U_i > 0$. After the transformation $f = f(y_i)$ is only a function of the spatial coordinates, u_i' is substituted for u_i, and T_{ij}, $\mathcal{F}_i$ and $\mathcal{Q}$ become

$$T_{ij} = \rho u_i' u_j' + [p - a_\infty^2 (\rho - \rho_\infty)] \delta_{ij} - \tau_{ij}, \tag{4.7}$$

$$\mathcal{F}_i = [\rho(u_i' - U_i)(u_j' + U_j) + \rho_\infty U_i U_j + p \delta_{ij} - \tau_{ij}] \frac{\partial f}{\partial y_j}, \tag{4.8}$$

$$\mathcal{Q} = [\rho(u_j' + U_j) - \rho_\infty U_j] \frac{\partial f}{\partial y_j}. \tag{4.9}$$

Eq. (4.6) is now in a convenient form to perform a Fourier transformation with the pair

$$\mathbb{F}[\phi(y_i, t)] = \phi(y_i, \omega) = \int_{-\infty}^{\infty} \phi(y_i, t) \exp(-i\omega t) dt \tag{4.10}$$

and

$$\mathbb{F}^{-1}[\phi(y_i, \omega)] = \phi(y_i, t) = \int_{-\infty}^{\infty} \phi(y_i, \omega) \exp(i\omega t) d\omega. \tag{4.11}$$

By renaming y_i to x_i and using the customary notation $p' = a_\infty^2 \rho'$, Eq. (4.6) becomes

$$\left\{ \frac{\partial^2}{\partial x_j^2} + k^2 - 2iM_j k \frac{\partial}{\partial x_j} - M_j M_k \frac{\partial^2}{\partial x_j \partial x_k} \right\} [H(f)p'(x,\omega)]$$

$$= -i\omega \mathcal{Q}(x,\omega)\delta(f) + \frac{\partial}{\partial x_j}[\mathcal{F}_j(x,\omega)\delta(f)] - \frac{\partial^2}{\partial x_j \partial x_k}[T_{jk}(x,\omega)H(f)], \qquad (4.12)$$

where $k = \omega/a_\infty$ is the wavenumber, and $M_j = U_j/a_\infty$. One has to assume that $\lim_{t\to\pm\infty} \mathcal{Q} = \lim_{t\to\pm\infty} \rho' = \lim_{t\to\pm\infty} \frac{\partial\rho'}{\partial t} = 0$ so that

$$[\exp(-i\omega t)\, \mathcal{Q}]_{-\infty}^\infty = [\exp(-i\omega t)\, \rho']_{-\infty}^\infty = [\exp(-i\omega t)\, \frac{\partial\rho'}{\partial t}]_{-\infty}^\infty = 0 \qquad (4.13)$$

for Eq. (4.12) to be correct.

The Green function G of this convected Helmholtz equation for $M < 1$ is obtained from a Prandtl-Glauert transformation of the 2D free-space Green function in the frequency-domain. Denoting the two-dimensional source points as y and the observer position as x, this Green function is given by

$$G(x,y,\omega) = \frac{i}{4\beta} \exp(iMkr_1/\beta^2) H_0^{(2)} \left(\frac{k}{\beta^2} \sqrt{r_1^2 + \beta^2 r_2^2} \right) \qquad (4.14)$$

where

$$r_1 = (x_1 - y_1)\cos\theta + (x_2 - y_2)\sin\theta \qquad (4.15)$$

$$r_2 = -(x_1 - y_1)\sin\theta + (x_2 - y_2)\cos\theta. \qquad (4.16)$$

The angle θ is defined via $\tan\theta = U_2/U_1$, $H_0^{(2)}$ is the Hankel function of the second kind of order zero, $M = \sqrt{U_1^2 + U_2^2}/a_\infty$ and $\beta = \sqrt{1 - M^2}$ is the Prandtl-Glauert factor.

The solution to Eq. (4.12) for $M < 1$ is now given by the following convolution integral over the entire two-dimensional space

$$\begin{aligned}
[H(f)p'](x,\omega) &= \int_{-\infty}^\infty G(x,y,\omega) \frac{\partial[\mathcal{F}_j(y,\omega)\delta(f)]}{\partial y_j} d\mathbf{y} \\
&- \int_{-\infty}^\infty G(x,y,\omega) i\omega \mathcal{Q}(y,\omega)\delta(f) d\mathbf{y} \\
&- \int_{-\infty}^\infty G(x,y,\omega) \frac{\partial^2[T_{jk}(y,\omega)H(f)]}{\partial y_j \partial y_k} d\mathbf{y}.
\end{aligned} \qquad (4.17)$$

The dipole term can be simplified by moving the Green function inside the derivative operator as follows:

$$
\int_{-\infty}^{\infty} G(x,y,\omega) \frac{\partial[\mathcal{F}_j(y,\omega)\delta(f)]}{\partial y_j} d\mathbf{y}
$$
$$
= \int_{-\infty}^{\infty} \frac{\partial[G(x,y,\omega)\mathcal{F}_j(y,\omega)\delta(f)]}{\partial y_j} d\mathbf{y} - \int_{-\infty}^{\infty} \mathcal{F}_j(y,\omega)\delta(f) \frac{\partial G(x,y,\omega)}{\partial y_j} d\mathbf{y}
$$
$$
= - \oint_{f=0} \mathcal{F}_j(y,\omega) \frac{\partial G(x,y,\omega)}{\partial y_j} dl. \tag{4.18}
$$

The integral of the divergence is zero which can be inferred from Green's theorem and the fact that $\mathcal{F}_j$ goes to zero at infinity. Note that the final integral in Eq. (4.18) is only a contour integral over $f = 0$. Application of similar manipulations to the quadrupole term yields the final solution for the far-field pressure fluctuations in the frequency-domain:

$$
[H(f)p'](x,\omega) = - \oint_{f=0} i\omega \mathcal{Q}(y,\omega) G(x,y,\omega) dl
$$
$$
- \oint_{f=0} \mathcal{F}_j(y,\omega) \frac{\partial G(x,y,\omega)}{\partial y_j} dl
$$
$$
- \int_{f>0} T_{jk}(y,\omega) \frac{\partial^2 G(x,y,\omega)}{\partial y_j \partial y_k} d\mathbf{y}. \tag{4.19}
$$

The Heaviside function $H(f)$ on the left-hand side of Eq. (4.19) implies that the solution at any point within the integration surface should be zero for all ω, which can be used as a check for the accuracy of the computations. One can also simplify the expressions for $\mathcal{Q}$, $\mathcal{F}_j$ and T_{jk} by removing constant terms which do not radiate sound, yielding

$$
\mathcal{Q} = \rho u_j n_j, \tag{4.20}
$$
$$
\mathcal{F}_j = [\rho(u_j - 2U_j)u_k + p\delta_{jk} - \tau_{jk}]n_k, \tag{4.21}
$$
$$
T_{jk} = \rho(u_j - U_j)(u_k - U_k) + (p - a_\infty^2 \rho)\delta_{jk} - \tau_{jk}. \tag{4.22}
$$

The required derivatives of the Green function can be evaluated analytically. The first derivatives, which are the only ones required if the quadrupole contribution is neglected, are

given by

$$
\begin{aligned}
\frac{\partial G(x,y,\omega)}{\partial y_1} &= -A(r_1,\omega)\frac{iMk}{\beta^2}\cos\theta H_0^{(2)}\left(\frac{kr_\beta}{\beta^2}\right)\\
&\quad + A(r_1,\omega)\frac{k}{\beta^2 r_\beta}(r_1\cos\theta - \beta^2 r_2\sin\theta)H_1^{(2)}\left(\frac{kr_\beta}{\beta^2}\right),\\
\frac{\partial G(x,y,\omega)}{\partial y_2} &= -A(r_1,\omega)\frac{iMk}{\beta^2}\sin\theta H_0^{(2)}\left(\frac{kr_\beta}{\beta^2}\right)\\
&\quad + A(r_1,\omega)\frac{k}{\beta^2 r_\beta}(r_1\sin\theta + \beta^2 r_2\cos\theta)H_1^{(2)}\left(\frac{kr_\beta}{\beta^2}\right),
\end{aligned}
\tag{4.23}
$$

where $r_\beta = \sqrt{r_1^2 + \beta^2 r_2^2}$, and $A(r_1,\omega) = \frac{i}{4\beta}\exp(iMkr_1/\beta^2)$.

Impenetrable Surfaces

The above expressions for the monopole and dipole terms given by Eqs. (4.20) and (4.21) can be further simplified when the source data is obtained on solid surfaces. Since for impenetrable surfaces $u_i = 0$, which implies that $u_i' = -U_i$, these terms simplify to

$$
\mathcal{Q} = 0 \quad \text{and} \quad \mathcal{F}_j = [p\delta_{jk} - \tau_{jk}]n_k.
$$

Note that the monopole term $\mathcal{Q}$ for impenetrable surfaces has no contribution to the frequency-domain solution and only the time history of the pressure is needed to calculate $\mathcal{F}_j$, which leads to considerable savings in memory and computational requirements.

Windowing

Most unsteady CFD calculations simulate fluid phenomena with flows that are dominated by tones and possess a periodic steady state. If the CFD calculations would give truly periodic results, only one period of the flow data would be sufficient to calculate the far-field pressure fluctuations with the above derived 2D FW-H equation in the frequency-domain. However, CFD calculations are hardly ever truly periodic, or it is infeasible to run them long enough to eliminate all transients. Additionally, the $\mathcal{Q}$ and $\mathcal{F}_j$ source terms can also be out of phase. This inherent aperiodicity in the data would lead to an erroneous result if a Fourier transformation is directly applied to it, because of the discontinuity between the first and last points. This leads to the idea of multiplying the existing data by some function that smoothly reduces the signal to zero at the end points, thus making the data

artificially periodic. This process is called "windowing", and the multiplying function is called a "window" or filter function.

The windowing should be applied to $\mathcal{Q}$ and $\mathcal{F}_j$ after the respective mean values are subtracted to minimize the errors incurred. The subtraction of the means has no effect on the calculated noise because the first derivatives of the Green function all contain ω (see Eq. (4.23)), and thus one can infer from Eq. (4.19) that there is no contribution to the pressure fluctuation or noise for $\omega = 0$ when the quadrupole term is neglected.

Standard window functions, such as the Hanning filter, significantly decrease the amplitudes of tonal dominated data and spread the energy over adjacent bands when only a few periods are included, which is the case for most unsteady CFD calculations. Thus, the window function proposed by Lockard [77] and shown in Figure 4.2 is used in this work since it keeps the correct amplitude for 3/4 of the input data.

Figure 4.2: The window function used to make the input data periodic.

The filter is essentially a Hanning filter on the ends with no scaling in the center region and is given by

$$
W_n = \begin{cases} 1 & \text{if } N/8 < n \leq 7N/8 \\ 0.5\{1 - \cos[8\pi(n-1)/(N-1)]\} & \text{otherwise} \end{cases} \tag{4.24}
$$

Here, n is an index that runs from 1 to N, the total number of points in the data sample.

The window is applied in an energy preserving manner by scaling the output of the Fourier transformation by $\sqrt{N/\sum W_n^2}$. This makes it easier to compare the time history of the predicted far-field pressure fluctuations to the one given by CFD calculation, but one has to keep in mind that this window function still preserves only energy and not peak amplitude. The small amount of time data typically available from a CFD calculation leads to inaccuracies in the windowed Fourier transformation in this frequency-domain formulation, but time-domain formulations suffer from the small amount of data available as well and are therefore not better.

Solution Process

In summary, the entire solution process to calculate the far-field pressure fluctuations via the 2D FW-H equation in the frequency-domain is as follows:

1. Define an integration surface $f(y_i) = 0$ that surrounds the object(s) in question

2. Compute $\rho(y_i, t)$, $u_i(y_i, t)$, $p(y_i, t)$ as well as the surface normals $n_i = \partial f/\partial y_i$ for a sufficient amount of source locations y_i on that surface

3. Calculate $\mathcal{F}_j$ and $\mathcal{Q}$ as given by Eqs. (4.21) and (4.20), respectively

4. Apply, if necessary, the window function (4.24) to $\mathcal{F}_j$ and $\mathcal{Q}$ after subtracting the respective mean

5. Perform the Fourier transformation given by Eq. (4.10) of $\mathcal{F}_j$ and $\mathcal{Q}$, preferably via a fast Fourier transformation (FFT)

6. Compute the Green function (4.14) and its first derivatives (4.23) for each ω used in the Fourier transformation as well as for each desired observer location x

7. Evaluate the line integrals in Eq. (4.19) for each observer location x and frequency ω to obtain $p'(x, \omega)$

8. If desired, the inverse Fourier transformation given by Eq. (4.11) of $p'(x, \omega)$ can be used via an inverse FFT to recover the pressure fluctuation in the time-domain $p'(x, t)$

A disadvantage of the frequency-domain formulation is that the source and observer are always a fixed distance apart, which means that Doppler effects are not accounted for. This is not a problem if one simulates experiments in a laboratory frame where the observer to source distances are typically fixed. However, comparisons for flyover experiments should include the Doppler effects, which can only be incorporated in a time-domain calculation, where the distance between the observer and the source can be changed for each time step.

4.3 Validation

In order to validate the program code for solving the 2D FW-H equation in the frequency-domain, two examples are presented in the following subsections in which the results for the far-field pressure fluctuations are compared to well-known analytical solutions. In the last subsection a direct comparison between the FW-H output and that obtained from a CFD simulation is performed to gauge the validity of the formulation for airframe generated noise.

4.3.1 Monopole in Uniform Flow

The first validation example considered is the acoustic field from a monopole line source. According to Greschner *et al.* [46], the complex velocity potential for a stationary monopole source placed at the origin in a uniform flow with velocity U_i and a flow angle $\tan\theta = U_2/U_1$ can be written as

$$\phi(x_1, x_2, t) = \mathcal{A}(x_1, x_2, t) H_0^{(2)}\left(\frac{k}{\beta^2}\bar{r}\right) \tag{4.25}$$

with

$$
\begin{aligned}
\mathcal{A}(x_1, x_2, t) &= A\frac{i}{4\beta}\exp(i\omega t + iMk\bar{x}/\beta^2) \\
\bar{r} &= \sqrt{\bar{x}^2 + \beta^2\bar{y}^2} \\
\bar{x} &= x_1\cos\theta + x_2\sin\theta \\
\bar{y} &= -x_1\sin\theta + x_2\cos\theta,
\end{aligned}
$$

where A is the amplitude, M is the Mach number, $\beta = \sqrt{1 - M^2}$, and $k = \omega/a_\infty$ is the wave number. The perturbation variables needed to calculate the monopole and dipole source

terms are obtained from the real parts of

$$p' = p - p_\infty = -\rho_\infty \left(\frac{\partial \phi}{\partial t} + U_1 \frac{\partial \phi}{\partial x_1} + U_2 \frac{\partial \phi}{\partial x_2} \right)$$

$$u_i' = u_i - U_i = \frac{\partial \phi}{\partial x_i}$$

$$\rho' = \rho - \rho_\infty = \frac{p'}{a_\infty^2}, \tag{4.26}$$

where

$$\frac{\partial \phi}{\partial t} = i\omega\phi$$

$$\frac{\partial \phi}{\partial x_1} = \frac{iMk}{\beta^2} \cos\theta\, \phi - \mathcal{A} \frac{k}{\beta^2 \bar{r}} (\bar{x} \cos\theta - \beta^2 \bar{y} \sin\theta) H_1^{(2)} \left(\frac{k}{\beta^2} \bar{r} \right)$$

$$\frac{\partial \phi}{\partial x_2} = \frac{iMk}{\beta^2} \sin\theta\, \phi - \mathcal{A} \frac{k}{\beta^2 \bar{r}} (\bar{x} \sin\theta + \beta^2 \bar{y} \cos\theta) H_1^{(2)} \left(\frac{k}{\beta^2} \bar{r} \right). \tag{4.27}$$

The source terms are calculated from these flow variables evaluated over one period $T_P = 2\pi/\omega$ on the integration surface, which is a circle with a radius of r_c. One hundred uniformly spaced points on this circle are used as source locations. For this example,

$$\theta = 20°, \quad M = 0.5, \quad \omega = 3000.0\, rad/s, \quad r_c = 2\, m,$$

$$A = 0.01\, m^2/s, \quad p_\infty = 1.00016 \cdot 10^5\, Pa \quad \text{and} \quad T_\infty = 300\, K,$$

which leads to

$$a_\infty = \sqrt{1.402 \cdot 287.05 J/(kg \cdot K) \cdot T_\infty} \approx 347.47\, m/s$$

$$\rho_\infty = p_\infty \cdot 1.402/a_\infty^2 \approx 1.161\, kg/m^3$$

$$U_1 = Ma_\infty \cos\theta \approx 163.26\, m/s$$

$$U_2 = Ma_\infty \sin\theta \approx 59.42\, m/s.$$

Figure 4.3 compares the directivity from the FW-H calculation to the analytic solution in the far-field at $r = 500\, m$, and Figure 4.4 makes a comparison for the time histories of the pressure fluctuations at $x_1 = 500\, m$ and $x_2 = 0\, m$. The agreement is excellent, demonstrating that the two-dimensional FW-H formulation is valid for problems with a uniform mean flow.

Figure 4.3: Directivity comparison for a monopole at $r = 500\,m$.

Figure 4.4: Time history comparison for a monopole at $x_1 = 500\,m$ and $x_2 = 0\,m$.

4.3.2 Scattering by an Edge

The second validation example is the acoustic radiation from a two-dimensional line vortex passing by a sharp edge of a half-plane. A schematic of the problem is shown in Figure 4.5.

Figure 4.5: Schematic of a line vortex moving around a half-plane.

A vortex of strength κ moves along the indicated path around the edge of a semi-infinite plate. The maximum speed of $M \equiv 0.01$ of the motion occurs at time $t = 0$, when the vortex is adjacent to the edge at $x_1 = \mathrm{b} \equiv 1\,m$ and $x_2 = 0\,m$. The general problem was solved analytically by Crighton [18] for low Mach numbers. He matched the velocity potential for the incompressible inner solution to the slightly compressible outer solution and applied a radiation condition to the outer solution at infinity. His solution for the non-dimensionalized velocity potential is given by

$$\phi(x_1, x_2, t) = \frac{2\sqrt{2}}{[M^2(r-t)^2 + 4]^{1/4}} \frac{\sin(\theta/2)}{r^{1/2}}, \tag{4.28}$$

where $r = \sqrt{x_1^2 + x_2^2}$ is the with b non-dimensionalized distance from the edge, θ is the angle measured relative to the positive x_1-axis, and t is the with b/a_∞ non-dimensionalized time. Again, in this example

$$p_\infty = 1.00016 \cdot 10^5\,Pa \quad \text{and} \quad T_\infty = 300\,K,$$

leading to

$$a_\infty = \sqrt{1.402 \cdot 287.05 J/(kg \cdot K) \cdot T_\infty} \approx 347.47\,m/s$$

$$\rho_\infty = p_\infty \cdot 1.402/a_\infty^2 \approx 1.161\,kg/m^3.$$

This time the perturbation variables required for the source terms are obtained from

$$
\begin{aligned}
p' = p - p_\infty &= -\rho_\infty \frac{\partial \phi}{\partial t} \cdot M \cdot \rho_\infty a_\infty^2 \\
u_i' = u_i &= \frac{\partial \phi}{\partial x_i} \cdot M \cdot a_\infty \\
\rho' = \rho - \rho_\infty &= \frac{p'}{a_\infty^2},
\end{aligned}
\tag{4.29}
$$

where

$$
\begin{aligned}
\frac{\partial \phi}{\partial t} &= \frac{\sqrt{2}}{[M^2(r-t)^2+4]^{5/4}} \frac{\sin(\theta/2)}{r^{1/2}} M^2(r-t) \\
\frac{\partial \phi}{\partial x_1} &= \frac{\partial \phi}{\partial r}\frac{\partial r}{\partial x_1} + \frac{\partial \phi}{\partial \theta}\frac{\partial \theta}{\partial x_1} = \frac{\partial \phi}{\partial r}\cos(\theta) - \frac{\partial \phi}{\partial \theta}\sin(\theta)/r \\
\frac{\partial \phi}{\partial x_2} &= \frac{\partial \phi}{\partial r}\frac{\partial r}{\partial x_2} + \frac{\partial \phi}{\partial \theta}\frac{\partial \theta}{\partial x_2} = \frac{\partial \phi}{\partial r}\sin(\theta) + \frac{\partial \phi}{\partial \theta}\cos(\theta)/r \\
\frac{\partial \phi}{\partial r} &= -\frac{\sqrt{2}(4 + M^2(r-t)(2r-t))}{[M^2(r-t)^2+4]^{5/4}} \frac{\sin(\theta/2)}{r^{3/2}} \\
\frac{\partial \phi}{\partial \theta} &= \frac{\sqrt{2}}{[M^2(r-t)^2+4]^{1/4}} \frac{\cos(\theta/2)}{r^{1/2}}.
\end{aligned}
\tag{4.30}
$$

Since the exact Green function for this geometry is not known, the free-space Green function in the frequency-domain, given by Eq. (4.14) with $M = 0$, has to be used. In order to take this into account, the integration surface is extended far enough such that most of the effective sources on the plate are enclosed by it. The surface extends from $-200\,m$ to $2\,m$ in x_1 with 180 equidistant points, and from $-2\,m$ to $2\,m$ in x_2 with 40 equidistant points, for a total of 440 points on the surface. A time history of the acoustic field from $-20.0\,s$ to $20.0\,s$ captures most of the features of the slowly varying signal as the vortex passes the edge of the half-plane. This problem is not periodic in nature; however, the source terms approach very small values for large negative and positive times so that they are naturally windowed. The pressure fluctuations over time shown in Figure 4.7 exemplify the behaviour of the source terms for large negative and positive times.

The directivity comparison between the exact and calculated solutions for observers at a radius of $50\,m$ from the edge is shown in Figure 4.6 and the time histories of the pressure fluctuations at $r = 50\,m$ and $-45°$ from the lower surface of the half-plane are compared in Figure 4.7. Again the agreement is excellent, showing that the two-dimensional FW-H approach is applicable to problems that are not dominated by a single frequency as well as to problems where the source of the acoustic radiation is spatially distributed.

Figure 4.6: Directivity comparison at $r = 50\,m$ for a vortex passing an edge.

Figure 4.7: Time history comparison at $r = 50\,m$ and $-45°$ from the lower surface of the half-plane for a vortex passing an edge.

4.3.3 Airfoil in Laminar Flow

In this subsection a direct comparison is presented between the pressure fluctuations calculated via the FW-H approach and those obtained from a CFD simulation. For more details about the numerical implementation of the FW-H equation see Appendix F. The laminar flow over the single-element NACA 0012 airfoil with a Reynolds number of 800, a free stream Mach number of 0.2, and an angle of attack of 20° is considered. At these conditions the airfoil experiences vortex shedding. A C-mesh with 848×395 nodes and a non-dimensional time step $\Delta t = 0.03$ is used. After the flow solver has reached a periodic steady state, 1800 time steps are taken, which cover about five vortex shedding cycles, and the solution is recorded. The fictitious or porous FW-H integration surface consists of one of the streamwise grid lines located at about $0.015c$ away from the airfoil, and the surface is closed at the trailing edge with one of the existing vertical grid lines.

Figure 4.8: Permeable FW-H integration surface and CFD probe locations.

For comparison purposes, six distinct locations with increasing distance from the airfoil are selected to probe the CFD results and extract the unsteady pressure fluctuations. The spatial locations of the six probe stations are displayed in Figure 4.8. The extracted CFD pressure fluctuations as well as those obtained from the FW-H solver are plotted in Figure 4.9 for three selected probe stations for more clarity and in Figure 4.10 for all six probe stations.

Figure 4.9: Comparison of pressure fluctuations calculated by CFD (solid line) and FW-H (dashed line) in selected probe locations.

The wavelength of the dominant tone of this quasi point source can be deduced from these figures and is given in non-dimensional units (chord lengths) by $\lambda = a_\infty/f = a_\infty \cdot T_P \approx 1 \cdot 9.2 = 9.2$. This explains why the pressure fluctuations in probe location 1 and 3 are almost in phase since these locations are about one wavelength apart from each other. In two dimensions one also expects that the sound intensity, which itself is proportional to the square of the sound pressure, is inversely proportional to the distance of an acoustic point source. This distance law is almost perfectly fulfilled by the pressure fluctuations which are calculated with the FW-H approach.

By comparing the pressure fluctuations probe location by probe location one can make the

Figure 4.10: Comparison of pressure fluctuations calculated by CFD (solid line) and FW-H (dashed line) in different probe locations.

following observations: At probe locations 2 and 3, which are relatively close to the airfoil, the pressure records from the CFD results and the FW-H approach are almost identical, except for the beginning and end of the data, where the window function tarnishes the result from the FW-H approach. The agreement at the first probe location is also fairly good, except for the underprediction of the amplitude by the FW-H calculation. It has been tried to resolve this problem by using different integration surfaces but without success. However, since in real applications the observer position is never so close to the integration surface this discrepancy is deemed to be a minor issue. At the fourth location the agreement in the low- to mid-frequency range (broadband noise component) is still quite good, but the CFD result shows attenuation of the high frequency (tonal noise) component, due to the coarser grid this far away from the airfoil and the low order accuracy of the flow solver. Lastly, the CFD results at probe locations 5 and 6 are basically useless, and it becomes apparent that an accurate propagation of the pressure signatures to the far-field for moderate cost is only achievable with an acoustic wave propagation code.

The directivities at a distance of ten chord lengths show the dipole nature of this problem

Figure 4.11: Variation of directivity with solid and porous integration surface.

in Figure 4.11 . The figure also displays a comparison between the directivity obtained using the porous integration surface described above and a solid surface that coincides with the airfoil. One can see a good agreement; however, as a vortex passes through the porous surface, a fictitious noise source is generated, which is caused by the time-varying force on the integration surface as the vortex passes through it. This apparent noise would be cancelled by the quadrupole term if it were included. However, the quadrupole contribution for this low-speed flow is relatively small, and hence good agreement is achieved, even though the quadrupole term is neglected.

The presented comparison confirms that FW-H calculations produce results that are equivalent to the more direct but costlier CFD approaches. Figures 4.10 and 4.9 show ample evidence of the ability of the FW-H code to calculate the pressure fluctuations without introducing too much amplitude or phase distortion. However, the FW-H results are only as good as the input data, and hence, care has to be taken to judiciously place the permeable integration surface and to use a fine enough mesh in the near-field region.

Chapter 5

RESULTS

After introducing all the components that are required to optimize airfoils in unsteady flows and to predict airframe generated noise in the previous chapters, it is time to present a wide spectrum of applications in this chapter. On the basis of these results, the unsteady optimization procedure can be validated and evaluated. Sections 5.1 and 5.2 deal with unsteady internal flow problems: the inverse design of a pulse in a one- and two-dimensional converging-diverging nozzle and the flow in a shock-tube are presented. The drag minimization for viscous flow around a rotating cylinder is presented in Section 5.3, and the attempt to mitigate the effects of transonic buffeting is covered in Section 5.4. In Section 5.5 the aeroacoustic shape design for unsteady trailing-edge flow is addressed, and in Section 5.6 the remote inverse designs of single- and multi-element airfoils at a high angle of attack are shown.

The final three sections address the validation of the hybrid URANS/FW-H optimization algorithm using remote inverse shape designs, and the application of the algorithm to turbulent blunt trailing edge flow and high-lift noise optimization.

5.1 Pulse in 1D and 2D Converging-Diverging Nozzle

As a first example the inverse design in one and two dimensions of a subsonic flow with a pulse in the static outflow pressure in a converging-diverging nozzle is considered (published in Rumpfkeil and Zingg [115]).

The one-dimensional case

The one-dimensional problem is governed by the quasi-1D Euler equations, and cubic spline interpolation with six control points is used to represent the nozzle shape. Since the control points at each end are fixed to ensure a well-posed design problem, there are four shape

design variables, $\bar{S}$, for this problem. The initial and target shapes of the nozzle together with the location of the control points are shown in Figure 5.1.

Figure 5.1: Initial and target converging-diverging nozzle shapes.

The pulse in the static outflow pressure is given by

$$p(t) = p_s + A \cdot \sin(2\pi F t), \tag{5.1}$$

where A and F are the given amplitude and frequency of the pulse, and p_s is a constant. At the inlet, constant stagnation conditions, p_0 and T_0, are enforced, and the remaining three boundary conditions are calculated through linear extrapolation as follows: at the inlet, the Riemann invariant $R_1 = u - \frac{2a}{\gamma-1}$ is used, and at the outlet, $R_2 = u + \frac{2a}{\gamma-1}$ and $H = E + p/\rho$. The flow solver is a one-dimensional implementation of the 2D solver described in Chapter 2. The BDF2 time-marching method is utilized for a time-accurate flow solve, and 100 equally-spaced nodes discretize the problem in space for all the presented cases. At $t = 0$, the unsteady flow solve is initialized with the steady state solution Q^0 of the quasi-1D Euler equations with $p(t = 0) = p_s$ (see Figure 5.2).

The control variables $Y = (A, F, \bar{S})$ are chosen, and two possible forms for the cost functional $\mathcal{O}$ are considered:

Figure 5.2: Initial and target pressure, velocity and density at $t = 0$.

1. The observation is only obtained for the final time T

$$\mathcal{O}_1 = \frac{1}{2} \sum_{j=1}^{100} \sum_{i=1}^{3} (Q_{j,i}^N - Q_{j,i}^{*N})^2 \tag{5.2}$$

2. The observation is distributed at assimilation times $0 \le t \le T$

$$\mathcal{O}_2 = \frac{1}{2} \Delta t \sum_{n=1}^{N} \sum_{j=1}^{100} \sum_{i=1}^{3} (Q_{j,i}^n - Q_{j,i}^{*n})^2 \tag{5.3}$$

Here, $Q_{j,i}^{*n}$ are the target or desired observations at node j, which are obtained as solutions of the flow problem with the control vector $Y^* = (0.05, 1.5, \bar{S}^*)$, where $\bar{S}^*$ are the four target shape design variables. There are also two different initial guesses $Y_1 = (0.04, 1.4, \bar{S})$ and $Y_2 = (0.08, 1.9, \bar{S})$ used for this optimal control problem, and $T = 1.0$ (in non-dimensional units) is chosen as the time horizon.

Matlab's command "fminunc" for unconstrained nonlinear optimization is used to solve the presented inverse design problem. The LargeScale option is set to "off" so that Matlab uses the BFGS Quasi-Newton method with a mixed quadratic and cubic line search procedure. The adjoint equations given in Appendix B are implemented in Matlab to calculate

the gradient. However, a slight modification is necessary to account for the required steady flow solve after the shape of the nozzle is modified due to new values of the design variables Y. Thus, one needs to add the steady contribution $\lambda^T R(Q^0, Y)$ to the Lagrangian, which leads to one extra adjoint equation for λ that needs to be solved

$$\lambda = - \left((\nabla_{Q^0} R)^T \right)^{-1} \left[(\nabla_{Q^0} \mathcal{R}^2)^T \psi^2 + \nabla_{Q^0} \mathcal{R}^1)^T \psi^1 \right]. \tag{5.4}$$

Once Matlab is provided with the necessary routines to compute the cost function and gradient, it is able to drive both objective functions $\mathcal{O}_1$ and $\mathcal{O}_2$, given by Eqs. (5.2) and (5.3), respectively, for the initial guess Y_1, to machine zero. The same is true for $\mathcal{O}_2$ with the initial guess Y_2, but for $\mathcal{O}_1$ (comparison only at the final time) and Y_2, BFGS gets stuck in a different minimum (see Figure 5.3).

Figure 5.3: Convergence plots for $\mathcal{O}_1$ (dashed) and $\mathcal{O}_2$ (solid) using $T = 1.0$ (for Y_1 as initial condition in the left column and for Y_2 in the right column.)

In order to gauge the accuracy of the adjoint gradient (ad) it is compared to the gradient computed via the complex-step (cs) method [133] at the first design iteration. The agreement is excellent with $\left(\left(\frac{\partial \mathcal{O}}{\partial Y_k} \right)_{ad} - \left(\frac{\partial \mathcal{O}}{\partial Y_k} \right)_{cs} \right) / \left(\frac{\partial \mathcal{O}}{\partial Y_k} \right)_{cs} \leq 10^{-11}$ for all k and both objective functions, showing that the adjoint approach yields a very accurate gradient.

The two-dimensional case

In order to solve the full two-dimensional version of the pulse problem, the 2D multi-block structured solver, TORNADO [97], is used in Euler mode with the BDF2 time-marching method. The pulse in the static outflow pressure is given by Eq. (5.1), and constant stagnation conditions at the inlet are specified for the remaining boundary conditions. Cubic spline interpolation represents the nozzle shape, however this time with only five control points, and since the inflow and outflow control points are fixed to ensure a well-posed design problem, there are only three shape design variables $\bar{S}$. The x-locations of the control points are 2.5, 5.0 and 7.5, respectively; the initial and target shapes of the nozzle are shown in Figure 5.4 with the grid consisting of 99×55 nodes.

Figure 5.4: Initial (red) and target (black) converging-diverging nozzle shapes in 2D.

The control vector is again given by $Y = (A, F, \bar{S})$ and the objective function is as follows

$$\mathcal{O} = \frac{1}{2}\Delta t \sum_{n=1}^{N} \sum_{j=1}^{Je} \sum_{k=1}^{Ke} \sum_{i=1}^{4} (\hat{Q}_{j,k,i}^{n} - \hat{Q}_{j,k,i}^{*n})^2,$$

where $\hat{Q}_{j,k,i}^{n}$ are the conservative flow variables at node (j, k) in the computational domain (the map of the curvilinear grid into a uniform and equally spaced grid). For this problem the following parameters are chosen: $Je = 99$, $Ke = 55$, and $N = 200$ with a constant time step $\Delta t = 0.1$, which yields $T = 20.0$ as final time. The objective function $\mathcal{O}$ is always scaled by a

factor such that the initial value is unity. The starting point Q^0 is the steady-state solution of the 2D Euler equations with $p(t\!=\!0) = p_s = 92 \; kPa$. The target flow variables $\hat{Q}_{j,k,i}^{*n}$ are obtained as the solution of the flow problem with the control vector $Y^* = (1000, 0.15, \bar{S}^*)$, and the non-dimensionalized target pressure at $t = 0$ is displayed in Figure 5.5.

Figure 5.5: Non-dimensionalized target pressure at $t = 0$ in 2D Nozzle.

The gradient of $\mathcal{O}$ with respect to the control variables Y is again calculated using the adjoint equations given in Appendix B with the one additional adjoint equation for λ given by Eq. (5.4).

In order to save computational time and storage, the flow field is only saved every five time steps, and thus the flowfield is compared with the target flowfield only every five time steps in the objective function as well. This means, in particular, that the transpose of the Jacobian has to be inverted only 40 times as opposed to 200 times in order to calculate the complete gradient. This approach has, of course, an influence on the accuracy of the gradient, as the following example demonstrates. Using $Y = (2500, 0.21, \bar{S})$ as an initial guess for the control vector and second-order central finite-differences (fd) with a stepsize of $h = 10^{-7}$ to calculate the gradient at the first design iteration (thereby comparing the flowfields at every time step) yields

$$\left(\frac{\partial \mathcal{O}}{\partial Y} \right)_{fd} = (-0.0519, \; 1.9142, \; -3.7971, \; 4.0757, \; 5.5990),$$

which is in good agreement with the gradient calculated via the adjoint method (ad)

$$\left(\frac{\partial \mathcal{O}}{\partial Y}\right)_{ad} = (-0.0519,\ 1.9142,\ -3.7661,\ 4.0911,\ 5.6017).$$

On the other hand, using the adjoint method while jumping over five time steps at a time ($ad5$) yields

$$\left(\frac{\partial \mathcal{O}}{\partial Y}\right)_{ad5} = (0.2219,\ 1.0391,\ -4.1309,\ 3.7740,\ 5.6894).$$

Nonetheless, one can see in the convergence plot for different initial guesses for A and F in Figure 5.6 that the objective function can be driven to machine zero in all the presented cases, where it is important to note that only about half of all initial guesses tried lead to convergence. It is also crucial to impose constraints on the shape design variables ($\bar{S} \in [0.7,\ 1.7]$) to ensure that the flow through the nozzle always stays entirely subsonic in the inverse design process. One has also to constrain the amplitude and frequency of the pulse ($A \in [-14000,\ 14000]$ and $F \in [-0.5,\ 0.5]$) to prevent pulses with excessively large amplitudes or frequencies.

Figure 5.6: Convergence plots for the inverse design of a pulse in a 2D nozzle.

5.2 The Inverse Design of Flow in a Shock-tube

In this section the inverse design of a flow in a 1D shock-tube is presented. This shows that unsteady optimization can be very useful in data assimilation problems, which try to determine a "best" estimate for the initial state that leads to the observed flow behaviour, given a set of actual measurements of this flow on $[0, T]$. This shock-tube problem has been explored before by Homescu and Navon [56], but here an analytic derivation of the adjoint model is incorporated, whereas they linearized the nonlinear forward model code line by line and viewed the resulting tangent linear model as the result of the multiplication of a number of operator matrices $O_1 O_2 \ldots O_M$. They then derived the adjoint model as the product of adjoint subproblems $O_M^T O_{M-1}^T \ldots O_1^T$.

The shock-tube problem can be described as follows: a tube that is filled with gas is initially divided by a membrane into two sections. The gas has a higher density and pressure in one half of the tube than in the other half, with zero velocity everywhere. At time $t = 0$, the membrane is suddenly removed and the gas is allowed to flow, which results in a net motion in the direction of lower pressure. Assuming uniform flow across the tube, there is variation in only one direction and the 1-D Euler equations apply. Thus, the same flow solver that was used for the one-dimensional converging-diverging nozzle problem can be applied.

The control variables for this problem are chosen to be $Y = (p_L, p_R, \rho_L, \rho_R)$, and the two forms of the cost functional $\mathcal{O}$ given by Eqs. (5.2) and (5.3), respectively, are applied here as well. This time the target or desired observations Q_j^{*n} are obtained as solutions of the shock-tube problem for two different sets of initial conditions:

$$Y_1^* = (p_L = 1.1, p_R = 0.2, \rho_L = 1.1, \rho_R = 0.2)$$
$$Y_2^* = (p_L = 1.5, p_R = 0.6, \rho_L = 1.6, \rho_R = 0.4).$$

The Sod shock-tube values [130]

$$Y = (p_L = 1.0, p_R = 0.1, \rho_L = 1.0, \rho_R = 0.125)$$

are used as an initial guess for the optimizer, and the time horizon is $T = 0.21$ (in non-dimensional units).

Figure 5.7 displays the different flow variables for the target observations at $t = 0.21$ obtained from the two different sets of initial conditions together with the observation of

Figure 5.7: Pressure, velocity and density: initial guess (dashed line) and target observation (solid line) at $t = T = 0.21$ using Y_1^* in the left column and Y_2^* in the right column.

the initial guess at the same output time (again using 100 equally-spaced spatial nodes and the BDF2 time marching method). In order to provide Matlab's BFGS algorithm with the necessary gradient, the adjoint equations given in Appendix B are used, but since this is a data assimilation problem, it is advantageous to write the gradient of $\mathcal{O}$ with respect to the design variables Y as follows:

$$\frac{\partial \mathcal{O}}{\partial Y} = \frac{\partial \mathcal{L}}{\partial Y} = \frac{\partial \mathcal{L}}{\partial Q^0} \frac{\partial Q^0}{\partial Y} = \left[(\psi^2)^T \nabla_{Q^0} \mathcal{R}^2 + (\psi^1)^T \nabla_{Q^0} \mathcal{R}^1 \right] \frac{\partial Q^0}{\partial Y}. \tag{5.5}$$

Matlab is able to drive both objective functions $\mathcal{O}_1$ and $\mathcal{O}_2$, given by Eqs. (5.2) and (5.3), respectively, for the two target observations Y_1^* and Y_2^*, to machine zero (see Figure 5.8).

Once again, the resulting adjoint gradients of the cost functionals with respect to the design variables at the first design iteration have been compared to the ones computed via the complex-step method [133]. The agreement of ten digits is also excellent, thus showing

Figure 5.8: Convergence plots for $\mathcal{O}_1$ (dashed) and $\mathcal{O}_2$ (solid) using $T = 0.21$ for the first set of initial conditions in the left column and for the second set in the right column.

that the framework presented in Section 3.3 for deriving the adjoint equations encounters no problems when dealing with discontinuities such as shocks.

5.3 Drag Minimization for Viscous Flow around a Rotating Cylinder

Since the accuracy of the unsteady adjoint gradient calculation has been established in the previous two sections, a more demanding problem can be investigated. In this section the drag minimization for viscous flow around a rotating cylinder is examined (published in Rumpfkeil and Zingg [115, 120]). The idea is that by rotating the cylinder and controlling the angular velocity the drag can be decreased through the Magnus Effect (also known as the Robin's Effect), which can be observed for rotating spheres as well as cylinders. A deep

understanding of the control strategies for flows past rotating bluff bodies can be very helpful in areas such as drag reduction, lift enhancement, vibration control, and last but not least, the particular interest of this thesis, noise control.

The laminar viscous flow past a circular cylinder has been comprehensively studied because of its simple geometry and its representative behavior of general bluff body wakes. There are various flow regimes, which are highly dependent on the Reynolds number ($\mathcal{R}e$) and can be identified by the character of the flow in the wake and boundary layer of the cylinder [16]. However, over a large range of Reynolds numbers ($47 < \mathcal{R}e < 10^7$) there are always eddies shed alternately from each side of the cylinder, forming rows of vortices in its wake, the so-called Karman vortex street [146].

In order to solve the underlying 2D unsteady Navier-Stokes equations, the 2D single-block structured thin-layer solver, PROBE [111], is used with the BDF2 time-marching method. The rotational boundary conditions are implemented by requiring the normal velocity on the surface of the cylinder to be zero and the tangential velocity to be equal to $\Omega \cdot r$, where Ω is the angular velocity and $r = 0.5$ the radius of the cylinder. It is convenient to introduce the Strouhal number

$$S_n = d \cdot f_n / u_\infty$$

for comparison purposes, where $d = 1$ is the diameter of the cylinder, f_n is the Karman vortex shedding frequency, and $u_\infty = M_\infty = 0.2$ is the free-stream velocity. Using an O-mesh with 140×90 grid nodes, an off-wall spacing of 10^{-4}, and the BDF2 time-marching method with a time step size of $\Delta t = 0.1$, the results from PROBE for the mean value of the drag coefficient $\bar{C}_D$ and the Strouhal number S_n are compared with computationally [52, 57] and experimentally [53, 148] obtained values by various authors in Table 5.1.

	$\bar{C}_D$		S_n	
Reynolds number	100	1000	100	1000
Present work	1.45	1.53	0.179	0.252
He *et al.* [52]	1.35	1.52	0.167	0.239
Homescu *et al.* [57]	1.42	1.68	-	-
Henderson [53]	1.35	1.51	0.166	0.237
Williamson [148]	-	-	0.164	-

Table 5.1: Mean drag coefficients and Strouhal numbers (the last two are experimental results).

There is a reasonable agreement for both Reynolds numbers shown. Most of the observed differences are likely due to the relatively large time steps and the relatively coarse grid. Also, the use of the thin-layer Navier-Stokes equations is questionable for a bluff-body flow and will deviate to some degree from a full Navier-Stokes solution. However, since the primary focus of this thesis is on the optimal control of unsteady flows, the trade-off between accuracy and performance is satisfactory, even though the computed unsteady flow is not grid converged.

The experimental work of Tokumaru and Dimotakis [137] motivated the attempt to find an optimal angular velocity in order to minimize the drag. Several researchers [57, 52] considered two control cases (but used different objective functions): the constant rotation case, $\Omega(t) = \Omega$ using $Y = \Omega$ as design variable, and the time harmonic rotary oscillation case, $\Omega(t) = A \cdot \sin(2\pi F t)$ with $Y = (A, F)$ as design variables.

The objective function of choice for the constant and harmonic rotating cases is a time averaged or mean drag minimization problem:

$$\mathcal{O} = \bar{C}_D = \frac{1}{N - N_c} \sum_{n=N_c+1}^{N} C_D^n, \tag{5.6}$$

where C_D^n is the cylinder's drag coefficient at time step n.

It is very important to have a practical knowledge of the design space to be able to choose a reasonable time step and control window. The effect of different values of Ω on the drag coefficient for the constant rotation case using a fixed time step of $\Delta t = 0.1$ is shown in Figure 5.9. The rotation starts impulsively, and after a transition period of about 1500 steps the mean drag coefficients of the rotating cylinders are all smaller than the mean drag coefficient of the stationary cylinder.

In order to reduce the computational costs in the actual optimization runs, one can "jump" over the adjusting or transition period as quickly as possible by taking a bigger time step $\Delta t_c = 0.5$ for $N_c = 300$ steps. This larger time step is chosen in such a way that the accuracy of the overall numerical solution is not significantly diminished. Once the domain where one wants to control the problem is reached (the control window is indicated by the box in Figure 5.9), a smaller time step $\Delta t = 0.2$ is used for another 500 steps, for a total of $N = 800$ time steps in each flow solve covering a time interval of $[0, 250]$. The corresponding adjoint equations for this situation are given in Appendix D and the time horizons are summarized in Table 5.2.

Figure 5.9: Drag coefficients for the constant rotation case for different values of Ω ($\Delta t = 0.1$).

N_c	Δt_c	$N - N_c$	Δt	N	Adjustment interval	Control interval
300	0.5	500	0.2	800	$[0, 150]$	$[150, 250]$

Table 5.2: Time horizons for the constant rotating cylinder.

The optimizer BFGS [153, 13] is able to minimize the mean drag with gradient norms of about 10^{-8} at the local minima when Ω is constrained to values between 0 and 1.9 to prevent excessively large rotation speeds. The resulting design space is shown in Figure 5.10 with the gradients at the design points represented by straight lines. One can see several local minima in this design space, with the global minimum in the given interval at $\Omega = \Omega^* \approx 1.16$ leading to $\bar{C}_D \approx 0.11$. This optimum value minimizes the mean drag value far beyond the extent of the control window, as can be seen in Figure 5.9; this behaviour was also observed by other researchers [57, 52].

Figure 5.10: The design space of the constant rotating cylinder $\Omega(t) = \Omega$.

Just like in the two-dimensional pulse case, one can try to save computational time and storage by saving the flowfield in the control time window only every other time step. This leads to an inexact gradient but also to only $300 + 500/2 = 550$ matrix inversions for the adjoint solution as compared to 800 in the original case. The result is also shown in Figure 5.10, and the gradients and objective function values are in reasonable agreement with each other, thus leading to similar convergence histories, except that in this case the local minima are slightly shifted (about 0.25 percent off) and the gradient norms only reduce to 10^{-3} at these minima. Trying to skip time steps in the adjusting period or more than every other time step in the control window did not work as well or did not converge at all.

In Figure 5.11 the effect of different values of A and F on the drag coefficient for the harmonic rotation case using a fixed time step of $\Delta t = 0.1$ is shown. The rotation starts

smoothly, and after a transition period of about 750 steps the mean drag coefficients of the harmonically rotating cylinders are again all smaller than the mean drag coefficient of the stationary cylinder.

Figure 5.11: Drag coefficients for the harmonic rotation case for different values of A and F ($\Delta t = 0.1$).

The chosen time horizons for this problem are shown in Table 5.3. Using the same objective function as for the constant rotating cylinder given by Eq. (5.6) and constraining the amplitude A to $[0, 1.9]$ and the frequency F to $[0, 0.3]$ to prevent rotations with excessively large amplitudes or frequencies, the optimizer could minimize the mean drag value with gradient norms of about 10^{-4} at the local minima.

The resulting design space is displayed in Figure 5.12, with the gradients at the different design points represented by arrows, and the objective function values given by a colour

N_c	Δt_c	$N - N_c$	Δt	N	Adjustment interval	Control interval
375	0.2	400	0.1	775	$[0, 75]$	$[75, 115]$

Table 5.3: Time horizons for the harmonic rotating cylinder.

scale with red representing the highest and blue the lowest values. Once again, several local minima can be seen, with a global minimum for $Y = Y^* \approx (0.98,\ 0.114)$ leading to $\bar{C}_D \approx 0.6832$, which again leads to a minimized mean drag value far beyond the extent of the control time window, as can be seen in Figure 5.11. Trying to skip any time steps while saving the flowfield is not pursued due to the already fairly coarse time steps for this highly oscillatory problem.

Figure 5.12: The design space of the harmonic rotating cylinder and a zoom into the most interesting region.

5.4 Transonic Buffeting Shape Optimization

This section describes the attempts to mitigate the effects of transonic buffeting with the help of unsteady turbulent shape optimization. The self-excited shock wave oscillations on a RAE2822 airfoil with $M_\infty = 0.71$, $Re = 20 \times 10^6$, and $\alpha = 7°$ form the test case. Instantaneous Mach contours are shown in Figure 5.13.

Figure 5.13: Instantaneous Mach contours for the RAE2822 airfoil.

Self-sustained shock wave oscillations on airfoils at transonic flow conditions are associated with the phenomenon of buffeting. The unsteady pressure fluctuations generated by these low-frequency large-amplitude shock motions are highly undesirable for the structural integrity and maneuverability of aircraft. Three distinct regions of transonic flight Mach numbers can be defined for a fixed free-stream Reynolds number [150]. Below a critical Mach number, the flow is steady and characterized by a weak shock wave near the midchord. Above this critical Mach number, the flow becomes unsteady with shock-induced flow separation and shock motions on the upper and lower surfaces of the airfoil which are out of phase. As the Mach number is further increased, a steady shock reappears which is again strong enough to induce flow separation. The physical mechanisms of the self-excited oscillation are not very well understood. However, the necessary but not sufficient condition for triggering periodic buffeting is a strong enough shock wave to cause boundary-layer separation [74]. Note that instead of increasing the transonic Mach number beyond the critical value one can observe the same effects by increasing the angle of attack for a fixed critical Mach number [150].

The unsteady turbulent shape optimization uses ten B-spline control points as shape design variables (five on the upper and five on the lower surface) and is started from three different initial shapes, which are shown in Figure 5.14:

1. The original RAE2822 airfoil (in red)

2. The airfoil that results from setting all ten design variables to their specified upper bounds (in blue)

3. The airfoil that results from setting all ten design variables to their specified lower bounds (in black)

Figure 5.14: The initial airfoil shapes.

The reason for the tight lower and especially tight upper bounds is that the flow solver is not very robust in this unsteady transonic flow regime and thus cannot handle larger shape changes. The flow solver PROBE [111] with the BDF2 time-marching method is used on a C-mesh with 198×60 nodes. The dissipation constant κ_2 is set to zero, so that the pressure switch Υ, given by Eqs. (2.32), which controls the first-order dissipation near shocks, is disabled. This leads to more accurate gradients since this pressure switch is not differentiated for the flow Jacobian in the current implementation.

Two objective functions are considered:

1. Mean drag minimization
$$\mathcal{O} = \bar{C}_D = \frac{1}{N - N_c} \sum_{n=N_c+1}^{N} C_D^n$$

2. Mean drag over mean lift minimization
$$\mathcal{O} = \frac{\bar{C}_D}{\bar{C}_L} = \frac{\sum_{n=N_c+1}^{N} C_D^n}{\sum_{n=N_c+1}^{N} C_L^n}$$

where C_D^n and C_L^n are the airfoil's drag and lift coefficient at time step n, respectively. Two thickness constraints are imposed to maintain a certain structural feasibility. They

are located at 35 and 99 percent chord length with a target thickness of $0.11c$ and $0.0015c$, respectively. The third initial shape (starting from specified lower bounds) slightly violates both thickness constraints.

After each shape modification the flow solve is warmstarted from the original RAE2822 airfoil periodic steady state solution, and the flow is allowed to evolve for some time to establish a new periodic steady state before the drag and lift coefficients are recorded (compare with Figure 5.18). The time horizons used for this unsteady shape optimization are summarized in Table 5.4 and the corresponding adjoint equations are given in Appendix D. Note that Δt_c is not larger than Δt for stability and robustness.

N_c	Δt_c	$N - N_c$	Δt	N	Adjustment interval	Control interval
200	0.2	400	0.2	600	$[0, 40]$	$[40, 120]$

Table 5.4: Time horizons for the buffeting shape optimizations.

Figure 5.15 presents the final improved airfoil shapes of the transonic buffeting shape optimizations. For the mean drag over mean lift minimization all three initial shapes converge to the same final shape shown in green. However, for the mean drag minimization each initial shape leads to a slightly different improved shape.

Figure 5.15: Final improved airfoil shapes of the buffeting shape optimizations.

The convergence histories of the mean drag minimizations are displayed in Figure 5.16. Starting from the original RAE2822 airfoil leads to the best shape with a reduction of about 17 percent in the mean drag. However, the gradient norms are reduced by less than one order of magnitude, implying that the optimizer did not converge due to stalls in the line search algorithm.

Figure 5.16: Convergence histories of the mean drag minimizations.

Figure 5.17: Convergence histories of the mean drag over mean lift minimizations.

The convergence histories of the mean drag over mean lift minimizations are shown in Figure 5.17. All three initial shapes converge to the same final shape and thus objective function value, which translates into a reduction in mean drag over mean lift of about 20 percent from the original RAE2822 airfoil. Once again, however, the gradient norms are reduced by less than one order of magnitude due to line search stalls.

The time histories of C_L and C_D for the original RAE2822 airfoil before and after the optimizations are shown in Figure 5.18. One can clearly see the unphysical adjusting period for the improved airfoils in the time interval $[0, 40]$ before they reach their new somewhat periodic steady state. A reduced mean drag for both improved airfoils is also visible. The mean drag over mean lift minimization leads to an increased mean lift as well, whereas the mean drag minimization actually decreases the mean lift. As a last observation, both objective functions lead to reduced oscillation amplitudes in both lift and drag. However, the mean drag minimization yields smaller amplitudes that even seem to approach a steady state with a fixed shock location, which is highly desirable from a structural integrity and maneuverability point of view.

Figure 5.18: Time histories of C_L and C_D for the RAE2822 airfoil before and after the optimizations vs. time ($\Delta t = 0.2$).

The above presented transonic buffeting shape optimizations look fairly promising, but a

more in-depth investigation is clearly required to try to resolve flow solver and optimizer convergence problems, and it should be stressed that the results have little practical importance at this stage.

5.5 Aeroacoustic Shape Design for Unsteady Trailing-Edge Flow

This section presents an unsteady aerodynamic noise reduction problem involving unsteady laminar trailing-edge flow (published in Rumpfkeil and Zingg [116, 119]). The airfoil geometry, which is a shortened version of the airfoil used in experiments by Blake [7], is shown in Figure 5.19. This geometry is very similar to the one used by Marsden *et al.* [82] in their noise minimization using a surrogate management framework. The thickness to chord ratio at one to ten is identical, and the leading and trailing edge geometry is duplicated as closely as possible. The free-stream Mach number is $M_\infty = 0.2$ with a Reynolds number of $\mathcal{R}e = 10,000$, and the angle of attack is $0°$.

Figure 5.19: Blake airfoil with the thickness constraint line (dashed). The fifteen B-spline control points which are used as design variables are shown as squares.

For unsteady laminar flow past an airfoil at low Mach number, the acoustic wavelength associated with the vortex shedding is typically long relative to the airfoil chord [82]. The noise generation from such an acoustically compact airfoil can be expressed using Curle's extension to the Lighthill theory [19], and a cost function $\mathcal{O}$, which is proportional to the total radiated acoustic power can be derived [84]:

$$\mathcal{O} = \overline{\left(\frac{\partial}{\partial t}\int_\mathcal{S} n_j p_{1j}(y,t)ds\right)^2} + \overline{\left(\frac{\partial}{\partial t}\int_\mathcal{S} n_j p_{2j}(y,t)ds\right)^2}. \tag{5.7}$$

Here p_{ij} is the compressive stress tensor, n_j are the normalized components of the outward normal to the airfoil surface $\mathcal{S}$, and y is the airfoil surface position vector. The overbar

denotes time-averaging over the chosen time interval, and repeated indices follow the usual Einstein summation convention. The radiation in this case is of dipole type, caused by the fluctuating lift and drag forces; see Wang *et al.* [147] for more details on airfoil self-noise due to vortex shedding.

The right half of the upper surface is allowed to deform in the optimization process and fifteen B-spline control points are used as shape design variables (see Figure 5.19). Since the cost of the adjoint approach is independent of the number of design variables, considerably more shape design variables are utilized than the five that Marsden *et al.* [82] could afford in their study using a surrogate management framework, thus giving the airfoil more freedom in the design space to take the most beneficial shape as given by the BFGS optimizer [13, 153]. However, Marsden's minimum thickness requirement is imposed here as well, which is given by a straight line connecting the left edge of the deformation region and the trailing edge, as shown in Figure 5.19, and is implemented via thickness constraints at the B-spline control point locations.

The algebraic grid movement algorithm is not capable of dealing with the occasional fairly large shape changes and therefore the quasi-linear elasticity mesh movement method [139, 140] with three increments is utilized instead. In order to solve the underlying two-dimensional unsteady compressible thin-layer Navier-Stokes equations, PROBE [111] with the BDF2 time-marching method is used on a C-mesh with 298×95 nodes, which is a good compromise between the accuracy of the flow solution and the computational effort required. Marsden *et al.* used a very similar non-dimensionalization to present their results as incorporated in PROBE. However, they used u_∞ instead of a_∞ as velocity scale. In order to convert the objective function value from PROBE's scaling to Marsden's scaling it must be divided by $(M_\infty)^6$, and PROBE's non-dimensionalized time must be multiplied by M_∞ to be comparable to Marsden's non-dimensionalized time. For the remainder of this section all the results are reported with Marsden's scaling for ease of comparison.

The laminar flow around the original Blake airfoil exhibits unsteady vortex shedding (see Figure 5.20), which leads to an oscillatory cost function, as shown in Figure 5.21 using a time step size of $\Delta t = 0.005$. The agreement between this cost function and the one shown in Marsden *et al.* [82] is reasonably good, even though the grid used here is about five times coarser.

In the actual optimization runs, the discrete version of the time-averaged cost function

Figure 5.20: Instantaneous pressure coefficient contours of the initial Blake airfoil.

Figure 5.21: Instantaneous (thin line) and time-averaged (thick line) cost function for the original Blake airfoil vs. time.

N_c	Δt_c	$N - N_c$	Δt	N	Adjustment interval	Control interval
300	0.01	1400	0.005	1700	$[0, 3]$	$[3, 10]$

Table 5.5: Time horizons for unsteady trailing-edge flow.

Figure 5.22: The initial airfoil shapes.

given by Eq. (5.7) is used once it is sufficiently converged and the chosen time horizons are displayed in Table 5.5. The optimization procedure is started from four different initial shapes, which are shown together with their objective function values (excluding the quadratic penalty for thickness constraint violation) in Figure 5.22:

1. The original Blake airfoil (in red)

2. The airfoil defined through the thickness constraint line (in green)

3. The airfoil that results from setting all fifteen design variables to their specified upper bounds (in blue)

4. The airfoil that results from setting all fifteen design variables to their specified lower bounds (in black)

The first three initial shapes do not violate the thickness constraint; however, the fourth one does.

The convergence histories of these aeroacoustic shape optimization problems are shown in Figure 5.23. The objective functions are always scaled with the initial objective function value of the original Blake airfoil ($J_0 = 1.33 \cdot 10^{-5}$) to make comparisons easier. One can see that all objective functions are driven to much smaller values in about two to ten design iterations, and the improvement after that is only marginal. Starting from the thickness constraint line leads to the best airfoil in terms of total radiated acoustic power. The gradient

Figure 5.23: Convergence histories of the aeroacoustic shape design problems using fifteen shape design variables.

norms are only reduced by one to two orders of magnitude, implying that the optimizer did not fully converge due to stalling of the line search algorithm. Nevertheless, the reduction in total radiated acoustic power is about 90 percent from the initial value, larger than the 80 percent achieved by Marsden *et al.* [82] using five design variables.

Figure 5.24 shows the final improved airfoil shapes together with their objective function values (this time with the quadratic penalty for thickness constraint violation included), which are interesting and unexpected. The increase in the trailing-edge angle to decrease the trailing-edge noise was also found by Marsden *et al.* and was theoretically predicted by Howe [60] for turbulent flow. However, the "wavy" part of the airfoil is to the best of the author's knowledge a novel result. Presumably Marsden *et al.* did not obtain similar "wavy"

Figure 5.24: Final improved airfoil shapes (solid) and initial airfoil shapes (dashed).

shapes due to the fact that they used only five design variables and thus did not give their optimizer enough freedom to come up with these novel shapes. This is partially confirmed in Figure 5.25 where the use of only six design variables with otherwise unchanged conditions leads to less wavy shapes and higher objective function values.

Figure 5.25: Final improved airfoil shapes (solid) and initial airfoil shapes (dashed) using only six shape design variables.

The four improved shapes using fifteen design variables lead to similar objective function values, indicating a relatively flat design space. It cannot be determined whether the four different shapes represent four distinct local minima, or we have been unable to fully converge to a unique minimum. The gradient has been reduced by one to two orders of magnitude, which is generally sufficient to indicate that the objective function is close to a minimum. The effect of the waviness is examined in Figure 5.26, where the best airfoil shape's objective function value is compared to another less wavy shape's objective function value. The second shape is a derivative of the best airfoil shape which preserves the steep trailing-edge angle and slimming of the airfoil while smoothing out the waviness. This result shows that the waviness is indeed improving the objective function value (in this case by more than a factor

of two). Reducing the Reynolds number to $5,000$ or Mach number to 0.175 leads to very similar shapes (not shown) implying that the presented results are not a special case for a particular set of operating conditions.

Figure 5.26: Best improved airfoil shape in comparison.

A comparison of the mean lift and drag coefficients for the initial and improved airfoils is displayed in Table 5.6. It is not necessary to add a lift constraint or a penalty for decreased lift to the objective function since the mean lift coefficients for all improved airfoils either stay about the same or increase in comparison to their initial values. The mean drag coefficients are decreased in all cases. This means the optimizer has not only produced aeroacoustically improved airfoils, but as a byproduct the initial airfoils have also been aerodynamically enhanced.

	Initial			Improved		
	$\bar{C}_L$	$\bar{C}_D$	$\bar{C}_L/\bar{C}_D$	$\bar{C}_L$	$\bar{C}_D$	$\bar{C}_L/\bar{C}_D$
Original Blake	0.284	0.076	3.75	0.284	0.049	5.79
Thickness line	0.265	0.054	4.95	0.283	0.049	5.77
Upper bound	0.134	0.119	1.12	0.285	0.049	5.82
Lower bound	0.305	0.055	5.57	0.282	0.049	5.75

Table 5.6: A comparison of the mean lift and drag coefficients for the initial and improved airfoils.

The time histories of C_L and C_D for the original Blake airfoil and the best airfoil after the optimization are shown in Figure 5.27. One can clearly see the unphysical adjusting period for the improved airfoil in the time interval $[0, 3]$ before it reaches its new somewhat

periodic steady state. A reduced mean drag as well as reduced oscillation amplitudes for the improved airfoil are also visible.

Figure 5.27: Time histories of C_L and C_D for the original Blake airfoil (dashed) and the best airfoil after optimization (solid) vs. time ($\Delta t = 0.005$).

An attempt was made to save computational time and storage by saving the flowfield in the control window only every second time step. However, in this case this approach does not work very well, since the optimizer is barely able to improve the initial airfoils even slightly with this inexact gradient information.

5.6 Remote Inverse Designs

The usual adjoint implementations for shape optimization calculate the gradient of a cost function which is computed from flow variables on the surface, for example of an airfoil, that is being modified. However, for many problems, such as inlet design, turbomachinery design

and airfoil-generated noise reduction, one wants to minimize an objective function using flow quantities that are not collocated at the points where the surface is being modified. This means one has to quantify the influence of geometric modifications on the flow variables at an arbitrary location, for example the near-field plane, within the domain of interest. This type of remote sensitivity calculation has been successfully used by Nadarajah *et al.* [91, 92, 95] for the steady case of sonic boom minimization. This section only focuses on controlling the near-field pressures of unsteady flows, which provide one of the inputs to a wave propagation program as discussed in Chapter 4. In particular, the remote inverse shape design of a single-element NACA 0012 airfoil at a high angle of attack in turbulent unsteady flow is presented in Section 5.6.1. Additionally, in Section 5.6.2 the remote inverse design of the multi-element NLR 7301 configuration [144] at a high angle of attack in laminar unsteady flow is addressed.

5.6.1 A Single-element Airfoil in Unsteady Turbulent 2D Flow

The first test case is a remote inverse shape design problem which involves turbulent unsteady flow over a single-element airfoil (published in Rumpfkeil and Zingg [115, 117]). The free-stream Mach number is 0.2 with a Reynolds number of 4×10^6, and the angle of attack is 20°. At these conditions the airfoil experiences vortex shedding. PROBE [111] with the one-equation Spalart-Allmaras turbulence model [131] and BDF2 as time-marching method is used to solve this unsteady turbulent flow problem. Only four shape design variables are used to keep the problem simple and to facilitate the comparison of the adjoint gradient with a finite-differenced one in order to validate the accuracy of the gradient calculation. The initial airfoil shape is the NACA 0012, and the four shape design variables are slightly perturbed to get a target airfoil shape, as shown in Figure 5.28.

Figure 5.28: The initial (red) and target (black) airfoil shapes.

The discrete cost function for a remote inverse design is given by

$$\mathcal{O} = \frac{1}{2}\Delta t \sum_{n=N_c+1}^{N} \sum_{NF} (p^n - p^{*n})^2, \tag{5.8}$$

where p^n is the near-field pressure obtained from the current airfoil, and p^{*n} is the target near-field pressure obtained from the target airfoil (both at time step n). The sum over NF implies a sum over all points that define the near-field plane. The choice for the near-field plane in this case is shown in Figure 5.29, and the required pressures are simply obtained on the grid nodes.

Figure 5.29: The mesh where the near-field plane is shown in black.

In Figure 5.30 the drag coefficients for the initial and target airfoil shapes are shown over time using a time step of $\Delta t = 0.05$. Both flow solves are warmstarted from a NACA 0012 periodic steady state solution; thus one can see an adjustment period for the target airfoil and the time horizons used in the remote inverse shape design are shown in Table 5.7.

The convergence history of this remote inverse shape design problem with the adjoint approach in comparison to a second-order central finite-difference approach with a step size

Figure 5.30: Drag coefficients for the initial and target airfoil shape ($\Delta t = 0.05$).

N_c	Δt_c	$N - N_c$	Δt	N	Adjustment interval	Control interval
300	0.1	200	0.05	500	$[0, 30]$	$[30, 40]$

Table 5.7: Time horizons for the single-element airfoil remote inverse shape design.

of $h = 10^{-7}$ is shown in Figure 5.31. The objective function is always scaled such that its initial value is unity. One can see that the objective function is driven to a small value in about twenty-six design iterations and that the two approaches show a reasonable agreement, which means that the adjoint approach for the gradient calculation is accurate. One can try to save computational time and storage by saving the flowfield in the adjusting period and in the control window only every fourth time step, leading to only $500/4 = 125$ matrix inversions for the solution of the adjoint equations. The result is also shown in Figure 5.31. The gradients and objective function values are in reasonable agreement with the original adjoint and finite-difference approach, thus leading to a similar convergence history while saving 75 percent of computational resources in the adjoint calculation.

Figure 5.31: Convergence histories of the remote inverse shape design problem with four design variables.

5.6.2 A Multi-element Airfoil in Unsteady Laminar 2D Flow

The remote inverse design problem in laminar unsteady flow over a multi-element airfoil, the NLR 7301 configuration [144], is the second test case (published in Rumpfkeil and Zingg [117, 120]). The free-stream Mach number is 0.2 with a Reynolds number of 800, and the angle of attack is again 20°. TORNADO [102] with BDF2 is used to solve the underlying 2D unsteady laminar Navier-Stokes equations. Three cases, two with two design variables each and one with four design variables, are considered, and the shapes are displayed in Figure 5.32:

1. The initial airfoil is the NLR 7301, and two shape design variables of the main element are slightly perturbed to get a target airfoil.

2. The initial airfoil is the NLR 7301, and the horizontal and vertical translation design variables are slightly perturbed.

3. The initial airfoil is the NLR 7301, and two shape design variables of the main element as well as the horizontal and vertical translation design variables are slightly perturbed.

1. Two shape design variables

2. Two translational design variables

3. Two shape and two translational design variables

Figure 5.32: The initial (red) and target (black) airfoils for the three test cases.

a) Square near-field plane

b) Rectangular near-field plane

Figure 5.33: The grid with the two near-field planes shown in black.

Two different choices for the near-field plane are considered, as shown in Figure 5.33, in order to judge the robustness of the remote inverse shape design with the distance of the near-field plane to the airfoil:

a) The near-field plane is a square that extends from -3 to 3 with a uniform spacing of 0.05 between points in both x- and y-directions.

b) The near-field plane is a rectangle that extends from -1 to 2 in the x-direction and from -1 to 1 in the y-direction with a uniform spacing of 0.05 between points in both directions.

The pressures (see Figure 5.34) at the points of the near-field plane are calculated using biquadratic interpolation involving the closest nodes of the grid to the point in question.

Figure 5.34: Instantaneous pressure coefficient contours of the initial NLR 7301 configuration with the rectangular near-field plane.

Figure 5.35 shows the drag coefficients for the initial and target airfoils for case 1 over time using a time step of $\Delta t = 0.1$. The chosen time horizons for the remote inverse shape design

are summarized in Table 5.8. Since the focus of this section is to show the feasibility of an unsteady remote inverse design, no grid convergence studies are performed and the relatively large time steps and the relatively coarse grid with about $31,000$ nodes are satisfactory.

Figure 5.35: Drag coefficient for the initial and target airfoils for case 1 ($\Delta t = 0.1$).

N_c	Δt_c	$N - N_c$	Δt	N	Adjustment interval	Control interval
200	0.2	300	0.1	500	$[0, 40]$	$[40, 70]$

Table 5.8: Time horizons for the multi-element remote inverse shape design.

The convergence histories of these remote inverse design problems with the adjoint approach in comparison to a second-order central finite-difference approach with a step size of $h = 10^{-7}$ are shown in Figure 5.36 for case 1, in Figure 5.37 for case 2 and in Figure 5.38 for the third case. The objective function given by Eq. (5.8) is again always scaled such that its initial value is unity. One can see that the two approaches show reasonable agreement, which implies that the adjoint approach for the gradient calculation is accurate. The figures also show that the distance of the near-field plane to the airfoil has not too much influence on the two approaches in terms of optimization iterations required to converge.

Figure 5.36: Convergence histories of the remote inverse design problem with two shape design variables.

Figure 5.37: Convergence histories of the remote inverse design problem with two translational design variables (note the log scale on all axes).

Figure 5.38: Convergence histories of the remote inverse design problem with two shape and two translational design variables (note the log scale on both axes for case 3a).

Once again, one can try to save computational time and storage by saving the flowfield in the adjusting period and in the control window only every fourth and even only every tenth time step, leading to only $500/4 = 125$ and $500/10 = 50$ linear solves for the solution of the adjoint equations, respectively. The result for the first case is shown in Figure 5.36, and the gradients and objective function values are in reasonable agreement with the original adjoint and finite-difference approach, thus leading to a somewhat similar convergence history while saving considerable computational resources.

Trying the same approach for the second case, namely saving the flowfield only every fourth and tenth time step, shows a different result (see Figure 5.37). This time the optimizer fails to converge if it uses only the information from every tenth time step. However, the information from every fourth time step is still sufficient to converge in a similar manner as the original adjoint. The flowfield is also saved only every fifth time step and one can see that this approach still works, although it comes with a huge increase in optimization iterations for the case 2a.

The third case shows yet another behaviour, as displayed in Figure 5.38. This time the optimizer fails to converge if it uses the information from every tenth and every fifth time step, but the information from every fourth time step is still sufficient to converge in a somewhat similar manner as the original adjoint.

5.7 Remote Inverse Design Using Hybrid URANS/FW-H

This section, unlike the previous section which controlled the near-field pressures, focuses on controlling the far-field pressures in an unsteady flow environment. This is also the first section in which the hybrid URANS/FW-H optimization algorithm is validated. Furthermore, the fourth-order ESDIRK scheme is used as time-marching method in addition to BDF2. Several remote inverse shape design problems with a discrete cost function given by

$$\mathcal{O} = \frac{1}{2}\Delta t \sum_{n=N_c+1}^{N} (p_{obs}^n - p_{obs}^{*n})^2, \tag{5.9}$$

are presented. Here, p_{obs}^n is the pressure at some far-field observer location at time step n obtained from a current airfoil shape, and p_{obs}^{*n} is the target pressure at the same observer location and time step obtained from the target airfoil shape. The target shape is given

through a perturbation in four shape design variables of the initial NACA 0012 airfoil and both shapes are shown in Figure 5.39. Once again, only four design variables are used to be able to compare the adjoint gradient with a finite-differenced one.

Figure 5.39: The initial (red) and target (black) airfoil shapes.

The unsteady flow conditions for this test case are exactly the same as the ones used in the validation of the acoustic propagation code in Subsection 4.3.3, namely a Reynolds number of 800, a free-stream Mach number of 0.2, and an angle of attack of 20°. However, a coarser mesh with only about 35,000 nodes is used to reduce the computational costs. Nonetheless, as displayed in Figure 5.40, the comparisons of pressure fluctuations calculated by CFD and FW-H for the initial NACA 0012 show a good agreement at a point about two chord lengths below the trailing edge for both time-marching methods.

Figure 5.41 shows the drag coefficients for the initial and target airfoils over time using a time step of $\Delta t = 0.05$ for BDF2 and $\Delta t = 0.5$ for ESDIRK4. One can see the adjustment period for the target airfoil. In order to reduce the computational costs in the actual optimization runs, a bigger time step of $\Delta t_c = 0.1$ is utilized for the first $N_c = 200$ steps with BDF2, and $\Delta t_c = 0.5$ for the first $N_c = 40$ steps is used with ESDIRK4. Once the domain where the pressures are compared is reached, a smaller time step $\Delta t = 0.05$ is used for another 1200 steps ($\Delta t = 0.5$ for 120 steps with ESDIRK4), leading to $N = 1400$ ($N = 160$ with ESDIRK4) time steps in total for each flow solve covering a time interval of $[0, 80]$. These time horizons are summarized in Table 5.9 and the corresponding adjoint equations for this situation are given in Appendices D and E for the BDF2 and ESDIRK4 time-marching method, respectively. For details on how to calculate the required derivative of the far-field pressure fluctuations with respect to the flow variables, see Appendix F.

	N_c	Δt_c	$N - N_c$	Δt	N	Adjustment interval	Control interval
BDF2	200	0.1	1200	0.05	1400	$[0, 20]$	$[20, 80]$
ESDIRK4	40	0.5	120	0.5	160	$[0, 20]$	$[20, 80]$

Table 5.9: Time horizons for hybrid URANS/FW-H remote inverse shape design.

Figure 5.40: Comparison of pressure fluctuations of the initial airfoil calculated by CFD (solid) and FW-H (dashed) about $2c$ below the trailing edge.

Figure 5.41: Drag coefficients for the initial and target airfoil shapes.

Figure 5.42: Convergence histories of remote inverse shape design problems using the hybrid URANS/FW-H algorithm with four design variables and two time-marching methods.

The convergence histories of some remote inverse shape design problems using the hybrid URANS/FW-H optimization algorithm are presented in Figure 5.42. The objective function is always scaled such that its initial value for either time-marching method is unity. The adjoint approach is compared to a second-order central finite-difference approach with a step size of 10^{-7} for a location that is about two chord lengths below the trailing edge. One can see that the objective functions are driven to small values in about forty to fifty design iterations, and that the two approaches show a reasonable agreement for both time-marching methods, which demonstrates that the adjoint approach for the gradient calculation is accurate. In particular, the gradient at the first design iteration with BDF2 using the finite-difference method (fd) yields

$$\left(\frac{\partial \mathcal{J}}{\partial Y}\right)_{fd} = (-52.83, \, -160.56, \, -56.68, \, -36.43),$$

which is in reasonable agreement with the gradient calculated via the adjoint method (*ad*):

$$\left(\frac{\partial \mathcal{J}}{\partial Y}\right)_{ad} = (-48.09, -162.26, -55.78, -36.68).$$

Using ESDIRK4, the same gradients are given by

$$\left(\frac{\partial \mathcal{J}}{\partial Y}\right)_{fd} = (-53.11, -164.44, -58.90, -37.60),$$

and

$$\left(\frac{\partial \mathcal{J}}{\partial Y}\right)_{ad} = (-48.37, -166.64, -57.89, -37.76).$$

The finite-difference approach for ESDIRK4 (dashed black line) does not fully converge, and the scaled objective function value stalls at about 10^{-8}. The reason for this is an inaccurate gradient due to error cancellation for such small values of the objective function in combination with the more involved time-marching method. The convergence history for a location eighty chord lengths below the leading edge using only the adjoint approach but both time-marching methods is shown in the same figure as well.

The results presented in this section prove that it is possible to recover far-field pressure fluctuations via a remote inverse shape design in an unsteady laminar flow. Further applications and validations of the hybrid URANS/FW-H optimization algorithm are presented in the following sections.

5.8 Turbulent Blunt Trailing Edge Flow

The shape of a NACA 0012 airfoil with a $0.03c$ thick blunt trailing edge in a turbulent flow is optimized in this section (the BDF2 results presented here are also published in Rumpfkeil and Zingg [118]). The free-stream flow conditions are given by $M_\infty = 0.2$, $Re = 2 \times 10^6$, $\alpha = 0°$, and the mesh consists of about $36,000$ nodes. First a remote inverse shape design problem is solved with the objective function given by Eq. (5.9) and a far-field observer located $40c$ below the leading edge. BDF2 and ESDIRK4 are again employed as time-marching methods, and only two shape design variables are used to enable a comparison between the adjoint gradient with a finite-differenced one and to thus validate the hybrid URANS/FW-H optimization algorithm for turbulent flows. The initial and target airfoil shapes are shown in Figure 5.43.

Figure 5.43: The initial (red) and target (black) airfoil shapes.

Figure 5.44: Comparison of pressure fluctuations calculated by CFD (solid) and FW-H (dashed) about $\frac{1}{3}c$ below the trailing edge of the initial airfoil for two time-marching methods.

The comparisons of pressure fluctuations calculated by CFD and FW-H in a location about $\frac{1}{3}c$ below the trailing edge of the initial airfoil are displayed in Figure 5.44 and show good agreement for both time-marching methods. Figure 5.45 shows the drag coefficients for the initial and target airfoil over time using a time step of $\Delta t = 0.005$ for BDF2 and $\Delta t = 0.025$ for ESDIRK4. Note that the target solution has not yet reached a periodic steady state, however, the computational cost are too high to cover the required time interval. The time horizons used in the remote inverse shape design for turbulent blunt trailing edge flow are shown in Table 5.10. The chosen time step sizes lead to the same computational effort for a flow or adjoint solution for the two time-marching methods, since the computational cost for one time step using ESDIRK4 is roughly five times more expensive than using BDF2.

Figure 5.45: Drag coefficients for the initial and target airfoil shapes.

	N_c	Δt_c	$N - N_c$	Δt	N	Adjustment interval	Control interval
BDF2	300	0.01	700	0.005	1000	$[0, 3]$	$[3, 6.5]$
ESDIRK4	60	0.05	140	0.025	200	$[0, 3]$	$[3, 6.5]$

Table 5.10: Time horizons for turbulent blunt trailing edge flow.

The convergence history of the remote inverse shape design problem for a turbulent blunt trailing edge flow using the hybrid URANS/FW-H optimization algorithm is presented in Figure 5.46. The objective function is again always scaled such that its initial value for either time-marching method is unity. The adjoint approach in comparison to a second-order central finite-difference approach with a step size of 10^{-5} is shown. One can see that the objective functions are driven to small values in about ten design iterations and that the two approaches show a reasonable agreement for both time-marching methods, which implies that the adjoint approach for the gradient calculation is accurate.

In particular, the gradient at the first design iteration using the finite-difference method

Figure 5.46: Convergence history of the remote inverse shape design problem with two design variables.

(fd) yields

$$\left(\frac{\partial \mathcal{J}}{\partial Y}\right)_{fd} = (-33.53,\, 34.18),$$

which is in good agreement with the gradient calculated via the adjoint method (ad):

$$\left(\frac{\partial \mathcal{J}}{\partial Y}\right)_{ad} = (-34.36,\, 35.11).$$

Similarly, the finite-difference approach for ESDIRK4 at the first design iteration leads to

$$\left(\frac{\partial \mathcal{J}}{\partial Y}\right)_{fd} = (-33.71,\, 34.74),$$

which can be compared to the adjoint gradient:

$$\left(\frac{\partial \mathcal{J}}{\partial Y}\right)_{ad} = (-34.29,\, 35.14).$$

Both approaches for ESDIRK4 do not fully converge and the scaled objective function values stall at about 10^{-10}. The reason is again an inaccurate gradient due to error cancellation

for such small values of the objective function in combination with the more complicated time-marching method.

After the validation of the hybrid URANS/FW-H optimization algorithm for turbulent flows using two time-marching methods, more practically relevant optimizations with two different objective functions are considered:

1. Mean drag minimization
$$\mathcal{J}_{\mathcal{D}} = \bar{C}_D = \frac{1}{N - N_c} \sum_{n=N_c+1}^{N} C_D^n \qquad (5.10)$$

2. Pressure fluctuation (noise) minimization
$$\mathcal{J}_{\mathcal{N}} = \sum_{n=N_c+1}^{N} (p_{obs}^n - \bar{p}_{obs})^2 = \sum_{n=N_c+1}^{N} (p_{obs}'^n)^2 \quad (5.11)$$

where $\bar{p}_{obs}$ is the mean pressure at the observer location, which is located $40c$ below the leading edge, and $p_{obs}'^n = p_{obs}^n - \bar{p}_{obs}$ is the pressure fluctuation in the observer location at time step n.

Figure 5.47: Initial shapes of the turbulent blunt trailing edge flow optimizations.

Eight B-spline control points are used as shape design variables which are all located in the aft 15 percent of the chord length (four on the upper and four on the lower surface). The unsteady shape optimizations are started from three different initial shapes, which are shown in Figure 5.47 together with their initial objective function values:

1. The initial airfoil (in red)

2. The airfoil that results from setting all eight design variables to their specified upper bounds (in blue)

3. The airfoil that results from setting all eight design variables to their specified lower bounds (in black)

Only the BDF2 time-marching method is used here and the time horizons are the same as given in Table 5.10 earlier in this section. Figure 5.48 presents the final optimized airfoil shapes of the turbulent blunt trailing edge flow optimizations together with their objective function values. All three initial shapes converge for each objective function to the same respective final shapes shown in blue and black for the mean drag and noise minimizations, respectively. As indicated in the figure, the mean drag value of the noise minimized airfoils is slightly higher than the mean drag value of the mean drag minimized airfoils and conversely, the pressure fluctuations of the mean drag minimized airfoils are a factor of two higher than the ones from the noise minimized airfoils. This shows that noise and drag improvements lead to qualitatively similar results to a first approximation, but they definitely do not yield the same optimized shapes.

Figure 5.48: Final improved airfoil shapes of the turbulent blunt trailing edge flow optimizations.

The convergence histories of the mean drag minimizations are displayed in Figure 5.49. The objective function values are always scaled with the mean drag value of the original airfoil, $J_D = 2.14 \cdot 10^{-2}$, to make comparisons easier. Since all three initial shapes converge to the same final optimized shape, they have the same objective function value, which translates into a reduction in mean drag of about 39 percent from the original airfoil. The objective function value is mostly reduced in the first few iterations, and the improvements after that are only marginal. The gradient norms are reduced by three to four orders of magnitude indicating that the optimizer has converged to a minimum in each case.

The convergence histories of the noise minimizations in Figure 5.50 show that this objective function is mainly reduced in the first five iterations and that the gradient norms

Figure 5.49: Convergence histories of the mean drag minimizations for turbulent blunt trailing edge flow.

Figure 5.50: Convergence histories of the noise minimizations for turbulent blunt trailing edge flow.

are reduced by two to three orders of magnitude. The sum of the pressure fluctuations for the optimized shape is reduced to 0.23 percent of the initial value of the original airfoil $J_N = 5.43 \cdot 10^{-7}$, which is again used to scale the objective function values to ease comparisons. Starting from the lower bound leads to a failed line search in the first iteration because all gradients indicate that it would be beneficial to "slim" the airfoil even more, which is not permitted by the box constraints imposed on the design variables to avoid grid movement and flow convergence problems.

Figure 5.51: Time histories of C_L and C_D before and after the optimizations vs. time.

The time histories of C_L and C_D for the original blunt trailing edge airfoil before and after the optimizations are shown in Figure 5.51 using a time step of $\Delta t = 0.005$. One can clearly see the adjusting period for the improved airfoils in the time interval $[0, 3]$ before they reach their new somewhat periodic steady state. A reduced mean drag and constant mean lift for both optimized airfoils is also visible, and both objective functions lead to reduced oscillation amplitudes in both lift and drag.

The hybrid URANS/FW-H optimization algorithm also works well in a turbulent flow environment, as shown by the results in this section. Finally, the last section of this chapter will address the attempt to change the shape of a high-lift airfoil to minimize the radiated noise while maintaining good flight performance.

5.9 High-lift Noise Optimization

It is experimentally well established that high-lift devices are significant contributors to airframe-generated noise in the mid- to high-frequency range [21, 27, 28, 51, 86]. In particular, the leading-edge slat and side edges of the flaps have been identified as dominant noise sources [71]. In this section, BDF2 is the time-marching method of choice and a three-element airfoil configuration, denoted as 30P30N [142, 143] and shown in Figure 5.52, is the starting point for the unsteady design optimization process.

Figure 5.52: The 30P30N high-lift airfoil configuration (red) with the FW-H integration surface (black dashed).

The deflections of both the slat and flap are set at 30°, hence the name 30P30N. The free-stream flow conditions under consideration are given by $M_\infty = 0.2$, $Re = 7.2 \times 10^6$ and $\alpha = 8°$ which are typical approach conditions. The mesh consists of about $100,000$ nodes. The comparison of pressure fluctuations calculated by CFD and FW-H for a location about $\frac{1}{4}c$ below the slat trailing edge in Figure 5.53 show a good agreement.

The flow is assumed to be fully turbulent except in the slat cove region where it is assumed to be quasi-laminar to eliminate excessive diffusive effects of the turbulence model on the resolved unsteady flow structures [70, 71]. Accordingly, the production term in the

Figure 5.53: Comparison of pressure fluctuations calculated by CFD (solid) and FW-H (dashed) about $\frac{1}{4}c$ below the slat trailing edge.

turbulence transport equation given by Eq. (2.27) is switched off in a limited zone that encloses the cove area. The removal of the excess damping allows the shear layer to set up large-scale disturbances that are self-excited.

The physical justification for this quasi-laminar assumption in the slat cove flow field is given in detail by Khorrami *et al.* [71], but it is basically based on two observations: Firstly, the slat boundary layer flow between the leading edge stagnation point and cusp is rapidly accelerated and is extremely thin because of a strong favorable pressure gradient and the short distance. Thus, it is basically laminar even up to flight Reynolds numbers. Secondly, the velocities in the recirculating zone of the slat cove area are relatively small leading to correspondingly small Reynolds numbers. As in the case of a shallow cavity most of the large scale structures become trapped in this zone, leading to an unsteady recirculating flow field which is again more or less laminar.

However, the quasi-laminar approach in the slat cove region in two-dimensional simula-

tion produces large-scale vortical structures within the slat cove region that are excessively energetic. This excess energy is caused by the absence of 3-D effects which would trigger the onset of secondary instabilities of the spanwise rollers and convert spanwise vorticity into streamwise vorticity [15]. Nonetheless, Khorrami *et al.* [70] believe that two-dimensional simulations still provide sufficient insight into the most important physical effects.

Only two design variables are used in the optimization, namely the horizontal and vertical translations which control the position of the slat. In order to get an insight into the required time horizon for this flow problem the two design variables are slightly perturbed to get a different slat position as shown in Figure 5.54.

Figure 5.54: The original 30P30N slat position (red) and a perturbed position (black).

Figure 5.55 shows the drag coefficients for the original 30P30N slat position as well as the perturbed position over time using a time step of $\Delta t = 0.005$. One can see that even the small movement of the slat leads to big changes in the drag fluctuations, and the mean drag is also about two percent higher for the perturbed position of the slat.

In the following it is attempted to minimize the far-field pressure fluctuations at an observer location $40c$ below the slat trailing edge by using the objective function given by Eq. (5.11). In the actual optimization runs the adjusting period visible in Figure 5.55 is "jumped" over with a time step of $\Delta t_c = 0.007$ for the first $N_c = 300$ steps. Once the time domain where the far-field pressure fluctuations are calculated is reached, the same time step for another 500 steps is used, leading to $N = 800$ time steps in total for each flow solve covering a time interval of $[0, 5.6]$. Unfortunately, the high sensitivity of the flow field to even the smallest movements of the slat leads to highly inaccurate gradients if calculated using a finite-difference approach as shown in Figure 5.56 for the first design iteration.

Figure 5.55: Drag coefficients for the original 30P30N slat position (red) and perturbed position (black) vs. time ($\Delta t = 0.005$).

Figure 5.56: The sensitivity of the gradient components to the step size of the finite-difference approximation for the first design iteration.

However, the finite-difference part of the adjoint approach is by far not as sensitive to step size changes as can be inferred from the same figure, and since the accuracy of the adjoint gradient has been validated in the previous sections it is assumed that the adjoint gradient is correct. Several optimization runs from various slat positions as starting points were conducted, and the resulting design space of the slat movement is displayed in Figure 5.57. The gradients at the different design points are represented by arrows, and the objective function values are given by a colour scale, with red representing the highest and blue the lowest values. The objective function values are always scaled with the sum of the pressure fluctuations of the original airfoil configuration $J_N = 9.60 \cdot 10^{-8}$ to make comparisons easier.

Figure 5.57: The design space of the slat movement and a zoom into the most interesting region.

As can be seen in the figure, the design space is very noisy and the gradient values are not greatly decreased. Nonetheless, the optimizer managed to reduce the objective function value in one of the runs by almost forty percent given by the slat position $(0.02137, 0.00408)$.

In conclusion, a much higher mesh density is most likely required for this case in order to make the flow solver much more accurate, and thus to hopefully reduce the high sensitivity of the finite-difference approach, which is one of the manifestations of the noisy design space. Khorrami and Lockard [70], for example, used for similar flow conditions and a similar three-element airfoil configuration 1.318 million grid points of which about sixty percent were clustered in the vicinity of the slat. Unfortunately, the $100,000$ nodes used here are already pushing the limits of the serial code since one function and gradient evaluation already takes about a day. Also, a hybrid URANS/LES or detached-eddy simulation (DES) [132] approach is much better suited for acoustic predictions and should be the preferred method of choice for such complicated flow problems. The results presented in this last section should be viewed as a proof of concept rather than solid facts, and a lot of future work has to be done by the CFD community and especially computer engineers before this particular optimization problem can be tackled in a meaningful way.

Chapter 6

CONTRIBUTIONS, CONCLUSIONS AND RECOMMENDATIONS

Contributions

As mentioned in Section 1.3 of the Introduction, the objectives of this thesis are two-fold and have both been accomplished. The contributions of this thesis can be summarized as follows:

1. A general framework has been developed to derive a discrete adjoint method for the optimal control of unsteady flows for any time and space discretization scheme, as described in Chapter 3. This framework also applies to remote designs as presented in Sections 5.6 to 5.9 and other approaches of simulating turbulence such as Large Eddy Simulations (LES) or Detached-Eddy Simulations (DES) [132]. It also allows the use of higher-order multi-stage time-marching methods (see Section 2.3 and Appendix E). Furthermore, more complicated grid movement algorithms [139, 140] can be incorporated via residual equations and additional Lagrange multipliers as well.

2. The general framework has been applied to several problems of interest including shock-tubes, pulses in converging-diverging nozzles, rotating cylinders, transonic buffeting, unsteady trailing-edge flow, and remote inverse shape designs of single- and multi-element airfoils (Sections 5.1 to 5.6). This large number of test cases allowed for a thorough validation of the framework.

3. The adjoint equations for a novel hybrid URANS/FW-H optimization algorithm have been derived (see Appendix F), and the accuracy of the adjoint gradients has been validated using remote inverse shape designs involving unsteady laminar flow in Section 5.7 and unsteady turbulent flow in Section 5.8.

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4. The novel hybrid URANS/FW-H optimization algorithm has been applied to airframe-generated noise reduction problems for a single-element blunt trailing edge airfoil in Section 5.8 and for a three-element airfoil configuration in Section 5.9.

Conclusions

Based on the results presented at the end of Chapter 4 and in Chapter 5 the following major conclusions can be drawn:

- The gradients computed using the discrete unsteady adjoint equations derived via the developed framework show good accuracy in comparison to second-order central finite-differenced gradients for a variety of two-dimensional results. Additionally, as mentioned in Sections 5.1 and 5.2, the adjoint gradients are in excellent agreement with the ones computed via the complex-step method [133] (ten digits) for the investigated one-dimensional problems.

- The developed general framework allows the use of more sophisticated, higher-order time-marching methods, since it is straightforward to derive the corresponding adjoint equations for them, as demonstrated for ESDIRK4 in Appendix E.

- The extension to unsteady turbulent flows of the two-dimensional turbulent Newton-Krylov based group codes PROBE and TORNADO maintained the efficiency of the steady flow solvers which can be inferred from the fact that only very few outer iterations with few inner iterations per outer iteration are required to converge.

- It takes about two to three times the computational time of an unsteady flow solution to calculate the corresponding gradient, due to a bad initial guess for the linear unsteady adjoint problem. The nonlinear unsteady flow solve problem on the other hand has a very good initial guess by using the flow solutions from the previous time steps, altogether leading to fewer linear iterations per time step. Nonetheless, the overall unsteady optimization algorithm utilizing a Newton-Krylov approach is very robust and fast. This made the presentation of a large number of very diverse test cases in this thesis possible.

- Some of the investigated problems produced novel and counterintuitive results, such as the wavy airfoils in Section 5.5 and the bulge close to the blunt trailing edge in Section 5.8.

- The comparisons of pressure fluctuations calculated by CFD and FW-H for different airfoils, flow conditions, and mesh densities show good agreement at locations which are reasonably close to the airfoil where the mesh spacing is still fine enough to give an accurate CFD solution. This establishes confidence in the ability of FW-H to predict far-field pressure fluctuations.

- The novel hybrid URANS/FW-H optimization algorithm developed for this thesis shows great potential to aid in reducing airframe-generated noise.

Other observations that can be made include:

- An absolute convergence tolerance for the unsteady flow residual $\mathcal{R}^n$ of 10^{-10} is a good balance between avoiding error propagation in the flow solution Q^n and spending too much computational time.

- The residual for the inexact linear solve, which results from applying Newton's method to the unsteady nonlinear flow equations, is reduced by two to three orders of magnitude for turbulent flows, whereas for laminar flows one order of magnitude is sufficient.

- The Spalart-Allmaras turbulence model works reasonably well for unsteady turbulent flows for most of the investigated cases, as also discussed in Rumsey *et al.* [121]. However, for the three-element airfoil configuration in Section 5.9 it shows excessive diffusive effects which could only be overcome by switching off the production term in the slat cove region. In general, none of the available turbulence models are tuned for unsteady flows, which can pose problems, as pointed out by Tucker [141].

- ESDIRK4 does not save computational time in comparison to BDF2 for the fairly coarse time steps used in this work. In addition, it can even lead to convergence problems since one has to use an approximately five times larger time step size in order to not have to pay a penalty in computational time.

- The linear systems in the adjoint equations are solved with an absolute convergence tolerance of 10^{-6}, which is equivalent to a relative convergence tolerance of 10^{-10} to 10^{-13} for most problems considered. This is again a good balance between avoiding error propagation and spending too much computational time.

- Bi-CGSTAB solves the unsteady adjoint equations up to fifty percent faster than GMRES. However, for a steady-state adjoint problem or the linear problem in the unsteady flow solve, Bi-CGSTAB does not work as well and thus GMRES is used instead.

- Marching with a bigger time step over unphysical adjusting periods as well as recording the flow solution only, for example, every fourth time step works well in practice for the simpler flow problems, thus resulting in significant savings in both memory and computational time for simple unsteady optimization problems.

- Convergence to only local minima is a well-known limitation of gradient-based methods. Attempts were made to verify the uniqueness of minima by starting from different initial shapes, which worked in the case of the turbulent blunt trailing edge flow in Section 5.8, but also showed the existence of several local minima in the rotating cylinder case in Section 5.3.

- The quadratic penalty formulation which is used to impose airfoil thickness constraints that prevent the occurrence of infeasible or undesired shapes performed well. This is most likely due to the fact that the number of constraints considered is relatively small.

- The gradient norm is usually reduced by several orders of magnitude. However, very noisy design spaces were encountered as well (e.g. the rotating cylinder, the laminar trailing-edge flow, and above all the high-lift noise reduction problem) where the gradient norms were hardly reduced, even though the objective function value was considerably improved.

- The algebraic mesh movement algorithm works well for most cases considered, but even the quasi-linear elasticity mesh movement method [139, 140] is computationally not too expensive for two-dimensional problems.

Recommendations

The conclusions drawn above immediately suggest a number of future research directions:

- Improvements to the flow solver

  - Matrix or CUSP dissipation [100], higher-order space discretizations [23], and the ability to predict boundary-layer transitions [29] would improve the accuracy of the flow solver and consequently, the accuracy of the optimization.

  - It would be desirable to be able to use a pressure switch for transonic flow optimization problems. However, the differentiation of the current pressure switch, Eqs. (2.32), is not well defined, since it contains a combination of discontinuous functions. It would also increase the bandwidth of the flow Jacobian. A different strategy to deal with shocks is probably required in order to improve the accuracy of the optimization.

  - For a more thorough investigation of the transonic buffeting case presented in Section 5.4 it is essential to improve the stability of the flow solver to avoid flow convergence problems after shape changes have taken place.

  - There is a dire need for turbulence models which are better suited for unsteady flows than the current ones.

  - It is necessary to have a parallelized code to allow the use of higher mesh densities, in particular for the three-element airfoil configuration investigated in Section 5.9.

  - A nonlinear frequency domain approach [93, 94, 136] can considerably reduce the computational cost for unsteady problems with dominant periodic behavior.

  - An extension to three dimensions in space [54, 85] is definitely required to simulate noise problems in an accurate and physically meaningful way since all significant acoustic phenomena are inherently three-dimensional [125].

  - Hybrid URANS/LES or DES approaches are better suited than URANS to simulate flows involving flow separation or for acoustic predictions.

- Improvements to the adjoint solver

  – An improved initial guess for the solution of the linear adjoint systems could decrease the computational effort greatly. Constant and linear extrapolations from previous solutions as well as simply using zero as the initial guess were all tried and resulted in a similar number of iterations to converge the residual to a pre-specified convergence tolerance.

  – In the debate about continuous versus discrete adjoint sensitivity analysis (see Appendix A), one of the big questions is whether a lower order model for the continuous adjoint approach could yield accurate enough gradients for optimization (e.g. use LES in the forward model and URANS with somehow averaged turbulent quantities in the adjoint model [61]).

- The use of more sophisticated optimizers, such as Sequential Quadratic Programming (SQP) methods [44], could decrease the number of objective function and gradient evaluations required for convergence and provide a more efficient treatment of constraints.

- Algorithms based on Newton-Krylov methods are promising for multidisciplinary optimization problems, such as aero-structural optimizations, since they are very robust and fast.

- Multipoint optimizations with several on- and off-design points are very important in a practical context [154] and should be considered for unsteady optimization problems.

- There are many more applications of interest for unsteady optimization algorithms

  – Active flow control through suction and blowing

  – Turbomachinery blades and helicopter rotors

  – Sonic boom (which can be treated as a steady problem, however, the use of remote sensitivities is still required)

- The adjoint variables are also very useful for error estimation and guidance for grid refinement [98, 99, 105].

All these future research directions could reinforce the role of CFD in the overall design process of future aircraft or for other applications such as automobiles.

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APPENDICES

Appendix A

THE DISCRETE AND CONTINUOUS ADJOINT APPROACHES

The difference between the discrete and continuous adjoint approaches is shown schematically in Figure A.1. The goal of both approaches is to derive a set of discretized adjoint equations which are suitable for a computer code. In the fully-discrete approach one starts by discretizing the nonlinear Partial Differential Equations (PDE's), and afterwards these equations are linearized and transposed. In the continuous adjoint approach, on the other hand, the PDE's are first linearized and then the adjoint problem is formed and discretized. One could even use an in-between approach by linearizing the original equations, discretizing them and then taking the transpose.

Figure A.1: Alternative approaches to forming discretized adjoint equations.

In principle, all three approaches should be consistent and converge to the correct analytic value for the gradient of the objective function $\frac{\partial \mathcal{J}}{\partial Y}$ in the limit of infinite grid and time resolutions and in the absence of shocks. However, for finite grids and time step sizes there will be a discrepancy in the computed results, and since there are important conceptual differences

between the different approaches, they all have important assets and drawbacks [43].
The advantages of the fully-discrete approach are

a) The exact gradient of the discrete objective function is obtained, which means that the optimization process can fully converge. It also implies that it is relatively easy to verify the programming implementation. In comparison, using the continuous approach one does not know whether a convergence failure is a consequence of the inexact gradient or a possible programming error.

b) The creation of the adjoint program is conceptually straightforward. In particular, the same iterative solution method that is used for the original linear matrix is also guaranteed to converge for the transposed matrix since they both have the same eigenvalues.

c) Automatic Differentiation can be used to substantially ease the development of the adjoint CFD code.

On the other hand, the advantages of the continuous approach are

a) The physical significance of the adjoint variables and the role of the adjoint boundary conditions are much more apparent. This better understanding of the nature of the adjoint solutions is especially advantageous when approaching more difficult problems, e.g. problems with shocks.

b) The adjoint program can be less complicated and require less memory than the fully-discrete code since one can discretize the adjoint PDE in any consistent way, which includes lower order time and space discretization schemes than the ones used in the original problem.

Appendix B

ADJOINT EQUATIONS FOR BDF2

In this Appendix, the discrete adjoint equations are derived which result from discretizing the time derivative in Eq. (3.5) with the second-order implicit backward difference (BDF2) time marching method. Since this method is not self-starting, the implicit Euler method is used for the first time step. The time-dependent flow solution $Q^n = J\hat{Q}^n$ is then implicitly defined through the following unsteady residuals:

$$
\mathcal{R}^1(\hat{Q}^1, \hat{Q}^0, Y) \ := \ \frac{\hat{Q}^1 - \hat{Q}^0}{\Delta t} + R(\hat{Q}^1, Y) = 0
$$

$$
\mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, \hat{Q}^{n-2}, Y) \ := \ \frac{3\hat{Q}^n - 4\hat{Q}^{n-1} + \hat{Q}^{n-2}}{2\Delta t} + R(\hat{Q}^n, Y) = 0 \qquad \text{for} \quad n = 2, \dots, N.
$$

The problem of minimizing the discrete objective function $\mathcal{J}$ as given by Eq. (3.3) is equivalent to the unconstrained optimization problem of minimizing the Lagrangian function

$$
\mathcal{L} = \sum_{n=1}^{N} I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\mathrm{con}}} C_j(Y) + (\psi^1)^T \mathcal{R}^1(\hat{Q}^1, \hat{Q}^0, Y) + \sum_{n=2}^{N} (\psi^n)^T \mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, \hat{Q}^{n-2}, Y)
$$

with respect to $\hat{Q}^1, \dots, \hat{Q}^N$, $\psi^1, \dots, \psi^N$ and Y. The Lagrange multipliers ψ^n must now be chosen such that $\nabla_{\hat{Q}^n}\mathcal{L} = 0$ for $n = 1, \dots, N$, which leads to

$$
\begin{aligned}
0 \ &= \ \nabla_{\hat{Q}^n} I^n + (\psi^n)^T \nabla_{\hat{Q}^n} \mathcal{R}^n + (\psi^{n+1})^T \nabla_{\hat{Q}^n} \mathcal{R}^{n+1} + (\psi^{n+2})^T \nabla_{\hat{Q}^n} \mathcal{R}^{n+2} \quad \text{for } n = 1, \dots, N-2 \\
0 \ &= \ \nabla_{\hat{Q}^{N-1}} I^{N-1} + (\psi^N)^T \nabla_{\hat{Q}^{N-1}} \mathcal{R}^N + (\psi^{N-1})^T \nabla_{\hat{Q}^{N-1}} \mathcal{R}^{N-1} \\
0 \ &= \ \nabla_{\hat{Q}^N} I^N + (\psi^N)^T \nabla_{\hat{Q}^N} \mathcal{R}^N.
\end{aligned}
$$

This can be written equivalently as

$$
\psi^N \ = -\left((\nabla_{\hat{Q}^N} \mathcal{R}^N)^T \right)^{-1} (\nabla_{\hat{Q}^N} I^N)^T
$$

$$
\psi^{N-1} = -\left((\nabla_{\hat{Q}^{N-1}} \mathcal{R}^{N-1})^T \right)^{-1} \left[(\nabla_{\hat{Q}^{N-1}} \mathcal{R}^N)^T \psi^N + (\nabla_{\hat{Q}^{N-1}} I^{N-1})^T \right]
$$

$$
\psi^n \ = -\left((\nabla_{\hat{Q}^n} \mathcal{R}^n)^T \right)^{-1} \left[(\nabla_{\hat{Q}^n} \mathcal{R}^{n+2})^T \psi^{n+2} + (\nabla_{\hat{Q}^n} \mathcal{R}^{n+1})^T \psi^{n+1} + (\nabla_{\hat{Q}^n} I^n)^T \right] \text{ for } n = N-2, \dots, 1.
$$

Finally, the gradient of $\mathcal{J}$ with respect to the design variables Y is again given by

$$\frac{\partial \mathcal{J}}{\partial Y} = \frac{\partial \mathcal{L}}{\partial Y} = \sum_{n=1}^{N} \nabla_Y I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\text{con}}} \nabla_Y C_j(Y) + \sum_{n=1}^{N} (\psi^n)^T \nabla_Y R(\hat{Q}^n, Y).$$

Appendix C

DERIVATION OF THE FW-H EQUATION

In order to derive the FW-H Equation one starts with the continuity and momentum equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \tag{C.1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial (p\delta_{ij} - \tau_{ij})}{\partial x_j}, \tag{C.2}$$

where $\rho = \rho_\infty + \rho'$, $u_i = U_i + u_i'$ and $p = p_\infty + p'$ are the total density, velocity and pressure, respectively. U_i are the components of the uniform mean velocity, a prime denotes a perturbation from the mean, δ_{ij} is the Kronecker delta, and τ_{ij} is the viscous stress tensor.

Now let the function $f(x_i, t) = 0$ define a control surface in arbitrary motion with $\frac{\partial f}{\partial x_i} = n_i$, where n_i is a unit normal vector that points into the fluid. The idea is that $f = 0$ as a function of space and time always surrounds a moving source region of interest such that $f > 0$ outside this region. $H(f)$ is the Heaviside function, which is one for $f > 0$ and zero for $f < 0$. The derivative of the Heaviside function $H'(f) = \partial H/\partial f = \delta(f)$ is the Dirac delta function, which is zero for $f \neq 0$, but yields a finite value when integrated over a region including $f = 0$. The following identity holds:

$$\frac{dH}{dt} = 0 = \frac{\partial H}{\partial f}\left(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x_i}\frac{\partial x_i}{\partial t}\right) = \frac{\partial H}{\partial t} + \frac{\partial H}{\partial x_i}\frac{\partial x_i}{\partial t}, \tag{C.3}$$

where one can define $v_i = \partial x_i/\partial t$ as the velocities of the control surface. This leads to

$$\frac{\partial H}{\partial t} = -\frac{\partial H}{\partial x_i}v_i = -\frac{\partial H}{\partial f}\frac{\partial f}{\partial x_i}v_i = -\delta(f)n_i v_i. \tag{C.4}$$

To take the presence of the moving source region into account, the continuity (C.1) and momentum (C.2) equations are multiplied by the Heaviside function $H(f)$, and $H(f)$ is

introduced inside the differential operators as follows

$$\frac{\partial \rho H}{\partial t} + \frac{\partial \rho u_j H}{\partial x_j} = \rho \frac{\partial H}{\partial t} + \rho u_j \frac{\partial H}{\partial x_j} \tag{C.5}$$

$$\frac{\partial \rho u_i H}{\partial t} + \frac{\partial \rho u_i u_j H}{\partial x_j} = \rho u_i \frac{\partial H}{\partial t} + \rho u_i u_j \frac{\partial H}{\partial x_j}$$
$$- \frac{\partial (p\delta_{ij} - \tau_{ij})H}{\partial x_j} + (p\delta_{ij} - \tau_{ij}) \frac{\partial H}{\partial x_j}. \tag{C.6}$$

Adding $-\rho_\infty \partial H/\partial t$ to Eq. (C.5), $\partial[a_\infty^2(\rho - \rho_\infty)H]/\partial x_j$ to Eq. (C.6), and rearranging yields

$$\frac{\partial(\rho - \rho_\infty)H}{\partial t} + \frac{\partial \rho u_j H}{\partial x_j} = [\rho(u_j - v_j) + \rho_\infty v_j]\frac{\partial H}{\partial x_j} \tag{C.7}$$

$$\frac{\partial \rho u_i H}{\partial t} + \frac{\partial a_\infty^2(\rho - \rho_\infty)H}{\partial x_j} = -\frac{\partial T_{ij}H}{\partial x_j}$$
$$+ [\rho u_i(u_j - v_j) + p\delta_{ij} - \tau_{ij}]\frac{\partial H}{\partial x_j}, \tag{C.8}$$

where a_∞ is the speed of sound in the undisturbed medium and T_{ij} is the so-called Lighthill stress tensor

$$T_{ij} = \rho u_i u_j + [p - a_\infty^2(\rho - \rho_\infty)]\delta_{ij} - \tau_{ij}. \tag{C.9}$$

Applying the operator $\partial/\partial t$ to Eq. (C.7), taking the divergence of Eq. (C.8), and subtracting the two resulting equations from each other leads to

$$\left\{ \frac{1}{a_\infty^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x_i^2} \right\} [a_\infty^2 \rho' H] = \frac{\partial}{\partial t} \left([\rho(u_j - v_j) + \rho_\infty v_j]\frac{\partial H}{\partial x_j} \right) + \frac{\partial^2}{\partial x_i \partial x_j}[T_{ij}H(f)]$$
$$- \frac{\partial}{\partial x_i} \left([\rho u_i(u_j - v_j) + p\delta_{ij} - \tau_{ij}]\frac{\partial H}{\partial x_j} \right). \tag{C.10}$$

Finally, defining the dipole term $\mathcal{F}_i$ and the monopole term $\mathcal{Q}$ as follows

$$\mathcal{F}_i = [\rho u_i(u_j - v_j) + p\delta_{ij} - \tau_{ij}]\frac{\partial f}{\partial x_j} \tag{C.11}$$

$$\mathcal{Q} = [\rho(u_j - v_j) + \rho_\infty v_j]\frac{\partial f}{\partial x_j} \tag{C.12}$$

yields the differential form of the FW-H equation, which is an exact rearrangement of the continuity and momentum equations into the form of an inhomogeneous wave equation

$$\left\{ \frac{1}{a_\infty^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x_i^2} \right\} [a_\infty^2 \rho' H(f)] = \frac{\partial}{\partial t}[\mathcal{Q}\delta(f)] - \frac{\partial}{\partial x_i}[\mathcal{F}_i\delta(f)] + \frac{\partial^2}{\partial x_i \partial x_j}[T_{ij}H(f)]. \tag{C.13}$$

Appendix D

ADJOINT EQUATIONS FOR BDF2 WITH TIME STEP SIZE CHANGE

In this Appendix, the discrete adjoint equations are derived in the form in which they are used to present all the results in this work except for the pulse in a converging-diverging nozzle (Section 5.1) and the shocktube problem (Section 5.2), which use the equations as given in Appendix B. The time-marching method of choice is the second-order accurate implicit backward difference (BDF2) method, the flow is controlled after a certain transition period, and one can use different time step sizes in the transition period and the control window.

The unsteady flow solve is warmstarted at some point in time which means that $\hat{Q}^0$ and $\hat{Q}^{-1}$ are known. In order to "jump" over the adjusting or transition period as quickly as possible, a bigger time step Δt_c for N_c steps is used. Once the domain where the problem is supposed to be controlled is reached, a smaller time step Δt for another $N - N_c$ steps is used for a total of N steps. To maintain the second-order time accuracy through this time step size change, the time-dependent flow solution $Q^n = J\hat{Q}^n$ is implicitly defined via the following unsteady residuals

$$\mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, \hat{Q}^{n-2}, Y) := \frac{3\hat{Q}^n - 4\hat{Q}^{n-1} + \hat{Q}^{n-2}}{2\Delta t_c} + R(\hat{Q}^n, Y) = 0$$
$$\text{for} \quad n = 1, \ldots, N_c$$

$$\mathcal{R}^{N_c+1}(\hat{Q}^{N_c+1}, \hat{Q}^{N_c}, \hat{Q}^{N_c-1}, Y) := \frac{2\Delta t + \Delta t_c}{\Delta t(\Delta t + \Delta t_c)}\hat{Q}^{N_c+1} - \frac{\Delta t + \Delta t_c}{\Delta t \Delta t_c}\hat{Q}^{N_c}$$
$$+ \frac{\Delta t}{\Delta t_c(\Delta t + \Delta t_c)}\hat{Q}^{N_c-1} + R(\hat{Q}^{N_c+1}, Y) = 0$$

$$\mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, \hat{Q}^{n-2}, Y) := \frac{3\hat{Q}^n - 4\hat{Q}^{n-1} + \hat{Q}^{n-2}}{2\Delta t} + R(\hat{Q}^n, Y) = 0$$
$$\text{for} \quad n = N_c + 2, \ldots, N.$$

The problem of minimizing a discrete objective function $\mathcal{J}$ as given by Eq. (3.3) is then equivalent to the unconstrained optimization problem of minimizing the Lagrangian function

$$\mathcal{L} = \sum_{n=N_c+1}^{N} I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\mathrm{con}}} C_j(Y) + \sum_{n=1}^{N} (\psi^n)^T \mathcal{R}^n(\hat{Q}^n, \hat{Q}^{n-1}, \hat{Q}^{n-2}, Y)$$

with respect to $\hat{Q}^1, \ldots, \hat{Q}^N$, $\psi^1, \ldots, \psi^N$ and Y. This leads to the following equations for ψ^n

$$0 = (\psi^n)^T \nabla_{\hat{Q}^n} \mathcal{R}^n + (\psi^{n+1})^T \nabla_{\hat{Q}^n} \mathcal{R}^{n+1} + (\psi^{n+2})^T \nabla_{\hat{Q}^n} \mathcal{R}^{n+2}$$
$$\text{for} \quad n = 1, \ldots, N_c$$
$$0 = \nabla_{\hat{Q}^n} I^n + (\psi^n)^T \nabla_{\hat{Q}^n} \mathcal{R}^n + (\psi^{n+1})^T \nabla_{\hat{Q}^n} \mathcal{R}^{n+1} + (\psi^{n+2})^T \nabla_{\hat{Q}^n} \mathcal{R}^{n+2}$$
$$\text{for} \quad n = N_c + 1, \ldots, N-2$$
$$0 = \nabla_{\hat{Q}^{N-1}} I^{N-1} + (\psi^N)^T \nabla_{\hat{Q}^{N-1}} \mathcal{R}^N + (\psi^{N-1})^T \nabla_{\hat{Q}^{N-1}} \mathcal{R}^{N-1}$$
$$0 = \nabla_{\hat{Q}^N} I^N + (\psi^N)^T \nabla_{\hat{Q}^N} \mathcal{R}^N,$$

which can be written equivalently as

$$\psi^N = -\left((\nabla_{\hat{Q}^N} \mathcal{R}^N)^T\right)^{-1} \left[(\nabla_{\hat{Q}^N} I^N)^T\right]$$
$$\psi^{N-1} = -\left((\nabla_{\hat{Q}^{N-1}} \mathcal{R}^{N-1})^T\right)^{-1} \left[(\nabla_{\hat{Q}^{N-1}} I^{N-1})^T + (\nabla_{\hat{Q}^{N-1}} \mathcal{R}^N)^T \psi^N\right]$$
$$\psi^n = -\left((\nabla_{\hat{Q}^n} \mathcal{R}^n)^T\right)^{-1} \left[(\nabla_{\hat{Q}^n} I^n)^T + (\nabla_{\hat{Q}^n} \mathcal{R}^{n+1})^T \psi^{n+1} + (\nabla_{\hat{Q}^n} \mathcal{R}^{n+2})^T \psi^{n+2}\right]$$
$$\text{for } n = N-2, \ldots, N_c+1$$
$$\psi^n = -\left((\nabla_{\hat{Q}^n} \mathcal{R}^n)^T\right)^{-1} \left[(\nabla_{\hat{Q}^n} \mathcal{R}^{n+1})^T \psi^{n+1} + (\nabla_{\hat{Q}^n} \mathcal{R}^{n+2})^T \psi^{n+2}\right]$$
$$\text{for } n = N_c, \ldots, 1.$$

A little care must be taken in calculating derivatives of $\mathcal{R}^{N_c+1}$ with respect to $\hat{Q}^n$ since the factors in front of $\hat{Q}^{N_c+1}$, $\hat{Q}^{N_c}$ and $\hat{Q}^{N_c-1}$ differ slightly from the usual scheme. Finally, the gradient of $\mathcal{J}$ with respect to the design variables Y is given by

$$\frac{\partial \mathcal{J}}{\partial Y} = \frac{\partial \mathcal{L}}{\partial Y} = \sum_{n=N_c+1}^{N} \nabla_Y I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\mathrm{con}}} \nabla_Y C_j(Y) + \sum_{n=1}^{N} (\psi^n)^T \nabla_Y R(\hat{Q}^n, Y).$$

Appendix E

ADJOINT EQUATIONS FOR ESDIRK4 WITH TIME STEP SIZE CHANGE

In this Appendix, the discrete adjoint equations for the fourth-order ESDIRK scheme are derived, where the flow is controlled after a certain transition period and different time step sizes can be used in the transition period and the control window.

The unsteady flow solve is warmstarted at some point in time which means that $\hat{Q}^0$ is known. In order to "jump" over the adjusting or transition period as quickly as possible, a bigger time step Δt_c for N_c steps is used. Once the domain where the problem that is being controlled is reached, a smaller time step Δt for another $N-N_c$ steps is used for a total of N steps. The time-dependent flow solution $Q^n = J\hat{Q}^n$ is implicitly defined via the following unsteady residuals where $\hat{Q}_1^n = \hat{Q}^{n-1}$ and $\hat{Q}^n = \hat{Q}_6^n$

$$\mathcal{R}_k^n(\hat{Q}_k^n, \dots, \hat{Q}_2^n, \hat{Q}^{n-1}, Y) \ := \ \frac{\hat{Q}_k^n - \hat{Q}^{n-1}}{a_{kk}\Delta t_c} + R(\hat{Q}_k^n, Y) + \frac{1}{a_{kk}}\sum_{j=1}^{k-1} a_{kj}R(\hat{Q}_j^n, Y) = 0$$
$$\text{for } n = 1, \dots, N_c \text{ and } k = 2, \dots, 6$$

$$\mathcal{R}_k^n(\hat{Q}_k^n, \dots, \hat{Q}_2^n, \hat{Q}^{n-1}, Y) \ := \ \frac{\hat{Q}_k^n - \hat{Q}^{n-1}}{a_{kk}\Delta t} + R(\hat{Q}_k^n, Y) + \frac{1}{a_{kk}}\sum_{j=1}^{k-1} a_{kj}R(\hat{Q}_j^n, Y) = 0$$
$$\text{for } n = N_c+1, \dots, N \text{ and } k = 2, \dots, 6.$$

The problem of minimizing the discrete objective function $\mathcal{J}$ as given by Eq. (3.3) is equivalent to the unconstrained optimization problem of minimizing the Lagrangian function

$$\mathcal{L} = \sum_{n=N_c+1}^{N} I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\text{con}}} C_j(Y) + \sum_{n=1}^{N}\sum_{k=2}^{6} (\psi_k^n)^T \mathcal{R}_k^n(\hat{Q}_k^n, \dots, \hat{Q}_2^n, \hat{Q}^{n-1}, Y)$$

with respect to $\hat{Q}_k^n$ and ψ_k^n for $n = 1, \ldots, N$ and $k = 2, \ldots, 6$ as well as Y. The Lagrange multipliers ψ_k^n must now be chosen such that $\nabla_{\hat{Q}_k^n} \mathcal{L} = 0$ for $n = 1, \ldots, N$ and $k = 2, \ldots, 6$, which leads to

$$\left. \begin{aligned} 0 &= (\psi_k^n)^T \nabla_{\hat{Q}_k^n} \mathcal{R}_k^n + \sum_{j=k+1}^6 (\psi_j^n)^T \nabla_{\hat{Q}_k^n} \mathcal{R}_j^n \quad \text{for } k = 2, \ldots, 5 \\ 0 &= (\psi_6^n)^T \nabla_{\hat{Q}_6^n} \mathcal{R}_6^n + \sum_{j=2}^6 (\psi_j^{n+1})^T \nabla_{\hat{Q}_6^n} \mathcal{R}_j^{n+1} \end{aligned} \right\} \quad \text{for } n = 1, \ldots, N_c$$

$$\left. \begin{aligned} 0 &= (\psi_k^n)^T \nabla_{\hat{Q}_k^n} \mathcal{R}_k^n + \sum_{j=k+1}^6 (\psi_j^n)^T \nabla_{\hat{Q}_k^n} \mathcal{R}_j^n \quad \text{for } k = 2, \ldots, 5 \\ 0 &= \nabla_{\hat{Q}_6^n} I^n + (\psi_6^n)^T \nabla_{\hat{Q}_6^n} \mathcal{R}_6^n + \sum_{j=2}^6 (\psi_j^{n+1})^T \nabla_{\hat{Q}_6^n} \mathcal{R}_j^{n+1} \end{aligned} \right\} \quad \text{for } n = N_c + 1, \ldots, N - 1$$

$$0 = (\psi_k^N)^T \nabla_{\hat{Q}_k^N} \mathcal{R}_k^N + \sum_{j=k+1}^6 (\psi_j^N)^T \nabla_{\hat{Q}_k^N} \mathcal{R}_j^N \quad \text{for } k = 2, \ldots, 5$$

$$0 = \nabla_{\hat{Q}_6^N} I^N + (\psi_6^N)^T \nabla_{\hat{Q}_6^N} \mathcal{R}_6^N,$$

which can equivalently be written as

$$\psi_6^N = -\left((\nabla_{\hat{Q}_6^N} \mathcal{R}_6^N)^T \right)^{-1} \left[(\nabla_{\hat{Q}_6^N} I^N)^T \right]$$

$$\psi_k^N = -\left((\nabla_{\hat{Q}_k^N} \mathcal{R}_k^N)^T \right)^{-1} \left[\sum_{j=k+1}^6 (\nabla_{\hat{Q}_k^N} \mathcal{R}_j^N)^T \psi_j^N \right] \quad \text{for } k = 5, \ldots, 2$$

$$\left. \begin{aligned} \psi_6^n &= -\left((\nabla_{\hat{Q}_6^n} \mathcal{R}_6^n)^T \right)^{-1} \left[(\nabla_{\hat{Q}_6^n} I^n)^T + \sum_{j=2}^6 (\nabla_{\hat{Q}_6^n} \mathcal{R}_j^{n+1})^T \psi_j^{n+1} \right] \\ \psi_k^n &= -\left((\nabla_{\hat{Q}_k^n} \mathcal{R}_k^n)^T \right)^{-1} \left[\sum_{j=k+1}^6 (\nabla_{\hat{Q}_k^n} \mathcal{R}_j^n)^T \psi_j^n \right] \quad \text{for } k = 5, \ldots, 2 \end{aligned} \right\} \quad \text{for } n = N - 1, \ldots, N_c + 1$$

$$\left. \begin{aligned} \psi_6^n &= -\left((\nabla_{\hat{Q}_6^n} \mathcal{R}_6^n)^T \right)^{-1} \left[\sum_{j=2}^6 (\nabla_{\hat{Q}_6^n} \mathcal{R}_j^{n+1})^T \psi_j^{n+1} \right] \\ \psi_k^n &= -\left((\nabla_{\hat{Q}_k^n} \mathcal{R}_k^n)^T \right)^{-1} \left[\sum_{j=k+1}^6 (\nabla_{\hat{Q}_k^n} \mathcal{R}_j^n)^T \psi_j^n \right] \quad \text{for } k = 5, \ldots, 2 \end{aligned} \right\} \quad \text{for } n = N_c, \ldots, 1.$$

Finally, the gradient of $\mathcal{J}$ with respect to the design variables Y is given by

$$\frac{\partial \mathcal{J}}{\partial Y} = \frac{\partial \mathcal{L}}{\partial Y} = \sum_{n=N_c+1}^N \nabla_Y I^n(Q^n, Y) + w_T \sum_{j=1}^{N_{\text{con}}} \nabla_Y C_j(Y) + \sum_{n=1}^N \sum_{k=1}^6 \left(\sum_{j=k}^6 (\psi_j^n)^T \frac{a_{jk}}{a_{jj}} \right) \nabla_Y R(\hat{Q}_k^n, Y)$$

with the definition $\frac{a_{11}}{a_{11}} = \frac{0}{0} := 0$.

Appendix F

IMPLEMENTATION DETAILS OF THE FW-H EQUATION

The far-field pressure fluctuations in the frequency-domain are given by Eq. (4.19). Assuming that the observer location x is outside the source region described by the function $f(y) > 0$ and neglecting the viscous stress tensor as well as the quadrupole contribution, they can be stated as follows:

$$
\begin{aligned}
p'(x, \omega) = \quad &- \oint_{f=0} i\omega \mathcal{Q}(y, \omega) G(x, y, \omega) dl \\
&- \oint_{f=0} \mathcal{F}_k(y, \omega) \frac{\partial G(x, y, \omega)}{\partial y_k} dl,
\end{aligned}
\tag{F.1}
$$

where the monopole term $\mathcal{Q}$ and dipole terms $\mathcal{F}_k$ in the time-domain are defined as

$$
\mathcal{Q}(y, t) = \rho(y, t) u_r(y, t) n_r(y)
\tag{F.2}
$$

$$
\mathcal{F}_k(y, t) = \Big[p(y, t) \delta_{kr} + \rho(y, t) \big(u_k(y, t) - 2 U_k(y) \big) u_r(y, t) \Big] n_r(y),
\tag{F.3}
$$

and the Green function $G(x, y, \omega)$ is given by Eq. (4.14).

In the actual code, $\mathcal{Q}(y, t)$ as well as $\mathcal{F}_k(y, t)$ are Fourier transformed using a FFT after subtracting their respective mean and applying the window function W_n given by Eq. (4.24) in an energy preserving manner. This yields for the monopole term in the frequency-domain

$$
\mathcal{Q}(y, \omega_l) = |W| \sum_{n=1}^{N} \hat{\mathcal{Q}}(y, t_n) \exp(-i\omega_l t_n) W_n \qquad \text{for} \quad l = 1, \dots, N
\tag{F.4}
$$

where $|W| = \sqrt{N / \sum W_n^2}$, $\omega_l = \big(2\pi(l-1) \big)/(N\Delta t)$, $t_n = (n-1)\Delta t$ and

$$
\hat{\mathcal{Q}}(y, t_n) = \mathcal{Q}(y, t_n) - \frac{1}{N} \sum_{n'=1}^{N} \mathcal{Q}(y, t_{n'}) \qquad \text{for} \quad n = 1, \dots, N.
\tag{F.5}
$$

One obtains similar expressions for the dipole terms $\mathcal{F}_k(y, \omega_l)$. The contour integrals in Eq. (F.1) are evaluated using the trapezoidal rule:

$$p'(x, \omega_l) = -\sum_{j=1}^{J} \frac{1}{2} \Delta s_j \Big[i\omega_l \mathcal{Q}(y_j, \omega_l) G(x, y_j, \omega_l) + i\omega_l \mathcal{Q}(y_{j+1}, \omega_l) G(x, y_{j+1}, \omega_l)$$
$$+ \mathcal{F}_1(y_j, \omega_l) \frac{\partial G(x, y_j, \omega_l)}{\partial y_{1j}} + \mathcal{F}_2(y_j, \omega_l) \frac{\partial G(x, y_j, \omega_l)}{\partial y_{2j}}$$
$$+ \mathcal{F}_1(y_{j+1}, \omega_l) \frac{\partial G(x, y_{j+1}, \omega_l)}{\partial y_{1j+1}} + \mathcal{F}_2(y_{j+1}, \omega_l) \frac{\partial G(x, y_{j+1}, \omega_l)}{\partial y_{2j+1}} \Big], \text{(F.6)}$$

where J is the total number of nodes which define the closed integration contour path, and $\Delta s_j = \sqrt{(y_{1j+1} - y_{1j})^2 + (y_{2j+1} - y_{2j})^2}$ is the distance between neighboring points. Note that variables with index $J + 1$ have the same value as those with index 1.

Differentiation with respect to the flow variables

If the FW-H equation is used as part of an objective function in the optimization framework, the derivative of the far-field pressure fluctuations with respect to the flow variables is needed explicitly. However, the derivative with respect to the design variables is obtained using fourth-order centered finite differences as explained in Section 3.3. Denoting the non-dimensional conservative variables given by Eq. (2.1) at source node location j and time step n as Q_j^n, the derivative of the far-field pressure fluctuations in the frequency domain with respect to the flow variables is given by:

$$\frac{\partial p'(x, \omega_l)}{\partial Q_j^n} = -\frac{1}{2} \Big(\Delta s_{j-1} + \Delta s_j \Big) \Big[i\omega_l G(x, y_j, \omega_l) \frac{\partial \mathcal{Q}(y_j, \omega_l)}{\partial Q_j^n}$$
$$+ \frac{\partial G(x, y_j, \omega_l)}{\partial y_{1j}} \frac{\partial \mathcal{F}_1(y_j, \omega_l)}{\partial Q_j^n} + \frac{\partial G(x, y_j, \omega_l)}{\partial y_{2j}} \frac{\partial \mathcal{F}_2(y_j, \omega_l)}{\partial Q_j^n} \Big] \qquad \text{(F.7)}$$

with

$$\frac{\partial \mathcal{Q}(y_j, \omega_l)}{\partial Q_j^n} = \Big[|W| \exp(-i\omega_l t_n) W_n - \frac{|W|}{N} \sum_{n'=1}^{N} \exp(-i\omega_l t_{n'}) W_{n'} \Big] \frac{\partial \mathcal{Q}(y_j, t_n)}{\partial Q_j^n}, \qquad \text{(F.8)}$$

and similar expressions for $\partial\mathcal{F}_1(y_j,\omega_l)/\partial Q_j^n$ and $\partial\mathcal{F}_2(y_j,\omega_l)/\partial Q_j^n$. Lastly, using the expressions for the monopole (F.2) and dipole terms (F.3) in the time-domain one finds

$$\frac{\partial\mathcal{Q}(y_j,t_n)}{\partial Q_j^n} = \begin{bmatrix} 0 \\ n_1(y_j) \\ n_2(y_j) \\ 0 \end{bmatrix} \tag{F.9}$$

$$\frac{\partial\mathcal{F}_k(y_j,t_n)}{\partial Q_j^n} = (\gamma-1)n_k(y_j) \begin{bmatrix} \frac{1}{2}[u_1^2(y_j,t_n)+u_2^2(y_j,t_n)] \\ -u_1(y_j,t_n) \\ -u_2(y_j,t_n) \\ 1 \end{bmatrix}$$

$$+ \frac{\mathcal{Q}(y_j,t_n)}{\rho(y_j,t_n)} \begin{bmatrix} -u_k(y_j,t_n) \\ 1 \\ 0 \\ 0 \end{bmatrix} + \big(u_k(y_j,t_n)-2U_k(y_j)\big) \begin{bmatrix} 0 \\ n_1(y_j) \\ n_2(y_j) \\ 0 \end{bmatrix}. \tag{F.10}$$

If, however, the derivative in the time-domain is required instead, the partial derivatives in Eq. (F.7) have to be Fourier transformed for each node j using an inverse FFT, that is

$$\frac{\partial p'(x,t_{\tilde{n}})}{\partial Q_j^n} = \frac{1}{N}\sum_{l=1}^{N}\frac{\partial p'(x,\omega_l)}{\partial Q_j^n}\exp(i\omega_l t_{\tilde{n}}). \tag{F.11}$$

Given the last equation, it is straightforward to differentiate the pressure fluctuation objective function used in Sections 5.8 and 5.9 and given by Eq. (5.11). Converted to the notation used in this Appendix it reads as follows

$$\mathcal{J}_N = \sum_{\tilde{n}=N_c+1}^{N}(p_{obs}^{\tilde{n}}-\bar{p}_{obs})^2 = \sum_{\tilde{n}=N_c+1}^{N}\big(p'(x,t_{\tilde{n}})-\bar{p}'(x,t_{\tilde{n}})\big)^2, \tag{F.12}$$

where $\bar{p}'(x,t_{\tilde{n}}) = \frac{1}{N-N_c}\sum_{n'=N_c+1}^{N}p'(x,t_{n'})$. Its derivative with respect to the flow variables is then given by

$$\frac{\partial\mathcal{J}_N}{\partial Q_j^n} = \frac{\partial\mathcal{J}_N}{\partial p'(x,t_{\tilde{n}})}\frac{\partial p'(x,t_{\tilde{n}})}{\partial Q_j^n} = 2\sum_{\tilde{n}=N_c+1}^{N}\big(p'(x,t_{\tilde{n}})-\bar{p}'(x,t_{\tilde{n}})\big)\frac{\partial p'(x,t_{\tilde{n}})}{\partial Q_j^n}. \tag{F.13}$$