Optimization of multiphysics problems: transient vibroacoustic and thermal-fluid systems

Dilgen, Cetin Batur

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Author:
Cetin Batur Dilgen

Main supervisor:
Associate Professor Niels Aage
Technical University of Denmark

Co-supervisor:
Professor MSO Jakob Søndergaard Jensen
Technical University of Denmark

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Centre for Acoustic-Mechanical Micro Systems (CAMM)
Department of Mechanical Engineering
Technical University of Denmark
Building 404, DK-2800 Kgs. Lyngby, Denmark
Preface

This thesis is submitted to the Technical University of Denmark (DTU) as partial fulfillment of the requirements for the degree of Doctor of Philosophy (PhD) in mechanical engineering. The PhD project has been funded by the Centre for Acoustic-Mechanical Micro Systems (CAMM). The work has been carried out at the Department of Mechanical Engineering, Section of Solid Mechanics, at DTU during the period from the 1st of February 2017 to the 1st of February 2020. The main supervisor has been Associate Professor Niels Aage and the co-supervisor has been Professor Jakob Søndergaard Jensen.

First of all, I would like to thank my supervisors, Niels and Jakob, for always being instantly available when I needed to discuss the work during my PhD studies, I greatly appreciate their inspiring support. A special thanks to Niels for stimulating discussions we had during "short-breaks" and giving me and Sümer a ride back to Nørrebro so many times.

I would also like to extend my thanks to fellow PhD students in the TopOpt and CAMM groups for countless scientific discussions and making my time at DTU very enjoyable.

Thanks to my family for always providing me the support and encouragement when I needed it, and of course, I would like to thank my beloved wife, Özge Dilgen, for her endless love and constant support. Finally, I would also like to thank my son, Selim Efe Dilgen, for bringing constant joy and happiness to our lives with his smile.
Abstract

The aim of this Thesis is to present efficient methods for advanced topology and shape optimization frameworks considering multiphysics systems. The Thesis is conducted in two parts: first part deals with the transient shape optimization of coupled acoustic mechanical interaction problems and the second part deals with the optimization of turbulent flow heat transfer systems.

Part I of the Thesis aims to develop a generalized shape optimization framework for transient vibroacoustic problems. Throughout the work, the geometry is implicitly defined using a level function as the interface between acoustic and structural domains is obtained from the zero iso-level of the level set function. The crisp representation of the geometry contained in the level set is then captured utilizing an immersed boundary method called the cut element method which operates on fixed background meshes. This way, accurate solutions to the strongly coupled vibroacoustic equations are obtained. Moreover, the utilized design parameterization allows the usage of gradient based optimizers for which the work employs a fully discrete adjoint approach for calculating the gradients of objective and constraint functions.

The calculated gradients with the developed transient optimization framework is validated and compared against the commonly utilized semi-discrete approach. The study highlights the importance of having consistent sensitivities obtained via the fully discrete adjoint method. Following this, the transient design formulation is also validated on a benchmark case, a simple acoustic partitioner design. The developed framework is further applied to the design of vibroacoustic pulse shaping devices.

The framework is extended to demonstrate a transient problem formulation that allows to optimize and control the wideband frequency response. To this end, the objective is defined in frequency domain and a fast Fourier transform (FFT) algorithm is applied on the transient response of the coupled system to obtain the frequency response. The capabilities of the proposed design method is then demonstrated on various vibroacoustic filter designs.

Part II of the Thesis aims to develop an efficient topology optimization framework for large-scale complex turbulent flow systems. The proposed methodology makes use of automatic differentiation (AD) in the derivation of discrete adjoints to calculate exact sensitivities without resorting to any simplifying assumptions. The work utilizes finite volume discretization for Reynolds-averaged Navier–Stokes equations which is also coupled to a two-equation turbulence closure model. The developed framework is demonstrated on the optimization of several 2D and 3D flow systems. The study also highlights the importance of including turbulence modeling in the proposed design method. Furthermore, the developed flow framework is then coupled to heat transfer in order to demonstrate the topology optimization of heat sinks with turbulent forced convection. Large-scale 3D heat sink design problems are demonstrated and the benefits of full 3D optimization are highlighted via the carried out comparisons.
Publications

The following international journal papers constitute a part of the Thesis:


**P5** Cetin B. Dilgen and Niels Aage. Transient shape optimization of vibroacoustic problems for broadband filter designs using cut elements, *Journal of Sound and Vibration*, To be submitted
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Introduction

This Chapter provides a brief introduction together with the motivation and goal for the presented work. Following this, the chapter presents a literature review to demonstrate the current state-of-the-art regarding the considered topics. After a brief summary on the contributions of the Thesis, the chapter lastly defines the structure of the thesis. Further details with the relevant references are given in Parts I and II.

1.1 Motivation and goal

In today’s world, the demand is ever increasing for high-fidelity performance of vibroacoustic devices such as hearing systems, head sets, mobile phones, etc. These devices generally constrained by a small, and often limited, design space. Micro acoustic-mechanical devices experience strong vibroacoustic coupling which renders the standard trial and error methods ineffective for obtaining intuitive solutions required to increase the performance. Shape and topology optimization methods, on the other hand, are well-suited to achieve significant performance improvements through geometric modifications and often result in novel design configurations.

Such devices usually operate with complex signals containing broad range of frequencies where controlling the explicit vibroacoustic response of the system is often of interest in industry. State-of-the-art methods commonly apply time-harmonic formulation for the modelling of broadband frequency response. However, the approach can easily become prohibitive when large number of frequency points are considered to accurately capture the system’s response. Employing transient formulation facilitates a viable alternative to handle this issue. This way, the broadband response of the system can be modelled in a straightforward way using a white noise excitation of the system. Time-domain formulation also allows to investigate transient phenomena which widens the application range of the method.

The main goal of the part I of the Thesis is to develop a transient optimization framework where the choice of the modelling approach is based on the findings of a comparative study. This way, within the optimization, accurate solutions to the strongly coupled vibroacoustic systems can be achieved for high frequency applications. The developed methodology will then be applied for the transient optimization of vibroacoustic systems demonstrating both transient and efficient broadband applications.

Industrial applications regarding fluid systems almost exclusively include fast and turbulent flows. Numerous methodologies are already developed for topology optimization of simplified laminar flow systems. However, including turbulence in the optimization process is imperative to obtain novel design configurations to realize increased performance of industrial flow systems. An efficient topology optimization framework for realistic flow systems can be achieved considering Reynolds-averaged
Navier-Stokes equations which describe the turbulence in steady-state with providing mean flow properties, which are often of interest in industry.

The part II of the Thesis aims to develop an efficient methodology to build a topology optimization framework for turbulent flows. Following this, part II will carry out the optimization of complex turbulent flow systems. Coupling to heat transfer will also be considered to optimize large scale heat sink devices that operate under a turbulent forced convection process.

1.2 Literature review

A summary of literature review is provided in this section regarding the specific subjects presented in parts I and II of the Thesis. The reader is kindly referred to the appended papers for a more exhaustive literature review on the considered topics.

For low frequency vibroacoustic design problems, density based topology optimization of coupled acoustic-mechanical interaction problems is demonstrated in [48] using a mixed finite element formulation. However, the lack of a clear boundary definition of density based methods together with the so called staircase (pixelated) boundary representation introduce issues when considering coupled multi-physics problems [27, 31].

Due to the noted potential drawbacks, level set methods are often employed as an alternative to the density design methodology especially for multi-physics problems. The level set method provides a crisp representation of the design from the zero contour of a level set function. An accurate modelling of the considered physics however, is obtained from the underlying numerical model and not the level set method itself.

For vibroacoustic applications considering frequency domain modelling, [35] employs an ersatz-type material model with a level set method for acoustic cavity designs. The application of a level set method with extensive remeshing at each design update, for an accurate modelling of acoustics, can be found in [22] which also considers topological derivatives. The works of [15, 40] utilize a Hamilton-Jacobi type design update scheme with again carrying out remeshing at design updates.

Using a complex and compact signal that contains broad range of frequencies is demonstrated in the works of [19, 20, 36] for transient topology optimization of antennas. Here, a proper time-domain input pulse is selected to excite a broad frequency range. However, the optimization only indirectly controls the broadband response of the system. Since, the objective function is also defined in the time-domain.

Considering fluid flow problems, topology optimization is first demonstrated using a Stokes flow model [11] where the large scale optimization of such problems is carried out by [3]. Later topology optimization studies consider Navier–Stokes equations under laminar flow conditions [14, 18, 26]. Moreover, including turbulent flows in the topology optimization framework is demonstrated in [37, 39] using the frozen turbulence assumption i.e, neglecting the variations of the turbulence field with respect to design variables. Later on, a continuous adjoint formulation, including a turbulence model in the sensitivity analysis, is presented in [25].
1.3 Contributions of the thesis

For coupled thermal-fluid problems, Stokes flow is considered in [24] where the optimization considered a combined objective function for the maximization of heat transfer and the minimization of pressure difference. Laminar flow conditions are studied in [13, 32, 46, 47] for the optimization of heat sink devices. Topology optimization of turbulent flow heat transfer systems is given in [39] using the simplifying frozen turbulence assumption. The continuous adjoint formulation including a turbulence model given in [25], also considers heat transfer applications.

1.3 Contributions of the thesis

Based on the appended papers, a short summary on the contributions of the Thesis is presented in this section

• A methodology for calculating exact sensitivities considering topology optimization of turbulent flows has been demonstrated for the first time and applied for the optimization of complex flow systems (P1).

• Topology optimization of turbulent flow heat transfer systems has been demonstrated (P2).

• A comprehensive comparative review has been conducted for topology optimization of acoustic mechanical interaction problems (P3).

• Transient shape optimization of vibroacoustic problems has been demonstrated for the first time (P4).

• The developed transient vibroacoustic optimization framework has been extended to include broadband applications and applied for the optimization of acoustic filter devices for the first time (P5).

1.4 Structure of the thesis

This thesis follows a summary style format and provides the reader with an overall overview of the appended papers. The Thesis consists of two separate parts due to the large differences in the content.

• Part I of the Thesis is largely based on papers P4 and P5 and deals with generalized shape optimization of transient vibroacoustic problems. Although paper P3 is not directly included in the summary, the utilized optimization and modelling methods in part I are based on the outcomes from the comparative review done in paper P3.

• Part II of the Thesis is based on papers P1 and P2 and deals with topology optimization of thermal-fluid systems considering turbulent flows.

It is noted that, each part contains a brief summary on the employed methods and presents the main results from the appended papers while ending with concluding remarks regarding the specific subjects.
Part I

Generalized shape optimization of transient vibroacoustic systems
[P3,P4,P5]
Modelling approach for the transient vibroacoustic problem

This chapter presents the governing equations for transient vibroacoustic problems. The governing equations are introduced in standard segregated form which is the most common approach for the modelling of multi-physics systems. Following this, the chapter provides a motivation on the utilization of an immersed boundary method. The method couples with the segregated governing equations through which the modelling of non-conforming boundaries are realized on fixed meshes. After a brief summary on the utilized immersed boundary method, the chapter lastly provides a short note on the implementation. The reader is kindly referred to papers P4 and P5 for thorough explanations of the finite element discretization of the governing equations and the implementation details of the immersed boundary method.

2.1 Governing equations

The standard segregated analysis is a common choice for the most commercial software that offers simulation of acoustic-mechanical interaction systems. The term segregated describes the way the coupled systems are numerically treated. That is, the acoustic wave equation is only solved in the acoustic domain $\Omega_a$ whereas the structural equation is only considered in the solid domain $\Omega_s$. The coupling between the two physics is realized through the shared interface that separates the solid and acoustic regions.

For a transient motion, the structure is governed by the linear elasticity equation which is written as

$$
\rho_s \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \mathbf{\sigma} + \rho_s \alpha_d \frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \left( \beta_d \frac{\partial \mathbf{\sigma}}{\partial t} \right) = 0 \quad \text{in} \quad \Omega_s \quad (2.1)
$$

$$
\mathbf{u} = 0 \quad \text{on} \quad \Gamma_{sd} \quad (2.2)
$$

$$
\mathbf{n}_s \cdot \mathbf{\sigma} = 0 \quad \text{on} \quad \Gamma_{sn} \quad (2.3)
$$

$$
\mathbf{n}_s \cdot \mathbf{\sigma} = p \mathbf{n}_a \quad \text{on} \quad \Gamma_{as} \quad (2.4)
$$

Here, the acoustic pressure is denoted by $p$ and the displacement vector is described by the vector $\mathbf{u}$. $\rho_s$ is the density of the solid material, $\mathbf{n}_s$ and $\mathbf{n}_a$ are the normal vectors defined at the interface pointing outwards from the acoustic $\Omega_a$ and the structural $\Omega_s$ domains, respectively. Throughout the work, the loss mechanism is reflected by employing a structural damping where $\alpha_d$ and $\beta_d$ are the so-called Rayleigh damping parameters. Moreover, $\mathbf{\sigma}$ is the Cauchy stress vector defined as $\mathbf{\sigma} = \mathbf{C}(E_s, \nu) \mathbf{\epsilon}$. The constitutive matrix $\mathbf{C}(E_s, \nu)$ utilizes plane stress assumption and is a function of the Young's modulus $E_s$ and the Poisson’s ratio $\nu$. Definition of the strain vector $\mathbf{\epsilon}$ can be found in papers P3 to P5.
Chapter 2. Modelling approach for the transient vibroacoustic problem

Considering the boundary conditions of the structural equation given in equation 2.1, the fully clamped boundary condition is given in equation 2.2 which is defined on $\Gamma_{sd}$. $\Gamma_{sn}$ given in equation 2.3 defines the traction free boundary condition. As it can be seen from the coupling condition for the structure given in equation 2.4, acoustic pressure fluctuations apply a pressure load onto the structure from the shared interface $\Gamma_{as}$.

Acoustic pressure response is found by solving the transient Helmholtz equation, which reads as

$$\frac{1}{K_a} \frac{\partial^2 p}{\partial t^2} - \frac{1}{\rho_a} \nabla^2 p = 0 \quad \text{in } \Omega_a \quad (2.5)$$

$$\mathbf{n}_a \cdot \nabla p = 0 \quad \text{on } \Gamma_{ad} \quad (2.6)$$

$$\mathbf{n}_a \cdot \nabla p = \rho_a \frac{\partial^2 (\mathbf{n}_s \cdot \mathbf{u})}{\partial t^2} \quad \text{on } \Gamma_{as} \quad (2.7)$$

$$\mathbf{n}_a \cdot \nabla p + \frac{1}{c_a} \frac{\partial p}{\partial t} = \frac{2}{c_a} \frac{\partial p_{in}}{\partial t} \quad \text{on } \Gamma_{ar} \quad (2.8)$$

where, $c_a$ and $\rho_a$ are the speed of sound and the density of the acoustic medium, respectively. $K_a$ defines the bulk modulus of the acoustic domain which is defined as $K_a = \rho_a c_a^2$. Furthermore, the hard-wall boundary condition is given in equation 2.6 which is defined on $\Gamma_{ad}$. Equation 2.7 gives the coupling condition to the structural domain defined on the shared interface $\Gamma_{as}$. The coupling boundary condition represents an acceleration boundary condition into the acoustic domain. Equation 2.8 gives the boundary condition for a plane wave radiation where $p_{in}$ is the amplitude of the incoming transient acoustic wave. Figure 2.1 gives a schematic illustration of the resulted coupled acoustic-structural system where the utilized boundary conditions are also shown. Throughout the work, temporal discretization of the coupled system is realized with employing the Newmark algorithm [23, 34] which is given in detail in papers P4 and P5.

![Figure 2.1: Schematic illustration of the coupled acoustic-structural system. Physical domains, the coupled interface and the boundary conditions are showed. The figure is taken from paper P5.](image-url)
2.2 Immersed boundary modelling

This section gives an introduction to the utilized immersed boundary modelling approach called the cut element method. The method is used with the segregated vibroacoustic equations to model the non-conforming boundaries. After a motivation is given on the choice of the immerse boundary method, the section introduces the geometry description that is used for modelling and the subsequent optimization. Lastly, the section gives a summary on the special integration scheme that is used in the elements that are cut by the non-conforming interface.

2.2.1 Motivation

As it is previously mentioned, segregated analysis is generally the most common approach for modelling the strongly coupled vibroacoustic systems. The approach is used with body-fitted meshes where the exact boundary representation is captured. Usually, the utilization of unstructured grid is required to mesh complex designs in the computational domain where a dedicated mesh generation software is used. Depending on the quality of the elements that are used to mesh the interface, a highly accurate modelling of the strongly coupled physics can be realized.

The expensive meshing operation however brings challenges for realizing an efficient parallel optimization framework. Since, the approach is usually coupled with classical level set based methods using the Hamilton-Jacobi update scheme where the re-meshing operation is done at every design update. The Hamilton-Jacobi update scheme (or a simplified advection-diffusion equation) also limits the optimization problem where considering multiple constraints create stability issues for the optimization process. Hence, although accurate solutions are obtained, the segregated analysis is not suitable to realize an efficient and general optimization framework for coupled multi-physics problems.

Another modelling approach for transient vibroacoustic systems can be obtained by modifying the structure equation given in equation 2.1 with introducing an auxiliary pressure variable to the equation in addition to the displacements. This way, pressure loads can be transferred without explicit boundary locations. The approach is called the so-called mixed formulation \[44, 49\] in which a single monolithic formulation that governs both physics can be obtained by changing the material properties of the system. The mixed formulation becomes the perfect candidate for density based topology optimization when the domain information (acoustic \(\Omega_a\) and structural \(\Omega_s\) domains present in \(\Omega\)) is tied to an indicator function which is relaxed to have intermediate values ("grey" pixels that are the mixture of both acoustic and structural domains). The material properties are then interpolated based on the indicator function to obtain a single solution without a clear definition of the interface between the two physics.

Although the most design freedom for optimization is obtained with density based topology optimization, the lack of physical interpretation of the grey areas together with the pixelized (stair-case) boundary representation create issues for multi-physics problems that are coupled through the shared interface. This is also shown in the comparative studies done in paper \(P3\) where simple optimized designs
are post-processed and analyzed with body-fitted meshes using segregated analysis. The resulted comparisons show around 30% discrepancies in objective function values.

Figure 2.2: Density based transient optimization of an acoustic pulse shaping design. (a) Shows an intermediate design in the optimization process and a figure showing the performance in which the black line is the desired pulse shape and the blue line is the calculated pulse shape. (b) Shows the end design and a figure showing the performance in which the black line is the desired pulse shape and the blue line is the calculated pulse shape.

Because of the high frequency content present in complex transient signals, strongly coupled vibroacoustic problems also show a high level of sensitivity to small design variations. When this is coupled with the lack of clear boundary definition as a result of the intermediate grey areas, the performance of the design suffers throughout the optimization. This is demonstrated in figure 2.2 where the optimization process of an acoustic pulse shaping device is shown. A brief explanation of the case setup for the optimization given in the figure is as follows: An acoustic pulse is radiated towards the structure in an acoustic channel. Due to the interaction between the acoustic pressure oscillations and the vibrations in the structure, the acoustic pressure is transmitted which is recorded at a point downstream in the channel. The case considers the optimization of an elastic structure in order to fit the pulse shape...
2.2. Immersed boundary modelling

(Envelope) of the recorded transmitted acoustic pressure into a specified pulse shape. As it can be seen from the figure 2.2a, a good agreement with the desired pulse shape is achieved when the optimizer is free to alter the wavelength with the grey areas in the design that lack physical interpretation. However, as the optimization progress (figure 2.2b) with using a filter-project scheme to obtain a crisp design, the performance of the design gets progressively worse. Overall, in the concept of density based topology optimization, issues remain for mixed formulation used for multi-physics problems that are coupled through an interface especially for high frequency applications.

Generally, the accurate modelling of the interface is crucial when considering strongly coupled problems such as vibroacoustics in order to capture the interactions between the two physics. To achieve this, the work utilizes an immersed boundary approach called the cut element method where the exact boundary representation is realized. The method avoids the cumbersome body-fitted meshing operation and the geometry is captured on a fixed regular mesh since elements are allowed to be cut by the non-conforming interface without modifying the underlying mesh.

Although the same governing equations are utilized with the segregated analysis, a fictitious domain approach is followed where the both physics are solved in the whole computational domain $\Omega = \Omega_s \cup \Omega_a$. This way, the acoustic and the structure domains can freely evolve during the optimization process without the need of re-numbering the degrees of freedoms. The fictitious domain approach realizes a void phase for the structure solution in the acoustic domain and a rigid phase for the acoustic solution in the structure domain. This is done, similar to the density based methods, by altering the material properties with a dimensionless contrast parameter. However, the contrast parameter is not relaxed to allow for grey areas (unphysical solutions). Meaning that, an element either belongs to the acoustic domain or to the structural domain. In terms of optimization, much like the density based methods, the same mesh is utilized both for the finite element analysis and the optimization which brings generality to build efficient parallel optimization frameworks for coupled multi-physics problems.

2.2.2 Geometry description

The work utilizes a scalar valued function $\bar{s}$ to implicitly define the geometry on a fixed regular grid. Discretely, the function $\bar{s}$ is stored on the nodes of the mesh and its values are used to identify the embedded acoustic and structure domains in the computational domain $\Omega$ that define the current design configuration. The embedded physical domains are identified using the following rule

\[\begin{align*}
\bar{s}(x) &> 0, \quad x \in \Omega_s \quad \text{(structural domain)} \\
\bar{s}(x) &= 0, \quad x \in \Gamma_{as} \quad \text{(interface)} \\
\bar{s}(x) &< 0, \quad x \in \Omega_a \quad \text{(acoustic domain)}
\end{align*}\] (2.9)

The rule given in equation 2.9 realizes a robust way of capturing implicitly defined complex geometries throughout the optimization. Here, the positive values of $\bar{s}$
specify the embedded structural domain $\Omega_s$ whereas the acoustic domain $\Omega_a$ is identified by the negative values of the function $\bar{s}$. Moreover, the shared interface $\Gamma_{sa}$ that couples the two physics is captured from the zero iso-level of the function $\bar{s}$. Since the function $\bar{s}$ is stored on the nodes of the fixed background mesh and it is discretized using linear shape functions, the extracted interface $\Gamma_{sa}$ forming the non-conforming boundary is represented by linear straight curves inside cut elements.

Figure 2.3: An example function $\bar{s}$ showing the embedded physical domains. (a) shows the rule that is used for specifying different physical domains embedded with the function. (b) finite element mesh where white color shows the uncut elements in the acoustic domain, gray color shows the uncut elements in the solid region and the blue color shows the cut elements. The figure is taken from paper P5.

The utilization of the rule given in equation 2.9 is illustrated in figure 2.3a where an example function $\bar{s}$ is used to identify the implicitly defined embedded physical domains ($\Omega_s$ and $\Omega_a$) along with the shared interface $\Gamma_{sa}$. Furthermore, before the cut element method is utilized to model the non-conforming boundaries inside cut elements, an element based indicator function marks each element for which the figure 2.3b visually illustrates the utilization of nodal values of the function $\bar{s}$ to mark the elements as cut or uncut. For uncut elements, if an element’s nodal $\bar{s}$ values are only positive ($\bar{s} > 0$) or only negative ($\bar{s} < 0$) then the element is set as an uncut element in $\Omega_s$ or in $\Omega_a$, respectively. Discretization of the coupled equations (Eqs. 2.1 and 2.5) does not require a special treatment in uncut elements where the standard finite element discretization is carried out. Integration in uncut elements utilizes the standard Gaussian quadrature rule for bilinear quadrilateral (Q-4) elements and
the fictitious domain solutions are realized with appropriately changing the material properties of the structure and acoustic equations.

2.2.3 Cut element method

This section introduces the cut element method which is employed for modelling the partial interfaces in cut elements. The method uses a special integration scheme to realize the non-conforming boundaries which means that the shape functions are not enriched and the discrete system’s degrees of freedoms are not modified. Moreover, the integration scheme is a local operation which makes it possible for a straightforward inclusion of the method into an existing parallel finite element framework.

Using the cut element method, the partial interface inside the cut element is realized through weighted integration for which the Gaussian quadrature rule is employed. Hence, it is crucial to correctly place the integration points. This is achieved by a simple triangulation algorithm where the parent element (cut element) is divided into sub-triangle elements. Triangulation step is carried out only to ensure the Gauss points are placed in correct positions for the sub-triangle and interface line.

Figure 2.4: Illustration of a sub-cell integration in a cut element. Physical domains are identified in the cut elements where the gray color is the structural domain, white color is the acoustic domain and the blue line is the interface. The figure shows the process of placing the Gauss points on iso-parametric triangle and line elements then mapping the integration points to the reference domain of the parent element for integration. The figure is taken from paper P5.
Chapter 2. Modelling approach for the transient vibroacoustic problem

elements. Similar to determining if an element is cut or uncut, again the nodal values of the function $\bar{s}$ is utilized to determine the location of the partial interface inside the cut element and the subsequent triangulation is carried out using the marching squares algorithm [30].

Figure 2.4 illustrates a cut element where the triangulation is done to obtain the sub-elements. As it can be seen from the figure, nodal values of the function $\bar{s}$ is used to assign further marks to sub-elements to set the domain information as either $\Omega_s$ or $\Omega_a$ which is used to set the correct material properties for both physics. This is done to realize fictitious domain solutions for the acoustic and structural equations inside the cut element.

Figure 2.4 also illustrates the sub-integration process which starts with inserting Gauss points in the reference domain of the sub-triangle element. These integration points in the iso-parametric triangle sub-element are then transferred to the reference domain of the parent quad element where the final integration is carried out. This way, the integration of the element matrices only contributes to the parent quad element without changing the sparsity of the system matrix throughout the optimization. For the integration in the parent quad element, the associated integration weights are also modified in order to keep the correct volume scaling between the sub and the parent elements.

The implementation of the coupling boundary conditions for the vibroacoustic system given in equations 2.4 and 2.7 is carried out on the partial interface inside the cut element where the integration process within the cut element method framework is also shown in figure 2.4. Firstly, the interface line element inside the cut element is identified in the sub-triangulation step. Following this, standard Gauss points are inserted considering the reference domain of an iso-parametric line element. The final integration is again considered in the parent quad element with the integration points that are mapped from the reference domain of the line element into the reference domain of the parent quad element. Different from the volumetric sub-integration, the associated integration weights defined in the sub-line element are directly used for the final integration in the parent quad element together with the mapped Gauss points. The reader is kindly referred to papers P4 and P5 for more detailed information on the cut element method.

2.3 A note on the implementation

The framework that is developed for solving strongly coupled vibroacoustic problems is implemented using C++. Parallelization of the developed code is achieved using the PETSc library [8–10] which is utilized for its parallel data management. For the solution of linear system of equations, the developed framework employs the parallel direct solver MUMPS [5, 6]. The code supports unstructured meshes for which quad and triangle elements are implemented. A text based user case configuration system is considered to be able to alter material properties, optimization parameters and boundary conditions of the problem without the need of recompiling the code with each parameter change. Both the segregated analysis that uses unstructured meshes and the immersed boundary method are included in the developed framework where
2.3. A note on the implementation

the choice of the modelling approach is done in the configuration files. Segregated analysis is mainly utilized for validation purposes throughout the work. For visualizing data (optimized design and state fields), the code outputs VTK files for which the open-source data visualization tool Paraview [4] is used.
The chapter introduces the design parameterization together with the general optimization problem used for broadband applications and the utilized design update scheme for the developed transient optimization framework for vibroacoustic problems. Furthermore, after a brief summary on the sensitivity analysis, the chapter also presents a gradient validation study with a further motivation on the choice of the discrete adjoint method for sensitivity analysis.

### 3.1 Design parameterization

The section introduces the design parameterization used for the developed transient optimization framework. The design parameterization describes the link between the mathematical design variable $s$ and the function $\bar{s}$ in which the current design configuration that is used in the finite element analysis is contained. Here it is noted that, the design variable $s$ is also discretely defined on the nodes of the mesh. The work utilizes a design parameterization that is similar to [7] which follows a level set type approach based on density methods where the design variable $s$ has the following bounds

\begin{equation}
0 \leq s \leq 1
\end{equation}

Using the above bounds in equation (3.1) for the design variable $s$, aligns the utilization of gradient based optimizers with the standard density based topology optimization methods. Moreover, an implicit limit is applied to the rate of the interface (zero iso-level) progress through design updates with the following mesh dependent mapping applied on the design variable $s$ as

\begin{equation}
-0.5h_e \leq \tilde{s}(s) \leq 0.5h_e
\end{equation}

where $h_e$ is the element edge length. Furthermore, a convolution filter is applied on $\tilde{s}(s)$ in order to regularize the optimization problem. Filtering step stabilizes the optimization process with increasing the zone of influence of the sensitivities which also speeds up the design process. The utilized filter is from the work of [28] which is based on a Helmholtz type differential equation. For realizing a stable solution, the filter equation is implemented employing the finite volume method in which variables are represented as piece-wise constants and stored in cell centers. The filter equation is written here as

\begin{equation}
-r^2 \nabla^2 \tilde{s}_c + \tilde{s}_c = \tilde{s}_c
\end{equation}
where \( r \) is the radius of the filtering and \( c \) denotes the variables which are stored in cell centers. Together with the added stability, finite volume discretization also allows the usage of any filter size \( r \) in the filter equation. The solution of the filter equation \( \bar{s}_c \) is then interpolated back to nodes resulting into the scalar function \( \bar{s} \) describing the current design configuration on which the cut element method is applied to carry out the finite element analysis. As it can be seen from the filter equation (Eq. 3.3), overall two interpolation operations are involved which are interpolating from nodes to element centers and from element centers to nodes. These interpolations result in extra implicit filtering which is present even in the case of setting the filter radius \( r \) to zero.

Here it is noted that, unlike density based methods, the presented design parameterization does not provide a minimum length scale for the optimization. This is because the zero iso-level of the scalar function \( \bar{s} \) determines the partial interfaces inside cut elements which makes the minimum feature size directly dependent on the element size used in the mesh. However, if needed, the so-called robust approach [7, 43] can be utilized to introduce a minimum length scale for the optimization. Similar to level set methods, when utilized for 2D optimization problems, the presented approach cannot introduce holes in the design throughout the optimization. The design updates in the optimization process are realized from the change in the interface (zero iso-level) of the design. However, 3D optimization with the presented approach does not have a such constraint. Thus, when considering 2D problems, the framework is termed a generalized shape optimization method.

### 3.2 Optimization problem and the design update scheme

The section introduces the general optimization problem considered for the optimization of broadband vibroacoustic problems. The optimization aims to tailor the frequency content of the transient response obtained from the time domain solution of the coupled vibroacoustic system. In order to achieve this, the objective function is defined in frequency domain. The frequency response of the coupled vibroacoustic system is obtained with a FFT operation which is applied on the transient response of the system. The considered optimization problem has the following form,

\[
\min_{\bar{s}} \quad \Phi = \sum_{m=0}^{M} \phi^m \left( U^n_f(\bar{s}) \right) \\
\text{s.t.} \quad \mathbf{R}^n(\bar{s}, U^n(\bar{s})) = 0, \quad \text{for} \quad n = 0, 1, \ldots, N \\
0 \leq \bar{s} \leq 1 \\
\psi_i \leq 0
\] (3.4, 3.5, 3.6, 3.7)

where the objective function is denoted as \( \Phi \), \( U^n \) is the vector of state variables for the current time step \( n \) and \( N \) is the total number of time steps considered in the transient solution of the coupled system. \( \mathbf{R}^n \) is the residual vector which is obtained from the discretization of the coupled system. The vector of state variables defined in frequency domain is denoted as \( U^n_f \) which is calculated with FFT applied on
3.3. Discrete adjoint method

The solution $U^n$. $M$ is the total number of discrete frequencies considered in the objective function and $\psi_i$ is the additional constraint function that is considered in the optimization problem.

Throughout the work, the method of moving asymptotes (MMA) algorithm [41] is employed for the solution of the optimization problem given in equations 3.4 to 3.7. The developed framework uses the method’s parallel PETSc implementation from [2].

The overall algorithm used for the developed optimization framework for the transient vibroacoustic problems is summarized as

1. Initialize the initial design variable $s$ (usually a structure having holes for increasing the design freedom).
2. Apply the design parameterization on $s$ to obtain $\bar{s}$.
3. Carry out the finite element discretization and apply the cut element method using $\bar{s}$.
4. Solve the transient coupled system.
5. Solve the adjoint equation
6. Calculate the sensitivities with respect to $\bar{s}$ and apply chain rule onto it to obtain the sensitivities with respect to the design variable $s$.
7. Update the design variable $s$ using the MMA algorithm.
8. Stop the interactions if the change in design is less then a given tolerance or continue from the step 2.

3.3 Discrete adjoint method

This section gives a summary on the sensitivity analysis for calculating the gradients of the objective and constraint functions with respect to the design variable. For general transient optimization problems, paper P4 provides a thorough explanation of the discrete adjoint method which is applicable to any time integration scheme. The given sensitivity analysis covers the summarized details for transient problems where the objective function is defined in frequency domain for which the derivation can be found in paper P5. Here, the considered gradient calculation with the discrete adjoint method considers the transformation from time domain to frequency domain via the FFT operation. The work employs the FFTW library [17] in order to apply the discrete Fourier transform to the transient response of the vibroacoustic system.

Time dependent sensitivity analysis is commonly carried out by the so called semi-discrete adjoint method for its ease of implementation. The term semi-discrete means that the problem is considered discrete in space but continuous in time. The derivation of the adjoint equation is done assuming the objective function is defined in time domain. Hence, the discrete FFT operation can not be incorporated within the semi-discrete approach. The work employs a discrete adjoint method to calculate
consistent and exact sensitivities where any objective or constraint function can be considered for gradient calculation.

For applying the discrete adjoint method, the objective function is augmented with a vector of Lagrangian multipliers $\Lambda$ realizing the Lagrangian function $L$

$$L = \Phi(U_f(U(\bar{s}))) + \sum_{n=0}^{N} \Lambda^n R^n (\bar{s}, U^n(\bar{s})) \quad (3.8)$$

As it can be seen from the above equation, the objective function $\Phi$ is a function of state variables in frequency domain $U_f$. The Lagrangian function $L$ recovers the original objective function $\Phi$ since the residual of the forward system is satisfied at each time step $R^n = 0$. Moreover, the derivative of the Lagrangian function with respect to $\bar{s}$ is

$$\frac{dL}{d\bar{s}} = \sum_{n=0}^{N} \left( \frac{\partial \Phi}{\partial U_f} \frac{\partial U_f}{\partial U} \right)^n \frac{\partial U^n}{d\bar{s}} + \Lambda^n T \left[ \frac{\partial R^n}{d\bar{s}} + \frac{\partial R^n}{dU^n} \frac{\partial U^n}{d\bar{s}} \right] \quad (3.9)$$

where the partial derivative of the objective function with respect to the transient state variable $\frac{\partial \Phi}{\partial U_f}$ is realized with the term $\left( \frac{\partial \Phi}{\partial U_f} \frac{\partial U_f}{\partial U} \right)^n$ in which the partial derivative $\frac{\partial U_f}{\partial U}$ is the utilized FFT operation. Furthermore, $\frac{\partial \Phi}{\partial U^n}$ is calculated with applying the partial derivatives in $\left( \frac{\partial \Phi}{\partial U_f} \frac{\partial U_f}{\partial U} \right)^n$ in reverse order. Meaning that, $\frac{\partial \Phi}{\partial U^n}$ is obtained, which is in time domain, by applying an inverse FFT on $\frac{\partial \Phi}{\partial U_f}$.

Using the fact that Lagrangian multipliers $\Lambda^n$ can be freely chosen, the adjoint equation is identified from the equation 3.9 to avoid the costly calculation of $\frac{\partial U^n}{d\bar{s}}$, which reads as

$$\frac{\partial R}{\partial U} T \Lambda = - \frac{\partial \Phi}{\partial U} \quad (3.10)$$

Here the adjoint equation contains the all time steps considered in the problem and hence the superscript $n$ is not used. The adjoint equation is solved with reverse pseudo time steps because of the transpose operation applied on $\frac{\partial R}{\partial U} T$. Moreover, after solving for the Lagrangian vector $\Lambda$ that satisfies the adjoint equation, the final sensitivity of the objective function is again calculated using the equation 3.9.

Having completed the sensitivity analysis, the gradient $\frac{\partial \Phi}{\partial \bar{s}}$ is obtained. Finally, the appropriate chain rule describing the design parameterization is applied on it to calculate the gradient of the objective function with respect to the design variable $\frac{\partial \Phi}{\partial \bar{s}}$.

### 3.4 Gradient validation

This section validates the implementation of the discrete adjoint method for gradient calculation. The method is also compared against the commonly used semi-discrete
3.4. Gradient validation

approach [12] in order to further motivate the discrete adjoint approach for transient optimization.

As it has been mentioned before, using the semi-discrete approach, the gradient calculation and the derivation of the adjoint equation is done analytically in time using only spatially discretized system of equations. Hence, the utilized time integration scheme does not play a role in the derivation process. This results in an adjoint equation having the same form as the spatially discretized forward problem where the time stepping algorithm used for the forward problem is commonly reused also for the adjoint equation.

A straightforward problem setup is used to validate and compare the calculated sensitivities. The schematic illustration of the problem is given in figure 3.1 in which the highlighted domain illustrates the region where the objective function is evaluated. The considered objective function is the summation of the absolute downstream acoustic pressure in the objective region over all time steps. For boundary conditions, the top and the bottom boundaries are realized as hard-wall conditions. An incoming sinusoidal acoustic plane wave having an amplitude of $p_{in} = 1$ kPa is applied at the left most boundary and the right most boundary realizes an open boundary. The study considers a simple circular structure in the middle of the acoustic channel and the calculated sensitivities will be investigated at the interface of the structure.

$$\mathbf{n_a} \nabla p = 0$$

$$\mathbf{n_a} \nabla p = 0$$

Figure 3.1: Schematic illustration of the sensitivity validation case showing the boundary conditions of the problem. Gray color shows the initial circle structure having the center at (2.25m, 1.0m) with a radius of 0.16m. Blue region illustrates the region where the objective function is evaluated. The figure is taken from paper P4.

For the first study, the gradients calculated with both semi and fully discrete adjoint methods are compared and checked against a finite difference calculation considering a backward difference method. A design variable from a cut element is randomly selected to carry out the investigation. For the comparison, different number of time steps are considered with keeping the time step size $\Delta t$ as constant in order to investigate the effect of the number of time steps on the quality of the calculated gradients with the both methods.

The result of the finite difference check study is presented in figure 3.2. As it can be seen from the figure, the correct first order convergence is demonstrated for the finite difference check of the discrete adjoint method for all of the considered number of time steps. Since, the quality of the gradients calculated with the discrete
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Sensitivity analysis does not depend on the number of time steps or the utilized time step size and the method always produces consistent sensitivities. However, for the semi-discrete approach, the calculated sensitivities approach the correct convergence behavior only with increasing the number of time steps.

Figure 3.2: Finite difference check for validating the calculated sensitivities. Blue color specifies the semi-discrete adjoint method and the black color is the discrete adjoint method. For both methods, dashed lines are 50 time steps, solid lines are 100 time steps and dash-dot lines are 200 time steps. The figure is taken from paper P4.

Figure 3.3: Calculated sensitivities $\frac{d\Phi}{ds}$ on the nodes of the mesh which are cut by the zero level set. Blue markers show the semi-discrete sensitivity calculation and black markers illustrate the discrete sensitivity calculation. The figure is taken from paper P4.
Following the finite difference check study, the produced gradients using both methods are numerically compared to each other. In order to carry out the comparison, the calculated sensitivities are extracted from the design variables which are located in the cut elements forming the lower half of the circular structure.

The result of the comparison is presented in figure 3.3 where the calculation considers 50 time steps for both methods. The figure shows that the calculated gradients follow the same trend in magnitude. However, the difference between the gradients calculated with the semi and the fully discrete adjoint methods becomes more apparent at the locations where the calculated sensitivities undergo a sign change. As it can be seen from the figure, inconsistent and wrong signed sensitivities are obtained with the semi-discrete approach which would drive the optimization process towards the opposite direction. Overall, the current findings motivate the usage of the employed fully discrete adjoint approach for calculating consistent sensitivities.
Applications

This chapter presents various numerical examples based on the developed framework for generalized shape optimization of transient vibroacoustic problems. The presented examples are mainly taken from the papers P4 and P5. The reader is kindly referred to the indicated papers for more in depth information and discussion regarding the presented results.

4.1 Acoustic pulse shaping

This section considers the design of a structure where the pulse shape of the averaged transmitted acoustic pressure at the outlet of an acoustic channel is to be fitted to a desired pulse shape after passing through a structural partitioner. The considered design problem is inspired from the work of [29] where the topology optimization of 1D pulse shaping designs are considered for wave propagation problems. The work extends the problem to 2D considering coupled vibroacoustic systems.

![Figure 4.1: Schematic illustration of the optimization case for acoustic pulse shaping at the outlet showing the boundary conditions of the optimization problem. Top red line specifies the symmetry plane and gray color shows the design domain. Input acoustic pulse and the desired pulse shape at the outlet are also shown. The figure is taken from paper P4.](image)

Figure 4.1 shows the schematic illustration of the computational domain for the optimization case in which the considered boundary conditions are also shown. As it is seen from the figure, the top boundary is set as a symmetry plane for both physics which is done to reduce the computational cost. For the bottom boundary, the structure is considered to be fully clamped and the hard-wall boundary condition is applied for the acoustic pressure. The right boundary (outlet of the acoustic channel)
realizes an open boundary with applying the absorbing boundary condition. The left boundary is also an absorbing boundary in which the incoming acoustic pulse which is composed of frequencies roughly between 1000 Hz and 3000 Hz is shown in the figure. The incoming acoustic pulse is realized as a plane wave. The figure also shows the desired pulse shape for the averaged acoustic pressure at the outlet of the acoustic channel. Furthermore, the structure in the design domain is chosen to be a rubber-like material and the acoustic domain is considered to be air.

Figure 4.2: Optimization for acoustic pulse shaping at the outlet. (a) Initial configuration $\Phi^* = 0.9945$. (b) Calculated acoustic pulse shape with the initial configuration, black line is the desired pulse shape and blue line is the calculated pulse shape. (c) Optimized design $\Phi^* = 0.0045$. (d) Calculated acoustic pulse shape with the optimized design, black line is the desired pulse shape and blue line is the calculated pulse shape. The figure is taken from paper P4.

Figures 4.2a and 4.2c show the initial configuration and the optimized design, respectively. The calculated envelope of the averaged transmitted acoustic pressure for the initial configuration is given in figure 4.2b together with the desired pulse shape. As it can be seen from the figure, after the initial impact of the incoming acoustic pulse has passed, the vibrations in the initial structure are quickly damped causing the transmitted acoustic pressure at the outlet to vanish. On the other hand,
4.1. Acoustic pulse shaping

the optimized design (figure 4.2c) realizes approximately 99.5% increase when the objective values given in the figure are compared. The performance increase is also apparent in figure 4.2d in which the calculated pulse shape of the averaged acoustic pressure at the outlet follows closely the desired envelope shape.

As it can be seen from comparing the initial guess to the optimized structure, the optimization mainly changes the shape and the size of the internal acoustic cavities through which the interaction between the acoustic and structural responses is increased significantly and the optimization is able to successfully tailor the transient response of the coupled system. Moreover, when the optimized design is re-analyzed with a stiffer material, the performance of the structure worsens significantly which shows that the desired performance is indeed achieved with utilizing the vibroacoustic coupling. Here it is noted that, a geometric robust approach should be included in the optimization process when considering fabrication since the optimized design is quite sensitive to boundary variations, or defects.

Figure 4.3: Sound pressure level [dB] contours of the optimized design for the second pulse shaping example. The given pressure field is from the time 0.007 s. The figure is taken from paper P4.

The sound pressure level field of the optimized design is given in figure 4.3 which is taken at the time step 0.007 s where the first peak occurs in figure 4.2d. It can be seen from the figure that the pressure has a uniform distribution across the outlet. Although, this is not the case for all time steps, uniform distribution is attained throughout majority of the considered time-span since the optimization tailors the averaged acoustic pressure pulse shape at the outlet of the acoustic channel. Moreover, as it is seen from figure 4.2c, two very small holes are present in the optimized design. When the sound pressure field plot (figure 4.3) is inspected, it can be said that these holes have a negligible intensity and hence, provide no significant contribution to the performance of the optimized pulse shaping device.


4.2 Broadband applications

In this section, the numerical setup which is utilized for the optimization of acoustic filter designs is presented. The objective function is defined in frequency domain in order to tailor the frequency content of the response of the coupled system.

\[
\begin{align*}
\mathbf{u} &= 0 \\
\mathbf{n}_a \nabla p &= 0
\end{align*}
\]

\[
\begin{align*}
\Omega_a & = 0.1 \text{m} \\
\Omega_s & = 0.3 \text{m}
\end{align*}
\]

\[
\mathbf{n}_a \nabla p &= 0
\]

\[
\begin{align*}
\Omega_a & = 0.1 \text{m} \\
p_{\text{out}} & = 0
\end{align*}
\]

\[
\begin{align*}
p_{\text{in}} & = 0 \\
p_{\text{out}} & = 0
\end{align*}
\]

Figure 4.4: Schematic illustration of the optimization case for the design of acoustic filters showing the boundary conditions of the optimization problem. Gray color shows the design domain. Incoming acoustic white noise and an example desired filter shape at the outlet are also shown. The figure is taken from paper P5.

The optimization considers wide frequency range in order to design efficient acoustic filters and a measure of transmission is defined to be able to apply various filter shapes to alter the response of the system. The transmission \( S(f) \) reads as

\[
S(f) = \frac{\hat{p}(f)}{\hat{p}_0(f)}
\]

(4.1)

Here, the \( \hat{\cdot} \) notation denotes the transmitted acoustic pressure signal which is averaged at the outlet of the considered acoustic channel and the subscript 0 illustrates the transmitted acoustic pressure for an empty channel (without any structural partitioner in the channel). Both \( \hat{p}(f) \) and \( \hat{p}_0(f) \) are calculated with applying discrete Fourier transform to \( \hat{p}(t) \) and \( \hat{p}_0(t) \) which are obtained from the transient response of the vibroacoustic system, respectively.

Throughout the optimization, the calculated transmission \( S(f) \) is fitted to a prescribed filter shape. When the value of \( S(f) \) is unity, a full transmission is achieved for a particular frequency. This means that the amplitude of the transmitted acoustic pressure with the presence of a vibrating structure inside the acoustic channel is equal to that of an empty duct. Similarly, when the value of \( S(f) \) is zero, no transmission is realized as the vibrating structure does not transmit acoustic pressure towards outlet of the acoustic channel. For a stable optimization, the transmission \( S(f) \) is not lowered to zero but to a small positive number i.e. \( 1 \times 10^{-3} \) or \( 1 \times 10^{-4} \). Realizing
three or four orders of magnitude decrease in the amplitude of the transmitted acoustic pressure compared to that of an empty channel was deemed sufficient to realize effective stop-band regions for the considered acoustic filters.

Figure 4.4 gives a schematic illustration of the design problem used for the optimization of acoustic filters. As it is seen from the figure, the hard-wall condition is enforced for the acoustic pressure at the top and bottom boundaries while the structure is clamped. Both left and right most boundaries are set as absorbing boundary conditions. The incoming plane wave from the left boundary is also shown in the figure. The incoming acoustic plane wave is set as a white noise having approximately constant energy content across all the frequencies present in the signal in which the random acoustic pressure values vary between $-1\text{Pa}$ and $1\text{Pa}$. This incoming wave is utilized to excite broad frequency range in the coupled vibroacoustic system. Furthermore, an example low-pass filter shape is also illustrated in the figure which is applied to the acoustic transmission $S(f)$ calculated at the outlet of the acoustic channel. The optimization aims to fit the calculated transmission $S(f)$ to the desired transmission shape and the presented numerical examples consider various filters for the optimization.

![Figure 4.5: Initial design that is used for the optimization of acoustic filters. The figure is taken from paper P5.](image)

The initial configuration that is used for the numerical examples presented in sections 4.2.1 and 4.2.2 is given in figure 4.5. The given initial design is selected such that nearly full transmission is realized for the frequency range that is considered by the optimization cases. Paper P5 also contains an initial guess study for the optimization of acoustic filters. Moreover, the acoustic domain is taken as air and the structure is considered to be a soft rubber-like material.

### 4.2.1 Band-pass and band-stop acoustic filter designs

This section firstly considers the optimization of an acoustic band-pass filter design. The frequency range considered for the band-pass filter is from 1000 Hz to 5500 Hz in which the frequencies between $2500 \text{ Hz} \leq f \leq 4000 \text{ Hz}$ define the pass-band region of the filter whereas the frequencies $1000 \text{ Hz} \leq f < 2500 \text{ Hz}$ and $4000 \text{ Hz} < f \leq 5500 \text{ Hz}$ form the stop-band regions of the filter. The optimization employs two objective functions $\Phi_1$ and $\Phi_2$ minimizing the difference between the calculated transmission $S(f)$ with the desired filter shape for pass-band and stop-band regions, respectively.

The initial configuration (which is given in figure 4.5) for the optimization has the objective function values of $\Phi_1 = 0.0154458, \Phi_2 = 1.15859 \times 10^8$. The large value
of the objective function $\Phi_2$ for the stop-band region of the filter is due to the inverse weighting that is utilized for the objective functions. The utilized inverse weighting was found to be efficient in the optimization of acoustic filters. A further study and a discussion on the choice of the objective functions are provided in Paper P5.

Figure 4.6: Optimization for an acoustic band-pass filter design. (a) optimized design. (b) transmission of the optimized design in the considered frequency range. Black line is the desired band-pass filter, blue line is the response of the optimized design, gray dashed line is the response of the initial guess design. (c) averaged SPL response of the optimized design calculated at the output, gray line is the empty acoustic duct, blue line is the response of the optimized design. The figure is taken from paper P5.

The result of the optimization for an acoustic band-pass filter design is given in figure 4.6. Moreover, figure 4.6a shows the optimized design where the objective functions are also given. When comparing the objective functions of the initial configuration and the optimized design, it can be seen that $\Phi_2$, which acts on the
4.2. Broadband applications

Stop-band region of the filter, is minimized significantly whereas $\Phi_1$ of the optimized design, which is active for the pass-band region, ends up at a higher value. This can also be visually inspected from figure 4.6b where the calculated transmission $S(f)$ of the initial and the optimized designs are presented. The figure shows that the initial design has a nearly full transmission across the frequencies 1000 Hz to 5500 Hz and the optimized design transmits frequencies while closely following the desired band-pass filter shape. It can be said that the performance drop of the pass-band region of the filter (frequencies between $2500 \text{ Hz} \leq f \leq 4000 \text{ Hz}$) is largely due to the transitions from the stop-band to pass-band and vice versa. The effectiveness of the optimized design for the considered band-pass filter can be further seen from figure 4.6c where the averaged sound pressure level (SPL) responses calculated at the outlet of the acoustic channel is given for the optimized design and the empty acoustic channel. As it can be seen from the figure, for the stop-band regions of the filter, the optimized design lowers the SPL values to approximately around 0 dB whereas the SPL response of the empty acoustic channel is clustered around 60 dB. At the pass-band, the design’s SPL response closely follow the SPL response of an empty acoustic channel.

When the initial configuration given in figure 4.5 and the optimized design in figure 4.6a is compared, it can be seen that the design process results in a significant topological change. It is interesting to note that, the optimized design (figure 4.6a) forms an acoustic cavity in the middle of the design domain which shows that the coupling from acoustic and structural interactions are utilized in the optimization. Overall, the developed transient optimization framework is applied successfully to tailor the frequency response of the coupled vibroacoustic system.

The framework is further applied to the design of an acoustic band-stop filter. The considered filter can be seen as the opposite of the pass-band filter previously demonstrated. Again the optimization considers the frequencies between 1000 Hz and 5500 Hz. The pass-band region of the filter is realized at the frequencies $1000 \text{ Hz} \leq f < 2500 \text{ Hz}$ and $4000 \text{ Hz} < f \leq 5500 \text{ Hz}$ and the stop-band is chosen to be at $2500 \text{ Hz} \leq f \leq 4000 \text{ Hz}$. The initial configuration is given in figure 4.5 which resulted in initial objective values of $\Phi_1 = 0.0552177$, $\Phi_2 = 5.8754 \times 10^7$.

Figure 4.7 presents the result of the optimized acoustic band-stop filter in which the optimized design can be seen in figure 4.7a. Moreover, figure 4.7b shows the desired band-stop filter and the calculated transmission $S(f)$ of the optimized and the initial designs. As it can be seen from both figure 4.7b and the objective values given in figure 4.7a, the transmission of the coupled system was successfully lowered to the desired level at the stop-band region of the filter. The optimized design’s calculated transmission closely follow the desired band-stop filter where sharp transitions from the pass-band to the stop-band (around 2500 Hz) and from the stop-band to the pass-band (around 4000 Hz) are realized.

Figure 4.7c shows the averaged SPL values calculated at the outlet of the acoustic duct for the optimized design and an empty channel. The figure further shows the performance of the optimized acoustic band-stop filter where the pass-band regions attain the overall 60 dB and approximately 0 dB is achieved at the stop-band region of the acoustic filter.
When the optimized designs given in figures 4.6a and 4.7a are compared, it can be said that the both designs resulted in highly different design configurations and underwent significant topological changes compared to the initial configuration (figure 4.5). Moreover, the lack of minimum feature size control for the optimization process can be seen from the small features of the optimized designs. As it is pointed out in section 4.1, the present results also signify the fact that a geometric robust approach is needed when considering fabrication. Overall, the developed framework is successfully applied for designing acoustic band-pass and band-stop filters.
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4.2.2 Validation study for an acoustic low-pass filter

This section considers the optimization for an acoustic low-pass filter design and aims to validate the performance of the optimized design using a commercial software. To this end, after the optimization is carried out, the optimized design is further processed and meshed using a body-fitted mesh and a segregated analysis is carried out using the COMSOL Multiphysics software [1]. As it has been introduced in previous sections, the transmission $S(f)$ of the design is calculated with applying FFT on the transient response of the coupled system when the system is excited with the incoming white noise realized with random pressure oscillations. However, in order to compare and validate the calculated transmission $S(f)$ of the design, instead of using a transient analysis, widely utilized time-harmonic frequency domain analysis is employed to realize a frequency-sweep on the system. This means that the system is solved at discrete frequencies for the frequency range that is considered by the optimization to realize steady-state solutions at each frequency. The system is excited with an incoming sinusoidal wave for each frequency. The calculated transmission $S(f)$ is then compared against the one obtained with the developed transient framework.

![Graph showing optimization results](image)

Figure 4.8: Optimization for an acoustic low-pass filter design. (a) optimized design. (b) transmission of the optimized design in the considered frequency range. Black line is the desired low-pass filter, blue line is the response of the optimized design, gray dashed line is the response of the initial guess design and the orange line is the COMSOL calculation done in frequency domain with body-fitted analysis.

The low-pass filter considered by the optimization acts on the frequencies between
500 Hz and 3500 Hz. The pass-band region of the filter is realized at the frequencies $500 \text{ Hz} \leq f \leq 2000 \text{ Hz}$ and the stop-band is at $2000 \text{ Hz} < f \leq 3500 \text{ Hz}$. Differently from the previous band-pass and band-stop filters, the stop-band of the current low-pass filter is lowered to $S(f) = 1 \times 10^{-4}$ in order to realize four orders of magnitude decrease in the amplitude of the transmitted acoustic pressure compared to that of an empty channel. The optimization utilizes the initial configuration given in figure 4.5 where the initial objective values are $\Phi_1 = 0.0385819$, $\Phi_2 = 5.8394 \times 10^3$.

![Figure 4.9: Time-harmonic frequency domain analysis of the optimized design for the acoustic low-pass filter showing the sound pressure level [dB] contours of the design. (a) The result from the pass-band at $f = 1100 \text{ Hz}$. (b) The result from the stop-band at $f = 2900 \text{ Hz}$.](image)

The result of the acoustic low-pass filter optimization is given in figure 4.8 in which the optimized design is shown in figure 4.8a. It can be seen that the optimized design resulted in significant topological changes compared to the initial configuration. The transmission $S(f)$ of the optimized design in the considered frequency range is given in figure 4.8b along with the desired low-pass filter and the transmission of the post-processed design obtained with frequency domain calculation using COMSOL. As it can be seen from the figure, the calculated transmission closely follows the pass-band of the filter and after a sharp transition from the pass-band into the stop-band region, which is around $2000 \text{ Hz}$, the transmission is successfully lowered to approximately $S(f) = 1 \times 10^{-4}$. The figure further compares the calculated transmissions obtained from the result of the optimization, using the transient framework with the cut element method, to the body-fitted segregated analysis done in frequency domain. As it is seen, the calculated transmission agrees well with the COMSOL calculation. The small discrepancies in the response can be explained from the fact that, the
frequency domain analysis realizes steady-state solutions at each discrete frequency whereas the developed framework utilizes a finite transient signal in order to obtain the transmission through the FFT operation. Meaning that the transient system is not solved to steady-state as it would be computationally unreasonable since the system is excited with random pressure oscillations. It should also be pointed out that, when the optimized design is extracted from the zero iso-level of $\bar{s}$ and meshed with unstructured meshes, a slight alteration of the interface is unavoidable. Overall, it can be said that the optimized design also shows a good performance as an acoustic low-pass filter when analyzed with frequency domain methods using body-fitted segregated analysis. The study validates the applicability of the developed transient framework for broadband applications considering coupled vibroacoustic systems.

Furthermore, figure 4.9 shows the SPL fields of the optimized design from the body-fitted COMSOL calculation. The pressure response at $f = 1100$ Hz which is given in figure 4.9a falls within the pass-band region of the considered frequency range. As it can be seen from the figure, the design allows the incoming wave to pass resulting in approximately constant SPL response at around 110 dB. On the other hand, figure 4.9b shows the response of the system at the frequency $f = 2900$ Hz which is in the stop-band region of the filter. As it is seen, through the interaction between the structural vibrations and pressure oscillations, the incoming wave is stopped and the design realizes SPL values of below 0 dB at the outlet of the acoustic channel.
This part of the thesis presents generalized shape optimization of vibroacoustic problems. The work extends the cut element approach to the coupled vibroacoustic problems and improves upon the state-of-the-art methods with applying transient optimization.

The developed framework utilizes a level set approach for the geometry description where the geometry is implicitly defined from the zero iso-level of a scalar function specifying the interface between acoustic and structural domains. In order to keep a fixed background mesh throughout the optimization, the work utilizes an immersed boundary cut element method which allows the elements to be cut by the interface boundary. Using the method's special integration scheme, the interface between the two physics is accurately resolved without the addition of extra degrees of freedom to the system. This way, the cut element method is easily be added into the existing parallel FEM frameworks.

For optimization, exact and consistent gradients of objective and constraint functions are calculated using the discrete adjoint method. Sensitivity analysis is done following a general derivation in order to allow for the inclusion of different time integration schemes. Moreover, for the cases where the objective function is defined in frequency domain which are used to realize wideband optimization, the implemented discrete adjoint approach also handles the FFT operation to calculate consistent sensitivities.

A simple numerical study is carried out for the validation of the calculated sensitivities using the discrete adjoint method. The study also compares the discrete and semi-discrete methods in order to provide a further motivation for the utilization of discrete adjoint approach. It is shown that the fully discrete approach always produces consistent sensitivities. However for the semi-discrete approach, the number of time steps used for the forward and adjoint equations significantly affect the quality of the calculated gradients. Because of the inconsistent gradient calculation within the semi-discrete approach, even wrong signed sensitivities can be calculated as it is shown for an extreme case.

The applicability of the developed framework is first demonstrated with a transient application in which the design of an acoustic pulse shaping device is considered. The system is excited with an incoming acoustic pulse consisting of frequencies between 1000 Hz and 3000 Hz. The optimization tailors the pulse shape of the transmitted acoustic pressure averaged at the outlet of the acoustic channel in order to fit it to a predefined shape. The optimized design realizes approximately 99.5% percent performance increase compared to the initial configuration and also shows topological changes mainly due to the versatility of the used optimization approach.

In order to demonstrate the advantages of transient optimization, the Thesis further presents the utilization of time-domain methods to realize broadband optimization in frequency domain considering coupled vibroacoustic problems. To achieve this, the optimization framework is applied to the design of acoustic band-
pass and band-stop filters, acting on the frequencies between 1000 Hz and 5500 Hz, where the both optimized designs resulted in efficient acoustic filters. Significant topological changes are realized for the optimized designs compared to the initial configuration, again demonstrating the versatility of the developed framework. The performances of the optimized designs can also be seen from the averaged SPL values calculated at the outlet of the acoustic channel where the pressure is lowered to around 0 dB in the stop-band for both filters. Furthermore, a validation study is carried out for the optimization of an acoustic low-pass filter where the result is post-processed and compared against a commercial software that uses widely utilized time-harmonic frequency domain analysis to realize a frequency-sweep on the system. As it is illustrated, the transmission of the design calculated with the developed transient framework agrees well with the one calculated with the frequency domain analysis done on the post-processed design. The study validates the applicability of the developed transient framework for broadband applications considering coupled vibroacoustic systems.

5.1 Future work

This section presents some ideas for future work which could be implemented to extend or improve upon the developed transient optimization framework for vibroacoustic systems.

- As mentioned before, the developed transient optimization framework utilizes parallel calculations and is built to be run on computer clusters. However, the solver employs a parallel direct solver for the solution of linear system of equations which do not exhibit scalability. Since the framework works on time-domain calculations, the utilization of iterative solvers can be incorporated into the framework (such as the multi-grid algorithm) which would greatly increase the scalability of the code. This would pave the way for the optimization of large-scale transient vibroacoustic systems.

- Even though implicit time-stepping schemes, such as the utilized Newmark algorithm, bring stability and allow for large steps to be taken in time-stepping, properly resolving vibroacoustic problems in time often require small time steps. Hence, explicit schemes such as the family of Euler methods that do not require solving a system for stepping in time can be considered to realize efficient and fast transient optimization.

- The utilized methods and the developed methodology can be readily extended to 3D calculations where i.e. a part of a hearing aid can be optimized. The optimized design can be manufactured with 3D printing which in turn could facilitate an experimental work for a further validation of the transient vibroacoustic optimization framework.

- Optimization of loudspeakers can be considered with applying the developed broadband optimization methodology to include wide frequency range in the optimization.
Part II

Topology optimization of turbulent flow and forced convection systems

[P1,P2]
6 Governing equations

6.1 Incompressible Reynolds-averaged Navier-Stokes equations

Throughout the work, the fluid flow is modeled with the steady-state incompressible Reynolds-averaged Navier-Stokes (RANS) equations which are written as

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = \nabla \cdot (2\nu S) - \frac{1}{\rho} \nabla p + \nabla \cdot \mathbf{T}_t - \lambda \chi(\gamma) \mathbf{u} \]  \hspace{1cm} (6.2)

where \( p \) is the pressure and the mean velocity vector is denoted by \( \mathbf{u} \), \( \rho \) and \( \nu \) are the density and the kinematic viscosity of the fluid, respectively. The standard Brinkman penalization is employed to model the effect of solid material on the fluid flow where \( \lambda \) is the so-called Brinkman parameter. \( \chi(\gamma) \) is a dimensionless function which takes values in the range of \( 0 \leq \chi(\gamma) \leq 1 \). The function \( \chi(\gamma) \) denotes a spatially varying porosity field where the lower (\( \chi(\gamma) = 0 \)) and the upper (\( \chi(\gamma) = 1 \)) bounds represents fluid and solid, respectively. Hence, no-slip boundary condition is approximated for solid-regions when \( \chi(\gamma) = 1 \) and a sufficiently large \( \lambda \) is used. The mean strain rate tensor \( S \) in equation 6.2 reads as

\[ S = \frac{1}{2} \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \]  \hspace{1cm} (6.3)

and the additional effects of turbulence are modeled with the Reynolds stress tensor given here as

\[ \mathbf{T}_t = -\mathbf{u}' \otimes \mathbf{u}' = 2\nu_t S - \frac{2}{3} k \mathbf{I} \]  \hspace{1cm} (6.4)

where the so-called turbulent fluctuating velocities are denoted with the prime notation and \( k \) is the turbulent kinetic energy per unit mass. In order to achieve closure, further equations are needed to define the turbulent eddy viscosity \( \nu_t \). The work utilizes the two-equation \( k-\omega \) model [45] which calculates the turbulent eddy viscosity \( \nu_t \) as

\[ \nu_t = \frac{k}{\tilde{\omega}}, \quad \tilde{\omega} = \max \left[ \omega, C_{lim} \sqrt{\frac{2S:S}{\beta^2}} \right], \quad C_{lim} = \frac{7}{8} \]  \hspace{1cm} (6.5)
Moreover, the turbulent kinetic energy $k$ and the specific dissipation rate $\omega$ are calculated from the solution of two additional steady-state transport equations

\[
\nabla \cdot (u k) = T_t; \nabla u - \beta^* \omega k + \nabla \left[ \left( \nu + \sigma^* \frac{k}{\omega} \right) \nabla k \right] - \lambda \chi(\gamma) k \tag{6.6}
\]

\[
\nabla \cdot (u \omega) = \frac{\alpha \omega}{k} T_t; \nabla u - \beta \omega^2 + \frac{\sigma d}{\omega} k \nabla \omega + \nabla \left[ \left( \nu + \sigma^* \frac{k}{\omega} \right) \nabla \omega \right] + \lambda \chi(\gamma) (\omega_b - \omega) \tag{6.7}
\]

More in-depth explanation for the $k$-$\omega$ model together with its closure constants are given in \textbf{P1}. The turbulent kinetic energy $k$ has a well defined boundary at walls given as

\[
k_b = 0 \tag{6.8}
\]

Similar to momentum equations, enforcing the above condition for solidified regions is done with using the Brinkman penalization as it can be seen from the last term on the right hand side of equation 6.6.

Contrarily, the specific dissipation rate $\omega$ has a singular behavior near a wall. Throughout the work, only the modelling of smooth walls are considered for which $\omega$ utilizes an approximate non-homogeneous Dirichlet type boundary condition as proposed by [33]

\[
\omega_b = \frac{60 \nu}{\beta_1 y_1^2}, \quad \beta_1 = 0.075 \tag{6.9}
\]

where $y_1$ is the distance from the wall to the cell center nearest the wall. Throughout the Thesis, $y_1$ is defined as the half cell length since the work employs uniform elements for meshing the computational domain for topology optimization of turbulent flows. Physically, the wall boundary condition $\omega_b$ ensures that turbulent eddies become infinitesimally small as a wall is approached. Again, as it is seen from the last term of equation 6.7, the Brinkman approach is used in order to enforce the non-homogeneous Dirichlet boundary condition $\omega_b$ in the solidified regions.

### 6.2 Conjugate heat transfer equation

Throughout the Thesis, the heat sink designs only consider forced convection where it is assumed that the temperature differences in the flow are small enough such that the fluid properties stay constant. Meaning that the system is only one way coupled where the flow field is obtained from the solution of RANS equations which is then supplied to the heat equation to calculate the temperature field.

The present method considers temperature variations both in fluid and solid regions which is obtained from the conjugate heat transfer equation given here as

\[
\chi_1(\gamma) \nabla \cdot (u T) = \nabla \cdot \left[ \alpha(\gamma) \nabla T \right] + Q(\gamma) \tag{6.10}
\]
where $T$ is the temperature. Through the convection term, which is in the left hand side of equation 6.10, the effect of fluid flow is provided to the given heat equation. The dimensionless function $\chi_t(\gamma)$ is used to turn on the convection term in fluid ($\chi_t(\gamma) = 1$) and turn it off in the solid regions ($\chi_t(\gamma) = 0$). The volumetric heat source $Q(\gamma)$ is made design dependent and only realized in solidified regions. In order to obtain the thermal diffusivity $\alpha$ based on the density variable $\gamma$, the function $\alpha(\gamma)$ interpolates between the thermal diffusivity of the fluid $\alpha_f$ and solid $\alpha_s$, which are

$$\alpha_f = \left( \frac{\nu}{Pr} + \frac{\nu_t}{Pr_t} \right)$$

$$\alpha_s = \frac{k_s}{c_s \rho_s}$$

where $Pr$ and $Pr_t$ are the laminar and the turbulent Prandtl numbers, respectively. Furthermore, the thermal conductivity is given by $k_s$, $c_s$ is the specific heat capacity and $\rho_s$ is the density of the solid.

### 6.3 Discretization

The presented RANS equations with the two equation $k$-$\omega$ turbulence model and the conjugate heat transfer equation are discretized using the finite volume method [16, 42] with unstructured grid formulation. A segregated approach, namely the SIMPLE (semi-implicit method for pressure-linked equations) algorithm [38] is followed to deal with the pressure-velocity coupling of the RANS equations. For computational fluid dynamics, due to its low memory requirements, the SIMPLE algorithm is one of the most attractive schemes and usually preferred over a fully coupled approach especially when considering large scale problems. Also, the method can handle both steady and unsteady flows.

As mentioned before, the buoyancy effects on the flow are ignored for the current study. This means that the fluid and the heat transfer equations are only weakly coupled. Hence, firstly the SIMPLE algorithm is utilized to obtain the fluid velocity and the pressure distribution of the flow. Afterwards, the scalar transport equation for the heat transfer is solved using the converged fluid velocity.

The developed framework for flow and heat transfer problems is written utilizing C++. The solutions of the linear system of equations are realized employing efficient parallel sparse solvers from the PETSc library [8–10]. A thorough explanation of the discretization details together with an experimental verification of the implemented fluid dynamics solver are given in paper P1.
Design parameterization and gradient calculation

7.1 Interpolation functions and the design parameterization

This section presents the interpolation functions that are used in the given thermal-fluid model and the design parameterization followed in the subsequent topology optimization.

Considering the momentum and turbulence equations, the interpolation between solid and fluid is realized using the function $\chi(\gamma)$ [11], which is given as

$$
\chi(\gamma) = \frac{1 - \overline{\gamma}(\gamma)}{q + \overline{\gamma}(\gamma)}
$$

(7.1)

Here, the curvature of the above function is controlled by the parameter $q$. The overline notation denotes the so-called physical design variable which means that $\overline{\gamma}$ is the current design configuration that is used in the flow and the subsequent heat analyses. $\overline{\gamma}$ is obtained by first applying a filter operation [28] on the design variable $\gamma$, which is then projected using a regularized Heaviside projection [43] to calculate $\overline{\gamma}$.

In order to effectively model impermeable solid regions in the computational domain, the Brinkman penalization parameter $\lambda$ must be chosen sufficiently high. Throughout the work, the choice of $\lambda$ is tied to the dimensionless Darcy number which is defined as

$$
Da = \frac{\nu U/L}{\lambda LU} = \frac{\nu}{\lambda L^2}
$$

(7.2)

The Darcy number represents the ratio of viscous forces to Darcy damping forces. Here, characteristic velocity and length scales are denoted as $U$ and $L$, receptively, and define the given flow problem. Regardless of problem scale, using the $Da$, the Brinkman penalization parameter $\lambda$ can be chosen consistently. Through the conducted numerical experiments, it can be said that choosing the $\lambda$ parameter that results in the Darcy number $Da \approx 10^{-5} - 10^{-6}$ is found to be sufficient to yield nearly impermeable modelling of solid regions.

In order to calculate temperature variations on the current design configuration $\overline{\gamma}$ (consisting of fluid, solid and intermediate regions), the following functions are utilized in the heat equation to interpolate the convection, the diffusion and the source terms as

$$
\chi_t(\gamma) = \overline{\gamma}(\gamma)^n
$$

(7.3)

$$
\alpha(\gamma) = \alpha_s + (\alpha_f - \alpha_s) \overline{\gamma}(\gamma)^n
$$

(7.4)

$$
Q(\gamma) = (1 - \overline{\gamma}(\gamma)^n) \frac{\dot{q}}{c_s \rho_s}
$$

(7.5)
Chapter 7. Design parameterization and gradient calculation

where the parameter $n$ controls the curvature of the interpolation functions in equations 7.3 to 7.5 and $\dot{q}$ is the volumetric heat source.

7.2 Discrete adjoint via automatic differentiation

This section summarizes the sensitivity analysis used for the developed framework of turbulent flows. The main motivation behind the utilization of automatic differentiation (AD) for sensitivity analysis is that, since the system of equations are treated with a segregated approach using an iterative scheme, the Jacobian of the residual system of equations is not explicitly formed. Moreover, following a hand-coded approach, the explicit calculation of the exact Jacobian for the discrete adjoint equation is a long and highly error prone process considering the complexity of the discretization. Hence, the work makes use of AD to simplify the calculation of exact gradients with a computationally cheap procedure.

AD allows to evaluate derivatives of functions implemented as a computer code using a set of software techniques. The main idea is that, every complex function is represented by a set of primitive operations with well-known derivatives. AD then records all of the primitive operations involved in the function evaluation and applies chain rule on them to obtain the gradient of any function implemented as a computer code. This way, the calculated derivatives are exact to machine precision. Utilization of AD is generally achieved with using operator overloading techniques in modern object oriented languages such as C++. Throughout the work, AD is employed in reverse-mode and the code uses the Adept: automatic differentiation library [21].

In what follows, the section briefly summarizes the discrete adjoint method applied with using AD. The developed methodology greatly increases the generality of the optimization framework since any objective and constraint functions can be included in the sensitivity analysis with minimum effort in implementation. Here it is noted that, the reader is kindly referred to paper P1 for an in-depth explanation of the utilization of AD in discrete adjoint method. The addition of heat transfer with the subsequent derivation of discrete adjoint equations is given in paper P2. In order to facilitate the sensitivity analysis efficiently, AD is used in a selective manner. Meaning that the AD is applied only for calculating the required partial derivatives for the adjoint equation and the gradient calculation. The overall implementation is done locally without the need of parallel communications.

Following the discrete adjoint method, the adjoint equation is identified as

$$
\frac{\partial R^T}{\partial U} \lambda = - \frac{\partial C}{\partial U}
$$

(7.6)

where $R$ is the residual vector and the state vector containing the solution fields is given as $U$. As it has been mentioned, AD is employed to calculate the Jacobian $\frac{\partial R}{\partial U}$ and the partial derivative of the objective function with respect to the state variables $\frac{\partial C}{\partial U}$. In order to efficiently calculate the Jacobian, the overloaded versions of cell-wise residual functions for state variables are implemented that return a scalar value for each cell. AD then records the call to each residual function evaluation in an element loop and applies the reverse-mode to obtain a row of the Jacobian matrix for each
7.2. Discrete adjoint via automatic differentiation

residual. Moreover, a similar strategy is also followed for calculating $\frac{\partial C}{\partial U}$. After the assembly of the Jacobian $\frac{\partial R}{\partial U}$, the adjoint equation given in equation 7.6 is solved using the iterative GMRES method for which a SIMPLER-like preconditioner is implemented to ensure rapid convergence. Using the solution of the adjoint equation, the final vector of gradients is evaluated as

$$\frac{dC}{d\gamma} = \frac{\partial C}{\partial \gamma} + \frac{\partial R}{\partial \gamma}^T \lambda$$

(7.7)

Again, AD is employed for evaluating the partial derivaties $\frac{\partial C}{\partial \gamma}$ and $\frac{\partial R}{\partial \gamma}$. 
This chapter presents a single optimization case for a heat sink device. For a broader discussion, the reader is kindly referred to paper P2 where heat sink devices are studied with various design configurations. Moreover, the results from paper P1 are omitted here for brevity where the optimization for flow manifolds, body-fitted mesh comparison and the investigation of the effect of frozen turbulence assumption on the calculated sensitivities are presented.

8.1 Optimization of a 3D heat sink

Figure 8.1: Computational domain for the 3D heat sink problem. Due to the symmetry, only a quarter of the domain is utilized for the optimization. Blue color represents the fixed fluid regions for inlet and outlet, green color shows the design domain $\Omega_d$ and the red color specifies the fixed solid region $\Omega_p$ (heated thin plate). The figure is taken from paper P2.

The presented case aims to optimize flow channels to increase the heat transport in order to minimize the temperature in a heated plate. The schematic illustration of the problem setup can be seen in figure 8.1 where only a quarter of the domain (highlighted sections) is considered in the optimization due to symmetry in both $y$ and $z$ directions. The fixed inlet and outlet channels are highlighted with the blue color and fully developed turbulent channel flow profiles are considered at the inlet with a bulk velocity of $U_b = 0.75 \, \text{m/s}$. Moreover, the design domain is shown with the green color and a thin heated plate is illustrated with the red color. The heated plate is treated as a fixed solid region for the optimization. A heat flux of $175 \, \text{kW/m}^2$ is applied from the bottom face of the heated plate. For the heat equation, a temperature of $300 \, \text{K}$ is applied at the inlet and other than the heated bottom surface, all other boundaries are realized as adiabatic walls. The
optimization problem considers the minimization of the integral of the temperature in the heated plate as an objective function. A volume constraint of 55% of the whole computational domain for the fluid along with a constraint for the allowable power dissipation are also considered in the optimization problem. Furthermore, the fluid is taken as air and the solid material is chosen as aluminum. As it can be seen from the figure, the geometry is scaled with the half the inlet channel height which is chosen as $H = 0.1 \text{ m}$. The resulted Reynolds number for the optimization problem is then calculated as $Re = U_b H/\nu = 5 \times 10^3$.

Figure 8.2: Topology optimization of 3D heat sink device for $Re = 5000$ with $k$-$\omega$ model. Red color specifies the heated plates at the top and the bottom of the design and blue color shows the optimized flow channels. The objective values of the end design is $C = 315$. The figure is taken from paper P2.

Figure 8.3: Lower half of the optimized flow channels, showing the streamlines of the flow. Streamlines on the right hand side are colored with the velocity magnitude $u \text{ [m/s]}$ while the left hand side is colored by the temperature $T \text{ [K]}$. The figure is taken from paper P2.
8.1. Optimization of a 3D heat sink

The computational domain is meshed with 216K hex cells which corresponds to 216K and 2.5M DOFs for the heat and the fluid problems, respectively. The result of the optimization is shown in figure 8.2 where the shaded red areas show the heated plates. The optimized flow channels shown in the figure exhibit rather flat and thin topology which is mainly parallel to the heated plates. For better visualization, figure 8.2b demonstrates the half of the optimized design which shows the upper surface of the channels shaped to speed up of the flow for more efficient cooling. Furthermore, figure 8.3 shows the resulted streamlines of the flow where it can be seen that the optimized channel’s input section directs the flow to all corners with covering the heated plate as much as possible resulting in almost uniformly heated flow towards the outlet region.

(a) Extruded 2D design.  
(b) 3D optimized design.

Figure 8.4: Streamlines of the flow colored by temperature $T$ [K]. Quarter of the flow channels are shown. The figure is taken from paper P2.

In order to present the importance of full 3D optimization considering heat sink devices, the section gives a further study where a 2D optimized heat sink is extruded and compared against the presented 3D heat sink device. The streamlines of the flows from the extruded 2D and the optimized 3D designs are compared in figure 8.4 where the streamlines are colored with the temperature field. As it can be seen from figure 8.4a, since the heat can not be transferred to the mid sections of the channel, the extruded 2D design results in an unevenly heated flow where the lower part of the flow is excessively heated. Meaning that the flow can not extract heat from the plate, realizing a low performing cooling device. On the other hand, through the enhanced flow circulations and larger contact surface area in the 3D optimized channel, the heat from the plate is extracted properly with uniformly heating the flow (figure 8.4b). Furthermore, the superior cooling performance of the 3D design can also be seen from figure 8.5 where the temperature distributions in the solid parts of the extruded 2D and the optimized 3D designs are compared. As it is seen from the figure, while the extruded 2D design results in an uneven cooling of the
heated plates (figure 8.5a), the 3D design realizes an efficient cooling of the heated plates as seen in figure 8.5b.

(a) Extruded 2D design, $C = 329$.
(b) 3D optimized design, $C = 315$.

Figure 8.5: Temperature $T$ [K] distribution of the solid regions of the optimized heat sinks. Figures show the half of the domain (cut in $z$ axis). The figure is taken from paper P2.
This part of the thesis presents the developed methodology for the application of Automatic Differentiation (AD) for obtaining exact sensitivities of 2D and 3D large scale turbulent flow topology optimization problems. As the framework provides a solution to the complex bookkeeping problems for coupled systems, easy accommodation of turbulence models is achieved with minimal effort on the implementation. The proposed adjoint solution procedure with the utilized preconditioner realizes a scalable and computationally cheap way of calculating gradients. The study also demonstrates that exact gradients can differ significantly when compared to gradients computed with a simplifying frozen turbulence assumption and the optimized designs using exact sensitivities outperform those optimized under the simplifying assumption.

Heat transfer coupling considering forced convection is added to the develop framework to demonstrate the ease of handling additional physics. The work includes an extensive study for topology optimization of heat sinks devices considering turbulent flows and highlights the importance of carrying out full 3D optimization for novel and better performing designs compared to simplified 2D approach. The work also provides a further motivation on including turbulent flows in the optimization process to allow for higher fluid velocities and increased design performance.

9.1 Future work

This section summarizes various ideas which could be implemented to improve the developed framework of topology optimization of turbulent flows.

- Immersed boundary modeling can be implemented to realize well defined boundaries throughout the optimization. This way, wall functions can be utilized in the RANS and turbulence model equations to optimize for higher Reynolds numbers without the need for extreme meshing.

- Coupling the immersed boundary modeling approach to a level set based topology optimization framework would facilitate the possibility of obtaining optimized topologies of even more complicated multi-physics problems.

- The developed flow framework can be considered for flow induced noise prediction problems to couple the optimization to acoustics. This can be achieved using aeracoustic analogies in which the turbulent flow field obtained from the RANS equations is utilized to calculate the acoustic pressure. Using the proposed methodology, the optimization framework can be applied to problems targeting noise reduction of realistic flow systems.
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Publications
Publication P1

Topology optimization of turbulent flows
Topology optimization of turbulent flows

Cetin B. Dilgen∗1, Sumer B. Dilgen1,2, David R. Fuhrman, Ole Sigmund, Boyan S. Lazarov3

Department of Mechanical Engineering, Technical University of Denmark, Nils Koppels Allé, Building 404, DK-2800, Denmark

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Highlights

• Presents a fast approach for topology optimization of turbulent flow systems.
• Demonstrates inclusion of turbulence models with minimal implementation effort.
• Demonstrates a scalable and computationally cheap procedure for gradient analysis.
• Demonstrates the shortcomings of frozen turbulence assumption.

Abstract

The aim of this work is to present a fast and viable approach for taking into account turbulence in topology optimization of complex fluid flow systems, without resorting to any simplifying assumptions in the derivation of discrete adjoints. Topology optimization is an iterative gradient-based design process which minimizes an objective and satisfies a set of selected design constraints by distributing material in a design domain. The gradients are obtained using adjoint sensitivity analysis which requires solutions of a forward state problem and an additional adjoint problem. In the presented article the forward solver is based on finite volume discretized Reynolds-averaged Navier–Stokes equations coupled with either one- or two-equation turbulence closure models, and the adjoint solver is obtained via automatic differentiation. The presented approach is demonstrated on the optimization of several 2D and 3D examples including a detailed comparison to designs and sensitivities obtained with different turbulence models and under a frozen turbulence assumption. The results demonstrate the importance of exact sensitivity analysis and open new possibilities for the design of large scale multiphysics problems involving turbulent flows.

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1. Introduction

Computational fluid dynamics (CFD) is an extremely important tool in the design of complex flow systems. Compared to experiments it offers a relatively inexpensive method for obtaining valuable information through virtual flow simulations in a computer environment. However, even for relatively simple fluid systems, due to the inherently complex nonlinear behavior, prior knowledge of potential design improvements is not often available. In such cases the pursuit of better (optimal) designs can easily be prohibited by the inefficiency of trial-and-error approaches. To this end, topology optimization [1] can provide valuable solutions by distributing a volume of material in a selected design domain through optimization of a chosen criterion, without defining any initial shape or topology prior to the optimization process.

Topology optimization is an iterative gradient-based design process. A material distribution is found by solving an optimization problem, while satisfying a set of design constraints and governing equations that define the problem physics. Ideally, the material distribution is represented by a density which takes values of either one and zero, representing the two materials considered in the problem, i.e. if a point in the design domain is occupied with fluid the density is equal to one, and if it is occupied with solid the density field is equal to zero. In order to utilize gradient-based optimization techniques the discrete zero/one problem is relaxed, and the density field is allowed to take intermediate values. Brinkman penalization is usually utilized to define a variable porous material which corresponds to the intermediate density values [2]. The earliest examples of utilizing topology optimization for fluid flow problems considered simplified Stokes flow models [2], with large scale examples found in [3]. More recently, [4] presented a locally cubically convergent algorithm for topology optimization of Stokes flows. Later optimizations of laminar flow problems using Navier–Stokes equations and Lattice Boltzmann methods have been demonstrated in [5–7] and [8–10], respectively. For general shape optimization, the derivation and the application of the topological sensitivities for Stokes and Navier–Stokes equations can be found in [11–13]. Considering the topology optimization of turbulent flows, [14, 15] utilized a simplified sensitivity analysis through the so-called frozen turbulence assumption, i.e., variations of the turbulence field with respect to design variables are neglected. Following the derivation of a continuous adjoint formulation for the Spalart–Allmaras turbulence model [16], recent work has demonstrated a topology optimization framework in [17].

In contrast to all previous works, the focus of the present paper is on the development of a discrete forward and adjoint Reynolds-averaged Navier–Stokes (RANS) solver for topology optimization with a scalable and computationally cheap procedure for gradient analysis where exact sensitivities are obtained for the considered discretization. The basic model will be coupled with different turbulence closures with minimal effort in terms of the required development time. It should be noted that, both continuous and discrete adjoint methods produce consistent sensitivities with the two approaches having their advantages/disadvantages (see [18, 19] for comparison between the two methods.). For complex CFD solvers, such as those utilizing segregated and iterative solution approaches such as SIMPLE algorithms [20], derivation of discrete adjoints by hand is a non-trivial and error-prone task. To this end, automatic differentiation (AD) [21, 22] will likewise be employed for calculating the exact gradients of the optimization objective and constraints in the topology optimization problems considered.

AD is a set of techniques enabling the exact numerical calculation of the gradients of a function implemented in a computer program. Similar to traditional sensitivity analysis, two modes can be clearly distinguished: forward and reverse modes, corresponding respectively to direct and adjoint differentiation. Depending on the capabilities of the programming language, AD can be implemented either by source code transformations or by operator overloading techniques; A detailed introduction can be found in [22]. The technique is mainly applied within shape and size optimization problems with a relatively small number of control/design variables. A source transformation AD tool is demonstrated in both reverse and forward modes to derive an exact adjoint version of the SIMPLE algorithm for shape optimization in [23]. Operator overloading is demonstrated in [24], where the OpenFOAM library [25] is differentiated in a black-box manner. The Dolfin-adjoint project [26] automatically derives the discrete adjoint given a differentiable forward model and an example of its application for topology optimization of Stokes flow problem is given in [27]. Also, both the FEniCS project [28] and COMSOL Multiphysics software [29] have automatic differentiation support. It should be pointed out that such black box differentiation brings immense memory requirements, and requires checkpoint algorithms [30] to store intermediate computations and to reduce the memory consumption. Alternatively, instead of differentiating the implemented code in a black box manner, the reverse mode of AD can be employed selectively, as demonstrated in [31, 32]. Herein, it is proposed to apply AD only in the formation of the exact discrete adjoint equation, thus enabling a significant reduction in memory requirements. The proposed approach requires...
the explicit solution of an adjoint system of equations, and the obtained adjoint solution times are similar to those of forward modes, in contrast to other results reported in the literature. The proposed methodology produces exact consistent sensitivities and can be easily applied to any set of partial differential equations. Similar approaches for shape optimization problems can be found in [31,33].

To the best of the authors’ knowledge, topology optimization of turbulent flows has not yet been demonstrated with exact sensitivities obtained with discrete adjoint approach and without any simplifying assumptions in the derivation of the discrete adjoints. Hence, the methodology developed in this paper can be seen as a contribution to the topology optimization of complex flow problems. The present work provides the foundation for additional applications, and for further investigation, development and expansion of the method on complex multiphysics problems.

This paper is organized as follows: First, the governing equations, along with the inclusion of Brinkman penalization, are described in Section 2. Topology optimization is introduced in Section 3, together with the associated adjoint sensitivity analysis. Automatic differentiation is then briefly presented in Section 4, and the implementation and the verification of discrete adjoint solvers for (two equation) \( k-\omega \) and (one equation) Spalart–Allmaras turbulence models are discussed in Section 5. Comparison with results based on a frozen turbulence assumption is likewise included. Finally, the developed techniques and methodology are demonstrated in the optimization of several 2D and 3D turbulent fluid flow problems in Section 6. Additional details on the employed finite volume discretization, the implementation and the validation of the implemented finite volume solver are presented in Appendixes A–C.

2. Governing equations

The considered problems are governed by the steady-state incompressible Reynolds-averaged Navier–Stokes (RANS) equations given as

\[
\nabla \cdot \mathbf{u} = 0 \tag{1}
\]

\[

\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = \nabla \cdot (2\nu \mathbf{S}) - \frac{1}{\rho} \nabla p + \nabla \cdot \mathbf{T}_t - \lambda \chi (\gamma) \mathbf{u} \tag{2}
\]

where \( \mathbf{u} \) is the mean velocity vector, \( p \) is the pressure, \( \nu \) is the kinematic viscosity of the fluid, \( \rho \) is the fluid density, and \( \lambda \) (formally having units of inverse time) is the so-called Brinkman penalization parameter. The dimensionless function \( \chi (\gamma) \) takes values ranging from zero to one, with these limits representing pure solid and fluid, respectively; The exact form of the interpolation function is discussed in Section 3. The Brinkman penalization term effectively models spatially varying porosity, and is utilized for representing the solid/fluid distribution in the optimization process. The penalization term with \( \chi (\gamma) = 1 \), and sufficiently large enough \( \lambda \), approximates a no-slip boundary condition at the fluid–solid interface. In the above, the mean strain rate tensor \( \mathbf{S} \) is defined as

\[
\mathbf{S} = \frac{1}{2} \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \tag{3}
\]

The additional effects of turbulence are modeled through the Reynolds stress tensor \( \mathbf{T}_t \), which accounts for additional normal and shear stresses on the fluid caused by turbulent eddies present in the flow. The Reynolds stress tensor is defined by invoking the so-called Boussinesq approximation as

\[
\mathbf{T}_t = -\overline{\mathbf{u}^t \otimes \mathbf{u}^t} = 2\nu_t \mathbf{S} - \frac{2}{3} k \mathbf{I} \tag{4}
\]

where \( \nu_t \) is the turbulent eddy viscosity, \( \delta_{ij} \) is the Kronecker delta, and

\[
k = \frac{1}{2} \overline{\mathbf{u}^t \cdot \mathbf{u}^t} \tag{5}
\]

is the turbulent kinetic energy per unit mass, with the prime superscript indicating fluctuating velocities. To achieve closure, an additional set of equations defining the eddy viscosity \( \nu_t \) is required. To this end, the present work considers two different closure models, namely, the (1) two-equation \( k-\omega \) model [34] and (2) the one-equation Spalart–Allmaras (SA) model [35], which are described in the following sub-sections. Implementation details are presented in Appendixes A and B, and a validation of the solver is demonstrated in Appendix C.
2.1. $k$–$\omega$ model

The $k$–$\omega$ model calculates turbulent eddy viscosity $\nu_t$ as

$$
\nu_t = \frac{k}{\omega}, \quad \omega = \max \left[ \omega_i, C_{lim} \sqrt{\frac{28.9}{\beta^*}} \right], \quad C_{lim} = \frac{7}{8}
$$

where $\cdot$ denotes the scalar product between two tensors (i.e. $\mathbf{a} \cdot \mathbf{b} = a_i b_j$). The turbulent kinetic energy (per unit mass) $k$ and the specific dissipation rate $\omega$ are obtained by solving two additional (steady state) transport equations

$$
\nabla \cdot \left( \nu \mathbf{u} k \right) = \mathbf{T}_i \nabla u - \beta^* \nu \mathbf{u} k + \nabla \cdot \left[ \left( \nu + \sigma \frac{k}{\omega} \right) \nabla k \right] - \lambda \chi(\gamma) k
$$

$$
\nabla \cdot \left( \nu \mathbf{u} \omega \right) = \frac{\alpha \omega \nu}{k} \mathbf{T}_i \nabla u - \beta^* \nu \mathbf{u} \omega + \frac{\sigma_d}{\omega} \nabla k \cdot \nabla \omega + \nabla \cdot \left[ \left( \nu + \sigma \frac{k}{\omega} \right) \nabla \omega \right] + \lambda \chi(\gamma) (\omega_0 - \omega)
$$

where $\beta^* = \beta_0 f_0$, $f_0 = \frac{1 + \nu_0}{1 + 0.05k}$, $\lambda \chi = \frac{\mu (\Omega_0^2 + 4 \Omega_0^2)}{\left( \rho^2 \Omega_0^2 \right)}$, $\Omega = \frac{1}{\gamma} (\nabla \mathbf{u} - \nabla \mathbf{u}^T)$, $\sigma_d = H(\nabla k \cdot \nabla \omega) \sigma_0$ and $H(\cdot)$ is the Heaviside step function which returns a unity if the argument is positive and zero otherwise. It should be noted that $\lambda \chi$ is zero for two-dimensional flows. The closure constants are $\alpha = 0.52$, $\beta_0 = 0.0708$, $\beta^* = 0.09$, $\sigma = 0.5$, $\sigma_d = 0.6$ and $\sigma_0 = 0.125$.

The turbulent kinetic energy $k$ has a well defined boundary at walls given as

$$
k_w = 0
$$

The specific dissipation rate $\omega_0$, on the other hand, has a singular behavior near a wall. For smooth walls (as uniformly considered herein), the approximate (non-homogeneous Dirichlet type) boundary condition proposed by [36] will be utilized, corresponding to

$$
\omega_0 = \frac{60 \nu}{\beta_1 \gamma_1}, \quad \beta_1 = 0.075
$$

where $\gamma_1$ represents the distance from the wall to the cell center nearest the wall. Assuming a uniform mesh in the optimization domain, the distance $\gamma_1$ is defined as half the cell height.

In the solidified regions, the penalization of wall boundary conditions for $k$ and $\omega$ (Eqs. (9) and (10), respectively) is enforced through the Brinkman penalization term present in the last terms on the right hand sides of Eqs. (7) and (8), respectively.

2.2. Spalart–Allmaras model

The second turbulence model utilized here corresponds to the one-equation Spalart–Allmaras model [35]. In the past it has been utilized mainly for aerodynamic simulations, however, later modifications [37] have significantly broadened its range of applicability, and the model has gained popularity due to its simplicity and good numerical characteristics. In this model the eddy viscosity $\nu_t$ is obtained as follows:

$$
\nu_t = \bar{\nu} f_{\nu}, \quad f_{\nu} = \frac{\chi^2}{\chi^2 + \nu_3^2}, \quad \chi = \frac{\bar{\nu}}{\bar{\nu}}
$$

with the viscosity parameter $\bar{\nu}$ obtained via solution of the following transport equation

$$
\nabla \cdot (\bar{\nu} \mathbf{u}) = P - D + \frac{c_{\rho_2}}{\sigma} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \frac{1}{\sigma} \nabla \cdot \left[ (\nu + \bar{\nu}) \nabla \bar{\nu} \right] - \lambda \chi(\gamma) \bar{\nu}
$$

Here the production $P$ and dissipation $D$ terms respectively read

$$
P = c_{\rho_1} \tilde{S} \bar{\nu}, \quad D = c_{\rho_1} f_\nu \left( \frac{\bar{\nu}}{D} \right)^2
$$

where $\tilde{S} = \Omega + \frac{1}{4} f_{\nu_2}$, $f_{\nu_2} = \sqrt{2 \Omega \Omega}$, $d$ is the distance from the closest wall, $r = \min \left[ \frac{k}{\alpha^2 \nu^2}, 10 \right]$, $f_{\nu_2} = 1 - \frac{r}{\nu^2 f_{\nu_2}}$, $f_{\nu_2} = g \left( \frac{1 + c_{\rho_1} \nu_2}{e_{\rho_1} + \nu_2} \right)$ and $g = r + c_{\rho_2} (r^6 - r)$. The closure constants are $c_{\rho_1} = 0.1355$, $c_{\rho_2} = 0.622$, $c_{\nu_3} = 7.1$, $\sigma = 2/3$, $c_{\rho_1} = \frac{4 \nu}{e_{\rho_1}^2} + \frac{4 c_{\rho_1}}{e_{\rho_1}^2}$, $c_{\rho_2} = 0.3$, $c_{\rho_3} = 2$ and $\kappa = 0.41$. 

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Since the turbulent kinetic energy \( k \) is not directly accessible in this model, the Reynolds stress tensor is calculated from \( T_{ij} = 2\nu \partial_i u_j \). From comparison with the full Boussinesq approximation (Eq. (4)) it is noted that this neglects turbulent normal stresses. The eddy viscosity parameter \( \nu \) in the Spalart–Allmaras model has a homogeneous Dirichlet boundary condition defined at walls as
\[
\nu_{wall} = 0
\] (14)
The additional penalization term, the last term on the right hand side of Eq. (12), approximates the wall boundary condition for \( \nu \) (Eq. (14)) in the solidified regions.

As it can be seen from the model closure coefficients, the Spalart–Allmaras turbulence model needs the distance to the closest wall \( d \). This is obtained by adopting a Poisson-like approach \([38,39]\). For the distance calculation, the Poisson equation has a homogeneous Dirichlet boundary condition on walls. In the presence of porous material, the equation is penalized the same way as in Eq. (12) to be able to calculate the distance field \( d \).

### 3. Topology optimization

A generic topology optimization problem, as utilized in the present work, can be defined as
\[
\min_{\gamma} C(\gamma, U(\gamma))
\] (15)
subject to
\[
\begin{align*}
R(\gamma, U(\gamma)) &= 0 \\
g_i(\gamma) &\leq 0, \quad \forall i = 1, \ldots, N \\
0 &\leq \gamma \leq 1
\end{align*}
\] (16)-(18)
where \( C(\cdot) \) is an objective function and \( \gamma \) represents the material (fluid/solid) distribution in the selected design domain \( \gamma \) is a vector which is a discrete representation of the density \( \gamma \), subject to an additional set of inequality constraints \( g_i \). \( U \) is the vector of state variables, and \( R \) is the vector of governing equations written in residual form.

As stated earlier, the values of \( \gamma \) take value zero for cells filled with impermeable solid material and one for fluid. The intermediate values can be interpreted as porous material with different porosities. The goal of the optimization is to find the porosity distribution which minimizes the objective and fulfills the set of constraints.

The interpolation between solid and fluid is realized with the help of a function \( \chi(\gamma) \) \([2]\), which is defined as
\[
\chi(\gamma) = \frac{1 - \gamma}{q + \gamma}
\] (19)
where the parameter \( q \) controls the curvature of the above interpolation function. The interpolation functions for three different values of \( q \) are presented in Fig. 1. Here it is seen that with \( q = 10 \) a near linear interpolation is realized. Lowering \( q \) increases the curvature of the interpolation function, resulting in a sharper transition between fluid and solid regions. In the presented results, all state fields, with the exception of \( \omega \), are penalized with \( q = 0.1 \). After a number of numerical experiments, it has been found that a sharper transition is needed in the \( \omega \) equation for robust convergence in the presence of intermediate density/porosity regions. Thus, \( q = 10^{-4} \) is used in the penalization of \( \omega \).

The values of \( \gamma \) are obtained from regularized Heaviside projection \([40]\), controlled by a sharpness parameter \( \beta \) and a threshold \( \eta = 0.5 \). The projection is applied on a PDE filtered density field \([41]\). A detailed discussion of this procedure, together with other alternatives, can be found in \([42]\). Gradients of the objective and constraints with respect to the original design field \( \gamma \) are subsequently obtained by applying the chain rule, which accounts for every field transformation.

The penalization parameter \( \lambda \), in all state equations, must be sufficiently high to effectively result in impermeable solid regions. If \( \lambda \) is relatively small, flow will diffuse through the porous media with finite velocity. On the other hand, large \( \lambda \) may result in slow convergence of the optimization process, convergence to poorly performing locally optimal solutions, and slow convergence of the forward state solver. To this end, the choice of \( \lambda \) is made based on the dimensionless Darcy number defined as:
\[
Da = \frac{\nu U/L}{\lambda U} = \frac{\nu}{\lambda L^2}
\] (20)
which represents the ratio of viscous forces to Darcy damping forces, where \( U \) and \( L \) are, respectively, characteristic velocity and length scales defining a given flow problem (to be clarified in what follows). Utilizing the (dimensionless)
Da enables selection of (dimensional) \( \lambda \) in a consistent manner, regardless of problem scale. Through testing, it has been found that selecting a sufficiently small Darcy number (\( Da \approx 10^{-5} - 10^{-6} \)) [43] is sufficient to yield nearly impermeable solidified regions.

The solution of the optimization problem is obtained with the help of the Method of Moving Asymptotes (MMA) [44,45]. Based on the gradients of the objective and the set of constraints, MMA updates the design field in an iterative fashion. The gradients are obtained by adjoint analysis. After obtaining the state solution, an adjoint system of equations is solved and the gradients of the objective and the constraints are computed with respect to the selected parametrization of the density field. Based on the gradients and the values of the constraints, MMA updates the design. Physically realistic designs require fine spatial resolution, resulting in a large number of degrees-of-freedom (DOFs) for representing the state solution, and high computational cost. Therefore, the state, the adjoint and the optimization solvers are parallelized, following the general strategy outlined in [46,47], in order to obtain a final design in a reasonable amount of time.

Apart from the parallel implementation, the main difficulty in the above outlined optimization process is the calculation of the gradients of the objective and the constraints with respect to the parametrization of the material distribution. This calculation represents one of the main novel contributions of the present work. For estimations based on finite differencing, the computational cost scales proportionally to the number of design parameters. Thus, for topology optimization problems, which are characterized by a large number of design variables and relatively small number of constraints, an adjoint-based sensitivity analysis is the preferred approach i.e. for each objective or constraint function only a single state and adjoint solution is necessary to evaluate all sensitivities. Here, a discrete adjoint approach is adopted, where the state problem is first discretized, followed by the evaluation of the objective, the constraints and gradients, utilizing the discrete solution to the state problem.

### 3.1. Discrete adjoint

The evaluation of the gradients will now be demonstrated for a generic objective or constraint function \( C(\gamma, U(\gamma)) \). The state solution \( U(\gamma) \) is required to satisfy the governing equation, which is written in residual form \( R(\gamma, U(\gamma)) = 0 \). The objective function is augmented with the help of a Lagrange multiplier vector \( \lambda \), and the Lagrangian function \( \mathcal{L} \) is written as

\[
\mathcal{L} = C(\gamma, U(\gamma)) + \lambda^T R(\gamma, U(\gamma))
\]  

(21)

For zero residual the Lagrangian coincides with the objective/constraint function. The derivative with respect to design parametrization can be written as
\[ \frac{dL}{d\gamma} = \frac{\partial C}{\partial \gamma} + \frac{\partial C}{\partial U} \frac{dU}{d\gamma} + \lambda^T \left( \frac{\partial R}{\partial \gamma} + \frac{\partial R}{\partial U} \frac{dU}{d\gamma} \right) \]

\[ = \frac{\partial C}{\partial \gamma} + \lambda^T \frac{\partial R}{\partial \gamma} + \frac{\partial C}{\partial U} + \lambda^T \frac{\partial R}{\partial U} \frac{dU}{d\gamma} \]

\[ \Rightarrow 0 \]

The term \( \frac{dU}{d\gamma} \) is computationally very expensive to evaluate. Thus, to avoid its computation the indicated part of the above equation is set to zero. This requirement provides the adjoint equation for the optimization problem, which is given as

\[ \frac{\partial R}{\partial U} \lambda = -\frac{\partial C}{\partial U} \]  \hspace{1cm} (23)

To obtain a Lagrange multiplier vector satisfying the adjoint equation, the final vector of gradients is evaluated as

\[ \frac{dC}{d\gamma} = \frac{\partial C}{\partial \gamma} + \frac{\partial R}{\partial \gamma} \lambda \]  \hspace{1cm} (24)

The adjoint procedure described above is applied to the already-discretized governing equations and a selected function. As this approach operates on the discrete level, where the boundary conditions are already accounted for, it can handle any cost function and governing equation in a robust way. Importantly, calculated sensitivities are always exact for the considered discretization.

### 4. Discrete adjoint via automatic differentiation

The Jacobian \( \frac{\partial R}{\partial U} \) in Eq. (23) is not formed explicitly during the state solution. Rather, the forward solution is obtained iteratively using the SIMPLE algorithm [20]. The explicit formation of the Jacobian is an error-prone and tedious task, due to the large number of coupled state fields and applied corrections required to ensure stability of the discretization. Towards this end the presented work utilizes automatic differentiation (AD) in order to simplify, and at the same time allow for, exact gradients in the evaluation [22].

AD calculates derivatives of a function implemented as a computer code. The basic idea behind AD is the fact that every evaluation of the function can be decomposed to a set of primitive operations which are easy to differentiate. AD keeps track of all primitive operations and calculates the gradient of any complicated function by invoking the chain rule. The calculated derivatives are thus exact to machine precision. Thus, AD should be considered as a tool which simplifies the evaluation of derivatives through software techniques. AD can be implemented through source code transformations [48] or by using operator overloading features of modern programming languages such as C++ and Fortran90 [49,50]. The advantages and disadvantages of the two approaches, as well as comparison to hand coded adjoints for several topology optimization problems, are discussed in detail in [32].

AD can differentiate a computer coded function using forward (tangent) and reverse (adjoint) modes. Forward mode provides derivatives in a single direction. Thus, the derivatives of all output variables are computed with respect to only one input variable in one forward sweep. A scalar valued function with \( n \) input arguments has to be executed \( n \) times for evaluating the gradients in forward mode. On the other hand, reverse mode can be seen as analogous to the discrete adjoint method described in Section 3.1. The approach calculates the full set of derivatives with respect to all input variables by applying the chain rule from outputs to inputs. Thus, considering a scalar valued function, its gradient vector can be obtained in a single call to a reverse AD routine after a record (a tape) of all primitive operations. The tape records all operations during the forward evaluation of the objective/constraints functions. For a large number of design parameters and long and complex evaluations the memory requirements can become prohibitive, and special check pointing schemes are necessary to avoid excessive use of memory, as well as to reduce the number of repetitive evaluations.

The considered topology optimization problems consist of one or a few constraints and a single objective. Therefore, the natural AD differentiation mode is reverse mode. As the overloading approaches require fewer modifications to the state solution solver, and a preliminary comparison in terms of speed between [50] and [49] did not reveal significant differences, the gradients evaluation was implemented using the Adept: automatic differentiation library [50]. Applying AD directly in the forward solution process combined with the following objective and
constraint evaluations would require check pointing and careful organization of the evaluation structure. As the linear algebra and the parallel communication libraries are not aware of the types and the structure of the AD differentiated code, the selected implementation utilizes AD selectively only for local operations. The exact process consists in forming a Jacobian, the right hand side of the adjoint equation, and finally evaluating the gradients using Eq. (24).

4.1. Implementation of residual vector functions

The developed incompressible Navier–Stokes solver utilizes a collocated (cell-centered) grid arrangement. Linearization of the governing equations results in additional variables, in the form of face fluxes, which are introduced and stored in the cell face centers. Due to the iterative nature of the forward algorithm, calculating face fluxes from the interpolated face velocities does not satisfy the momentum residuals at convergence, i.e. during the iteration sequence, residuals are satisfied through both convected (nodal) and convecting (face flux) velocities. For a hexagonal cell the number of state variables is 12. These include the face fluxes and the state variables for the turbulence model. The inclusion of the SA model in the adjoint analysis follows the same steps as for the k-ω model, hence its presentation is omitted here for brevity.

The residual and the state vectors for the discrete model are given as

\[ \mathbf{U} = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3 \quad \mathbf{p} \quad \mathbf{f}_1 \quad \ldots \quad \mathbf{f}_6 \quad \mathbf{k} \quad \mathbf{ω}]^T \]

\[ \mathbf{R} = [\mathbf{R}^{u1} \quad \mathbf{R}^{u2} \quad \mathbf{R}^{u3} \quad \mathbf{R}^f \quad \mathbf{R}^{f1} \quad \ldots \quad \mathbf{R}^{f6} \quad \mathbf{R}^k \quad \mathbf{R}^ω]^T \]

where \( N_e \) is the total number of cells in the domain. \( \mathbf{u}_1, \mathbf{u}_2 \) and \( \mathbf{u}_3 \) denote the vectors of velocity components and \( \mathbf{f}_i \) is the vector of face fluxes with \( i = 1, \ldots, 6 \) for a hexagonal cell.

Residual calculations of the velocity components (\( \mathbf{R}^{u1}, \mathbf{R}^{u2}, \mathbf{R}^{u3} \)) and turbulence model variables (\( \mathbf{R}^k, \mathbf{R}^ω \)) are easily differentiated, as for each cell, they reflect the governing equations and the transport equations for \( k \) and \( ω \). The generic explicit discrete form of these equations is given for a single cell as

\[ \mathbf{R}^φ = A_φ \phi_f - \sum_N A_N \phi_N - S_b \approx 0 \]

where \( φ \) stands for any variable other than pressure and fluxes (for more details see Appendix A).

The pressure residual is obtained from the iterative procedure and at convergence \( p'^{l} \approx p'^{l-1} \), where the superscript indicates the iteration stage. Thus, a residual for the pressure can be derived from its correction, Eq. (B.13),

\[ R^p = p_p - \left( p_p - \frac{\partial p}{\partial p} \sum_N \alpha_N p_N - \sum_f F^* \right) \approx 0 \]

(27)

where \( F^* \) is calculated as in Eq. (B.9). In the SIMPLE algorithm, the pressure correction is zero at convergence (\( p' \approx 0 \)), therefore in the adjoint solver it is not necessary to declare the pressure correction as an independent variable, and it is hence set to zero for differentiation. With the above modification (taking out the terms with pressure correction) the residual for the pressure is calculated as

\[ R^p = p_p - \left( p_p - \frac{\alpha_p}{\partial p} \sum_f F^* \right) \approx 0 \]

(28)

Residual functions for fluxes are derived from their correction, Eq. (B.14), using the fact that \( p' \approx 0 \)

\[ R^f_i = F_i - F^*_i \approx 0 \]

(29)

where subscript \( i \) denotes the face number.

All of the above residual functions are implemented in a cell-wise manner. The derivative of the residual vector with respect to the state variables will be different than zero only for indices of state variables corresponding to a limited number of cells located around the considered cell. Taking into account all convective and diffusive schemes employed for the discretization, the stencil width for each row in the Jacobian is up to 33 for 3D, and up to 13 for 2D, problems.
4.2. Assembly of Jacobian matrices

Efficient calculation of the Jacobian matrices \( \frac{\partial R}{\partial U} \), \( \frac{\partial R}{\partial \gamma} \) is crucial to yield good performance in the discrete adjoint solver. To this end, instead of directly computing the Jacobian matrices (by differentiating the whole residual vector), the implemented single-output residual functions are differentiated in an element loop. Thus, for each residual function, a row in the Jacobian is obtained through AD. This approach is beneficial, not only in terms of memory requirements, but also for parallel calculation, as all differentiations are performed locally without the need of any parallel communications.

Active input variables are accompanied by a map structure containing the local and global indices of the current stencil. Thus, the calculated gradients are assembled directly into the global matrix. Algorithm 1 illustrates the general steps taken to differentiate the residual functions and assemble the Jacobian matrix.

\begin{algorithm}
\caption{Jacobian assembly}
\begin{algorithmic}
\For {Element \( n_i, i = 1, \ldots, N_e \)}
\State Extract the required stencil for element based residual evaluation.
\State Initialize active input variables (\( u_1, u_2, u_3, p, \ldots \))
\For {Every residual \( r = 1, \ldots, N_R \)}
\State Start new recording
\State Call overloaded residual function
\State Reverse sweep on the recording
\For {\( j = 1, \ldots, N_{\text{stencil}} \)}
\State Extract the gradients
\State Insert the gradients into the matrix
\EndFor
\EndFor
\EndFor
\end{algorithmic}
\end{algorithm}

In the above algorithm \( N_R \) is the number of residuals per cell. For a hexahedron and the \( k-\omega \) turbulence model \( N_R = 12 \). After differentiation and assembly, the Jacobian matrix has the following form:

\[
\frac{\partial R}{\partial U} = \begin{bmatrix}
R_{u_1}^{u_1} & R_{u_1}^{u_1} & R_{u_1}^{u_1} & \ldots & R_{u_1}^{u_1} \\
R_{u_1}^{u_2} & R_{u_1}^{u_2} & R_{u_1}^{u_2} & \ldots & R_{u_1}^{u_2} \\
R_{u_1}^{u_3} & R_{u_1}^{u_3} & R_{u_1}^{u_3} & \ldots & R_{u_1}^{u_3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
R_{u_1}^{p} & R_{u_1}^{p} & R_{u_1}^{p} & \ldots & R_{u_1}^{p} \\
R_{u_1}^{f} & R_{u_1}^{f} & R_{u_1}^{f} & \ldots & R_{u_1}^{f} \\
\end{bmatrix}_{(12N_e) \times (12N_e)}
\]

Each block, i.e. \( R_{u_1}^{u_1} \), in the matrix has size \( N_e \times N_e \) where the subscripts define with respect to which variable the differentiation is done. The Jacobian has a highly sparse structure which is exploited in terms of storage. As can be seen from Eqs. (23) and (24), the adjoint equation requires the transpose of the matrix. In order to avoid the transpose operation on the assembled system, the assembly is therefore performed directly on the transposed matrix.

4.3. Assembly of gradient vectors

Gradient vectors in the adjoint equation are solely based on the differentiation of the cost function \( C(\gamma, U(\gamma)) \) with respect to either the design variables \( \gamma \) or state variables \( U \). For any scalar valued cost function, first an overloaded
version is implemented, where the active inputs have size corresponding to the number of elements. After recording the call to the overloaded objective function, gradients are computed and then extracted in an element loop. The process is demonstrated in Algorithm 2.

**Algorithm 2 Gradient vector assembly**

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Initialize active input variables ((u_1, u_2, u_3, p, ... ))</td>
</tr>
<tr>
<td>2</td>
<td>Start new recording</td>
</tr>
<tr>
<td>3</td>
<td>Call overloaded objective function</td>
</tr>
<tr>
<td>4</td>
<td>Reverse sweep on the recording</td>
</tr>
<tr>
<td>5</td>
<td><strong>for</strong> Element (n_i, i = 1, ..., N_e) <strong>do</strong></td>
</tr>
<tr>
<td></td>
<td>Extract the gradients</td>
</tr>
<tr>
<td></td>
<td>Insert the gradients into the corresponding vectors</td>
</tr>
<tr>
<td><strong>end for</strong></td>
<td></td>
</tr>
<tr>
<td>Resulting vectors with sizes of: (\frac{\partial C}{\partial U} \rightarrow (N_R \times N_e) \times 1)</td>
<td></td>
</tr>
<tr>
<td>(\frac{\partial C}{\partial \gamma} \rightarrow (N_e) \times 1)</td>
<td></td>
</tr>
</tbody>
</table>

### 4.4. Adjoint solution method

The assembled adjoint equation is given as

\[
\frac{\partial R^T}{\partial U} \lambda = -\frac{\partial C}{\partial U} \tag{31}
\]

The solution can be obtained by a direct factorization method, though such an approach does not scale well for large problems. Thus, an iterative solution technique would be preferable. The robustness of these solvers is controlled by the supplied preconditioners. Here the GMRES iterative method implemented in the PETSc library, in combination with a SIMPLER-like preconditioning scheme, ensures rapid convergence. Following the same idea behind the implemented forward flow solver, where pressure–velocity coupling has been dealt with by employing the SIMPLE algorithm, a similar preconditioner is set-up for the dual velocity–pressure coupling in the adjoint variables, without employing any under-relaxation. The considered preconditioner is implemented by only utilizing the upper left \(4 \times 4\) block of \(\frac{\partial R^T}{\partial U}\) (individual blocks of \(\frac{\partial R^T}{\partial U}\) can be seen from Eq. (30)). Coupling to the rest of the system (adjoint fluxes and turbulent variables) is ignored, and block-wise preconditioning is implemented for these remaining adjoint variables. Hence, the following equation is considered

\[
\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix}
=
\begin{bmatrix}
b_1 \\
b_2
\end{bmatrix} \tag{32}
\]

where each sub-block can be written as

\[
A_{11} = \begin{bmatrix}
(R^{u_1}_n)^T & 0 & 0 \\
0 & (R^{u_2}_n)^T & 0 \\
0 & 0 & (R^{u_3}_n)^T
\end{bmatrix}, \quad A_{12} = \begin{bmatrix}
(R^{p}_n)^T \\
(R^{p}_n)^T \\
(R^{p}_n)^T
\end{bmatrix} \tag{33}
\]

\[
A_{21} = \begin{bmatrix}
(R^{p}_n)^T \\
(R^{p}_n)^T \\
(R^{p}_n)^T
\end{bmatrix}, \quad A_{22} = \begin{bmatrix}
(R^{p}_n)^T
\end{bmatrix} \tag{34}
\]

The approximate Schur complement matrix is calculated as

\[
S = A_{22} - A_{21} \tilde{A}_{11}^{-1} A_{12} \tag{35}
\]

where, \(\tilde{A}_{11}\) is a diagonal matrix, whose entries are the diagonal part of the \(A_{11}\). With the matrices defined above, the following steps define the application of the preconditioner on a vector \((r_u, r_p)\) with the resulting vector \((\tilde{r}_u, \tilde{r}_p)\)

\[
\tilde{r}_p = S^{-1} \left[ r_p - A_{21} \tilde{A}_{11}^{-1} r_u \right] \tag{36}
\]
\[ \mathbf{r}_u = A_{11}^{-1} \left[ \mathbf{r}_{u'} - A_{12} \mathbf{r}_p \right] \]  
(37)

\[ \Delta \mathbf{r}_u = A_{11}^{-1} \left[ \mathbf{r}_{u'} - (A_{11} \mathbf{r}_u + A_{12} \mathbf{r}_p) \right] \]  
(38)

\[ \Delta \mathbf{r}_p = S^{-1} \left[ \mathbf{r}_p' - (A_{31} (\mathbf{r}_u + \Delta \mathbf{u}) + A_{32} \mathbf{r}_p) \right] \]  
(39)

\[ \mathbf{r}_u = \mathbf{r}_u + \Delta \mathbf{r}_u - A_{11}^{-1} A_{12} \Delta \mathbf{r}_p \]  
(40)

\[ \mathbf{r}_p = \mathbf{r}_p + \Delta \mathbf{r}_p \]  
(41)

which follows closely the steps in the SIMPLER preconditioner [51,52]. Unlike utilizing SIMPLE-type methods as iterative solvers, above operations (Eqs. (36)–(41)) are applied for preconditioning GMRES iterative solvers.

### 4.5. Objective and constraint functions

In the following examples the selected objective corresponds to volume-based power dissipation. An expression for power dissipation stems from the energy equation, and can be derived with the scalar multiplication of the momentum equations and the velocity vector. Taking into account the extra body force acting on the momentum equation due to power dissipation stems from the energy equation, and can be derived with the scalar multiplication of the momentum equations

\[ C = \int_V \left( 2 \nu \nabla \chi (\gamma) \mathbf{u} \cdot \mathbf{u} \right) dV \]  
(42)

The fluid volume is bounded, and the constraint is given as

\[ g_i(\gamma) = \frac{\Delta V_i}{V} \gamma_i - 1, \quad i = 1, \ldots, N_e \]  
(43)

where \( \Delta V_i \) and \( \gamma_i \) are respectively the cell volume and design variable of the \( i \)th cell, \( V \) is the total volume of the design domain, and \( f \) is the prescribed fluid volume fraction.

For flow manifold optimization problems (Sections 6.2 and 6.3) multiple outlets are constrained, such that specified mass flow rates across the outputs are obtained. The flux constraints are formulated as

\[ g_2(\mathbf{U}(\gamma)) = \frac{\int_{A_i} \mathbf{n} \cdot \mathbf{u} dA}{-q_i F_{in}} - 1 \leq \epsilon \]  
(44)

where \( m \) is the number of constrained outlets, \( F_{in} \) is the fixed inlet flow rate calculated at the input boundary, \( q_i \) is the desired mass flow fraction at outlet \( i \), and \( \epsilon \) is the tolerance on the flux constraint. A tight tolerance corresponding to \( \epsilon = 1 \times 10^{-4} \) is utilized. It should be noted that, in terms of implementation, the above flux constraint \( g_2 \) is a function of face flux \( F \), which is a state variable. Hence, for each constrained outlet, an adjoint equation has to be solved in order to calculate the gradient of the constraint in Eq. (44) with respect to the design variables. For every adjoint equation, AD is utilized only in the formation of the gradient vector \( \frac{\partial g_2}{\partial \gamma} \), which is the source term of the adjoint equation. Jacobian matrices \( \frac{\partial g_2}{\partial \gamma} \) remain unchanged.

## 5. Gradient calculation

### 5.1. Sensitivity verification in a channel bend problem

The focus in this section is on verification of the adjoint sensitivity analysis. As an example, the considered computational domain for a channel bend problem is shown in Fig. 2a. As seen, the domain consists of an empty box, having a single inlet and outlet. Half of the input channel height is taken to be \( H = 0.1 \) m. A fully developed turbulent flow profile is imposed as a boundary condition for velocities and turbulence model variables, obtained directly through an a priori simulation. The inlet bulk velocity is set to \( U_b = 3 \) m/s and the kinematic viscosity of the fluid is taken as \( \nu = 5 \times 10^{-6} \) m²/s. The Reynolds number, defined with half inlet height and bulk velocity, is tailored to be \( Re = U_b H / \nu = 10^5 \); \( H \) and \( U_b \) are likewise taken as the characteristic scales defined in Eq. (20). The computational domain consists of 13 162 hexahedral cells clustered near the walls to ensure accuracy in the primal solution. The distance of the first cell to the walls in wall coordinates is kept as \( y^+ = y U_f / \nu < 1 \), where \( U_f \) is the friction velocity. A contour plot of the velocity magnitude from the primal solution utilizing the \( k-\omega \) model, along with resulting streamlines, is presented in Fig. 2b.
The design domain, which coincides with the computational domain, is initialized with fluid only, i.e. $\gamma = 1$ is set everywhere in the domain. The interpolation function, Eq. (19), is utilized in computing the Brinkman penalization with curvature parameter $q = 0.1$ and penalization parameter $\lambda = 10^3 \text{ s}^{-1}$. The finite difference approximation for an arbitrary cell is obtained as

$$\frac{dC}{d\gamma_i} \approx \frac{C(\gamma_i + \Delta h, U(\gamma_i + \Delta h)) - C(\gamma_i, U(\gamma_i - \Delta h))}{2\Delta h}$$  \hspace{1cm} (45)$$

Thus, for each cell, two forward solutions are necessary for estimating the gradients of the selected objective by the central finite difference scheme. The step size is selected to be $\Delta h = 10^{-6}$.

Simulations using both the SA and $k$–$\omega$ turbulence models have been performed. It should be stressed that throughout the present work the dependence of the distance function in the SA turbulence model on the design variables is neglected in the differentiation. The effect of this simplification on the calculated sensitivities with the adjoint SA model is illustrated in Fig. 6. For the selected verification case, the design domain is occupied only by fluid, and the distance function is not penalized. This allows for direct comparison between the gradients evaluated by finite difference and the AD adjoint for the SA model.

Tables 1 and 2 provide comparisons of calculated sensitivities at randomly selected cells in the computational domain, using finite difference, full turbulence adjoint, and a frozen turbulence model. As can be seen, the estimated sensitivities agree well between the finite difference and the adjoint evaluations. As expected, utilizing a frozen turbulence assumption results in inconsistent sensitivities. Furthermore, the frozen turbulence assumption is seen to sometimes result in gradients having opposite sign, which would lead to anti-optimization steps! This effect is demonstrated in Figs. 3 and 4, which compare calculated sensitivity fields (with and without the frozen turbulence approximation), utilizing the $k$–$\omega$ and SA turbulence closure models, respectively. Although the sensitivities obtained with frozen turbulence and exact adjoint follow the same general trend, consistent evaluation clearly requires the

$$\begin{array}{l}
\text{Table 1} \\
\text{Validation of calculated sensitivities for the channel bend problem with the k–o adjoint solver. Cells are chosen arbitrarily.}
\end{array}$$

<table>
<thead>
<tr>
<th>Derivative sparingly and Frozen turbulence</th>
<th>Finite difference</th>
<th>Adjoint k–o</th>
<th>Frozen turbulence</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CV_1$</td>
<td>$-4.016668 \times 10^{-3}$</td>
<td>$-4.016381 \times 10^{-3}$</td>
<td>$-2.993492 \times 10^{-3}$</td>
</tr>
<tr>
<td>$CV_2$</td>
<td>$-7.641710 \times 10^{-4}$</td>
<td>$-7.649730 \times 10^{-4}$</td>
<td>$-9.143874 \times 10^{-4}$</td>
</tr>
<tr>
<td>$CV_3$</td>
<td>$+3.366152 \times 10^{-3}$</td>
<td>$+3.360705 \times 10^{-3}$</td>
<td>$-8.757109 \times 10^{-4}$</td>
</tr>
<tr>
<td>$CV_4$</td>
<td>$-2.655306 \times 10^{-2}$</td>
<td>$-2.655305 \times 10^{-2}$</td>
<td>$-2.665780 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Fig. 2. Simulation setup and velocity contours for the channel bend problem.
Validation of calculated sensitivities for the channel bend problem with the SA adjoint solver. Distance function is not penalized. Cells are chosen arbitrarily.

<table>
<thead>
<tr>
<th>Derivative $\frac{dC}{d\gamma}$</th>
<th>Finite difference</th>
<th>Adjoint SA</th>
<th>Frozen turbulence</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{V1}$</td>
<td>$-1.488273 \times 10^{-3}$</td>
<td>$-1.488297 \times 10^{-3}$</td>
<td>$-2.571103 \times 10^{-3}$</td>
</tr>
<tr>
<td>$C_{V2}$</td>
<td>$+1.476542 \times 10^{-3}$</td>
<td>$+1.470075 \times 10^{-3}$</td>
<td>$-6.637291 \times 10^{-4}$</td>
</tr>
<tr>
<td>$C_{V3}$</td>
<td>$+1.538834 \times 10^{-3}$</td>
<td>$+1.538780 \times 10^{-3}$</td>
<td>$-6.786502 \times 10^{-4}$</td>
</tr>
<tr>
<td>$C_{V4}$</td>
<td>$-2.530123 \times 10^{-2}$</td>
<td>$-2.530116 \times 10^{-2}$</td>
<td>$-2.572755 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

(a) Discrete $k$–$\omega$ adjoint solver. (b) Discrete $k$–$\omega$ adjoint solver with frozen turbulence.

Fig. 3. Calculated sensitivity field of the power dissipation objective function $C$ with respect to all design variables $\gamma$ for the channel bend problem. The cell values are scaled with cell volumes.

including the turbulence model variables in the gradient evaluation. A detailed comparison can be further seen in Fig. 5, where, the gradients along a line connecting the lower left corner to the upper right corner of the computational domain are presented in a one dimensional plot. Similar conclusions can be drawn from Fig. 6, which depicts the sensitivities along the line $(x, 0.5)$.

The distance function in the SA turbulence model accounts for changes in the topology of the design by penalization techniques. However, in the adjoint analysis this dependence is neglected. As demonstrated in Fig. 6, the obtained gradients agree very well with those which have taken into account changes in the topology and been computed by finite difference techniques. As the present work demonstrates optimization using exact gradients for the $k$–$\omega$ turbulence model, further investigations on the effect of this simplifying assumption in the SA model are left for future studies.

6. Topology optimization of turbulent flow examples

In this section the proposed sensitivity adjoint analysis will be utilized directly within several topology optimization examples. The first will consider detailed comparisons between designs obtained under the frozen turbulence assumption and with numerically exact gradients. The effect of different parameters will likewise be studied in detail. Finally, comparison to baseline designs will demonstrate the advantage of topology optimized solutions. The final
examples, involving 2D and 3D manifold designs, will demonstrate the applicability of the presented techniques to more complex, and computationally intensive, problems.

6.1. 2D U-bend

The first example considers the optimal configuration of a 2D U-bend, utilizing both $k-\omega$ and SA turbulence models. The objective is given by Eq. (42), i.e. the aim is to minimize the energy dissipation in a 2D channel. The effect
Fig. 6. Sensitivity $\frac{\partial C}{\partial \gamma}$ along the line $(x, 0.5)$ in the channel bend problem, showing the effect of neglecting the density dependence on the distance function in the sensitivity analysis. The solid line represents the full turbulence SA adjoint, the dashed line represents frozen turbulence, markers — finite difference calculations.

Fig. 7. Schematic illustration of the 2D $U$-bend problem. Here $\Omega_d$ specifies the design domain. Blue and gray colors represent fixed fluid and solid regions, respectively. At the inlet, fully developed turbulent channel flow profiles are imposed for velocity and turbulent model variables. The geometry is scaled with the half inlet channel height $H$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 3
Flow properties for the 2D $U$-bend problem.

<table>
<thead>
<tr>
<th>$U_b$ [m/s]</th>
<th>$H$ [m]</th>
<th>$\nu$ [m$^2$/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.1</td>
<td>$4.0 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

of the frozen turbulence assumption on the final design will be investigated by comparing against the full-turbulence (numerically exact gradients) solutions. Moreover, the obtained designs will be further assessed by comparing the performance of body-fitted meshes and a baseline $U$-bend channel.

The problem setup and domain boundaries can be seen in the definition sketch, Fig. 7, where, the geometry is scaled with the half-inlet channel height $H$. The Reynolds number in the considered optimization problem is $Re = U_b H/\nu = 5 \times 10^3$, where $U_b$ is again the bulk velocity. Table 3 lists the properties utilized in the simulation. The considered optimization parameters are likewise shown in Table 4.

The total number of optimization cycles in the simulation is set to 500. During the optimization cycle, the projection parameter $\beta$ is increased by a factor 1.5, starting from $\beta = 1.5$, after every 50 iterations. During the last 100 iterations,
it is fixed at $\beta = 14$ which results in a relatively sharp interface between solid and fluid regions. The convergence history of the optimization process with the $k$-$\omega$ turbulence model is shown in Fig. 8. Once the volume constraint is satisfied, the objective value starts decreasing monotonically.

The obtained topologies with both $k$-$\omega$ and SA turbulence models, including comparison of designs obtained under a frozen turbulence assumption, are shown in Figs. 9 and 10. Even though the frozen turbulence assumption results in inconsistent sensitivities, the objective functions $C$ for the obtained designs are very close to those obtained using exact sensitivities, in this example. This is due to the confinement of the losses in the immediate vicinity of the solid/fluid boundary and to the similar length of these inter-phase boundaries. For faster flows and more confined boundary layers it might be necessary to use logarithmic transformation of the objective in order to reflect the nature of the problem on the design topology. In the current setup, a smooth curved topology is necessary to decrease the pressure difference between the entrance and outlet sections. This appears due to high inertial effects, and is clearly observed in the designs obtained with consistent sensitivities.

A cross check demonstrating the optimality of the obtained full turbulence designs is presented in Table 5. This demonstrates that the turbulence model is reflected exactly in the optimization process, and further improvement of the design performance can, in principal, only be obtained by further improving the ability of the models to describe the physical flow within the system.

The performance gain of the optimized designs with respect to a reference design, both using a body fitted mesh, is demonstrated in Tables 6 and 7. The body fitted profiles, shown in Fig. 11, are obtained using the threshold $\eta = 0.5$. The inlet and the outlet in the simulations have been extended sufficiently in order to allow for fully-developed turbulent profiles to enter in the design domain, and to avoid back flow in the computational domain. Power dissipation objective values are calculated only in the design domain, corresponding to the section of the optimized pipes given

### Table 4

<table>
<thead>
<tr>
<th>Parameter settings in the topology optimization of the 2D $U$-bend problem.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$ [s$^{-1}$]</td>
</tr>
<tr>
<td>$2 \times 10^3$</td>
</tr>
</tbody>
</table>

### Table 5

Cross check of the optimized designs from the $k$-$\omega$ and SA turbulence models for the 2D $U$-bend problem. The blue color indicates that a specific design outperforms all others for the corresponding physical models utilized in the optimization.

<table>
<thead>
<tr>
<th>$k$-$\omega$ Sim</th>
<th>SA Sim</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00355394</td>
<td>0.00615163</td>
</tr>
<tr>
<td>0.01000547</td>
<td>0.00989088</td>
</tr>
</tbody>
</table>

Fig. 8. Convergence of the constrained optimization problem involving the 2D $U$-bend.
Fig. 9. Topology optimization of the 2D U-bend problem for $Re = 5000$ with $k$-$\omega$ model. The presented velocity contours are non-dimensionalized with the bulk velocity. $C$ is the objective function given by Eq. (42) and computed for the final designs.

in Fig. 11. Unstructured meshes are utilized in the simulations. For the boundary layers the distance (in dimensionless wall units) from the first cell center to the wall is kept well below unity.

The estimated performances clearly demonstrate the advantage of utilizing consistent sensitivity analysis in the optimization process. Designs obtained under a frozen turbulence assumption possess sharper corners and connections. Although, all optimized designs exhibit significant improvements over the baseline, in both tables the (two-equation) $k$–$\omega$ full turbulence design achieves the largest improvement (in percentage gain over the baseline). The worst of the optimized designs is that obtained with (one-equation) SA model using a frozen turbulence assumption.

As expected (see again Tables 6 and 7), the objective values calculated on the body fitted meshes are found to be smaller than those computed with Brinkman penalization. The main reasons for this difference are the existence of the gray transition regions between the solid/fluid phases and the mesh resolution utilized for the optimization, which is $y^+ \approx 10$. For further investigation, the convergence of the penalized model to the body fitted one for increasing penalization is demonstrated in Fig. 12. The simulations are performed with the $k$–$\omega$ turbulence model and the penalization coefficients are obtained with increasing projection level, which brings the topology optimized solution near to a crisp 1–0 design. The convergence trend can be clearly observed and the predicted power dissipation agrees on the first significant digit to the body-fitted result for a near crisp 1–0 design. It should be stressed that for sharper transitions a refinement of the mesh around the transition region would be necessary in order to have a further
Fig. 10. Topology optimization of the 2D U-bend problem for Re = 5000 with the SA model. Presented velocity contours are non-dimensionalized with the bulk velocity. C is the objective function for the optimized designs.

Fig. 11. Comparison of topology optimized 2D U-bend profiles to the standard baseline model for Re = 5000. The body fitted meshes are constructed from the presented curved boundaries.
agreement with the body fitted model. However, it is not presently computationally feasible to refine the optimization mesh to use a resolution of $y^+ \approx 1$.

Finally, comparisons of forward solutions of the optimized design with the $k-\omega$ model and of the baseline design are presented in Figs. 13 and 14. The pressure distribution demonstrates that the pressure difference between the inlet and the outlet is greatly reduced for the optimized case. The reason for the high performance gain can be explained by closely examining the flow separation presented in Fig. 14, which is the main source of power dissipation.

6.2. 2D flow manifold

The second example considers the optimization of a 2D flow manifold. The objective is to minimize the power dissipation calculated using Eq. (42) and restrict the mass flux at the outlets. The setup is shown in Fig. 15. The $k-\omega$ turbulence model is utilized in the computations. The parameters utilized in the simulations and the optimization process are shown in Tables 8 and 9. The Reynolds number is $Re = 3500$ and is again defined using the half inlet channel height $H$ and the bulk velocity $U_b$. Fully developed turbulence profiles are set for the stream-wise velocity.
Fig. 13. Optimized channel on a body fitted mesh for $Re = 5000$, showing the pressure field in comparison with that from the baseline model. The simulations are performed with the $k-\omega$ turbulence model.

Fig. 14. Optimized channel on a body fitted mesh for $Re = 5000$, showing the velocity magnitude in comparison to that from the baseline model. This figure highlights that the main separation regions which occur in the baseline model are largely prevented in the optimized design. The simulations are performed using $k-\omega$ turbulence model.

turbulent kinetic energy $k$ and the specific dissipation rate $\omega$ at the inlet. During the optimization process, the projection parameter $\beta$ is increased in the same manner as in Section 6.1.

The optimized topology is shown in Fig. 16. The resulting velocity and the kinetic energy distribution are shown in Fig. 17. The diameter of the inner flow channels is smaller than the outlets. The optimization procedure links the inner network of channels to the outlets by minimizing the power dissipation and distributing material only in the design domain. The geometry of the outlets is fixed using Brinkman penalization, which results in rough jumps
Table 8
Flow properties used in the 2D flow manifold problem.

<table>
<thead>
<tr>
<th>$U_b$ [m/s]</th>
<th>$H$ [m]</th>
<th>$\nu$ [m$^2$/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.1</td>
<td>$5.7 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 9
Parameter settings in the topology optimization of the 2D flow manifold problem.

<table>
<thead>
<tr>
<th>$\lambda$ [s$^{-1}$]</th>
<th>$q$</th>
<th>$r$</th>
<th>$\beta$</th>
<th>$f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2 \times 10^3$</td>
<td>0.1</td>
<td>0.028</td>
<td>1.5–14</td>
<td>0.43</td>
</tr>
</tbody>
</table>

Fig. 15. Schematic illustration of the 2D flow manifold problem. Here $\Omega_d$ specifies the design domain. Blue and gray colors are fixed fluid and solid regions, respectively. Fully developed turbulent channel flow profiles are imposed for velocity and turbulence model variables at the inlet. The geometry is scaled with the half inlet channel height $H$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

at the connection between the inner channels and the outlets. In order to ensure smooth transition a prescribed set of boundary conditions are enforced on the topology during the PDE filtering step [53]. These do not require any changes in the optimization setup, and can provide computationally cheap enforcement of topological features, accounting for physical characteristics, design, and manufacturing constraints not taken into account by the model.

6.3. 3D flow manifold

The final example considers topology optimization of a 3D manifold, as depicted in Fig. 18. The aim of this example is to demonstrate the applicability of the proposed techniques on a real 3D large-scale problem. The $k$–$\omega$ turbulence model is utilized in the optimization. The computational domain is scaled with the input pipe radius $H$. The inlet length is $4H$ and the outlets are $8H$. The design domain is a cube with dimensions $10H \times 10H \times 10H$. A fully developed turbulent pipe flow profile is mapped at the inlet boundary for the stream-wise velocity and turbulence model variables. The Reynolds number considered corresponds to $Re = U_b H / \nu = 3500$, where $U_b$ is the bulk inlet velocity. Flow properties corresponding to the turbulent pipe inlet are presented in Table 10. The optimization parameters are likewise specified in Table 11. The optimized design is shown in Fig. 19.

The problem is discretized using 1.3M cells, corresponding to 16M DOFs for the forward and the adjoint solutions. Every optimization step requires one forward solution and four adjoint solutions (one for the objective function and
Fig. 16. Topology optimization of a 2D flow manifold problem for $Re = 3500$ using the $k-\omega$ turbulence model. The objective value of the end design corresponds to $C = 2.3 \times 10^{-3}$.

(a) Velocity magnitude $u \,[\text{m/s}]$. (b) Turbulent kinetic energy $k \,[\text{m}^2/\text{s}^2]$.

Fig. 17. Primal solutions on the topology optimization of a 2D flow manifold problem for $Re = 3500$ with the $k-\omega$ model.

three for the constraints). The optimized design, presented in Fig. 19, is obtained overnight after 200 iterations on 400 CPU cores (Intel(R) Xeon(R) CPU E5-2680 v2 @ 2.80 GHz). The projection parameter $\beta$ is multiplied by 1.5 every 20 iteration with a maximum value of 8. The design domain at the initial optimization step is filled with fluid only.

Similar to other large scale problems reported in the literature [41,46,47], most of the computational time is spent in solving the forward and the adjoint problems. The forward problem is solved iteratively using the SIMPLE algorithm. During the first several optimization iterations the topology changes significantly. Once the rough shape of the design is fixed during the initial optimization steps, the following designs are obtained by small incremental changes, mainly
Table 10
Flow properties for the 3D flow manifold problem.

<table>
<thead>
<tr>
<th>$U_b$ [m/s]</th>
<th>$H$ [m]</th>
<th>$\nu$ [m$^2$/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.1</td>
<td>$5.7 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 11
Parameter settings in the topology optimization of 3D flow manifold problem.

<table>
<thead>
<tr>
<th>$\lambda$ [s$^{-1}$]</th>
<th>$q$</th>
<th>$r$</th>
<th>$\beta$</th>
<th>$f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2 \times 10^3$</td>
<td>0.1</td>
<td>0.028</td>
<td>1.5–8</td>
<td>0.12</td>
</tr>
</tbody>
</table>

Fig. 18. Computational domain for the 3D flow manifold problem. Constrained outlets are shown with the specified mass flow rates. The visible box corresponds to the design domain, whereas pipes are fixed throughout the optimization.

on the boundaries of the fluid/solid interface. These incremental changes lead to small changes of the fluid velocity and pressure distribution fields, thus requiring significantly fewer iterations. The same behavior can be observed in the adjoint solution. Thus, the computational cost per optimization step, initially requiring 500–800 iterations for solving the forward and adjoint problems, decreases significantly towards the end of the optimization process, resulting in 25 to 50 forward and adjoint iterations. The actual iteration time is often lower than the time required for assembling the problem. These numbers demonstrate some of the advantages of the proposed schemes in terms of computational time. Furthermore, the proposed adjoint and forward algorithms are scalable. The only serial step is the construction (the action on a vector) of the Schur complement matrix given by Eq. (35). Thus, larger problems can be easily optimized, provided that the implementation addresses efficiently the construction of the adjoint preconditioner.

7. Conclusions

The article demonstrates the application of Automatic Differentiation (AD) for obtaining exact sensitivities of 2D and 3D large scale turbulent flow topology optimization problems. Easy accommodation of new physics and turbulence closure models is achieved with minimal implementation effort. The developed methodology demonstrates a solution of the complex bookkeeping problem for coupled problems. The proposed adjoint solution provides a
scalable and computationally cheap procedure for gradient analysis. It is shown that exact discrete gradients can differ significantly from those computed under a simplifying frozen turbulence assumption, confirming similar observations in the literature [16]. Optimized results are obtained using two different models for turbulence closure, corresponding to the one-equation Spalart–Allmaras model and the two-equation \( k-\omega \) model. The optimized designs without any simplifying assumptions in the derivation of discrete adjoints outperform those optimized under a frozen turbulence assumption.

It should be pointed out that improved preconditioners are necessary for more robust behavior and even lower computational cost. Future research is required to demonstrate the applicability of the methodology to coupled fluid-heat transfer problems and more complex multiphysics.

Acknowledgment

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Appendix A. Discretization overview

The solution of the state equations is obtained by finite volume discretization on a non-uniform grid. The discretized Reynolds-averaged Navier–Stokes equations are solved using a segregated approach for the pressure–velocity coupling, with the help of the SIMPLE (semi-implicit method for pressure-linked equations) algorithm [20]. The SIMPLE method and its variants are widely used in computational fluid dynamics due to their low memory requirements and the ability to simulate both steady and unsteady flows. The implementation is based on the PETSc library [54,55], which is utilized mainly for its efficient parallel sparse solvers.

The discretization procedure is demonstrated for a standard transport equation. All variables are stored in cell centers (collocated grid arrangement). The fluxes are derived through a linearization procedure, and are stored in cell face centers. Fig. A.20 illustrates two neighboring cells, where \( \mathbf{d} \) is the vector connecting the cell centers \( P \) and \( N \). \( \mathbf{A} \) is the normal area vector of the common face \( f \), pointing outwards from the current cell \( P \). A generic scalar transport equation for the scalar variable \( \phi \) is given below in vector notation, where the discretization of all spatial terms is presented.

\[
\nabla \cdot (\mathbf{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi \tag{A.1}
\]

Fig. 19. Iso-views of the optimized 3D flow manifold for \( Re = 3500 \) with the \( k-\omega \) turbulence model. Streamlines are colored based on the velocity magnitude m/s. The objective value for the end design is \( C = 0.83 \). Constrained mass flux fractions are shown on outlets. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
After integrating over a cell, and applying the Gauss divergence theorem, the following discrete form of the above transport equation is obtained:

$$\sum_{f} F_{f} \phi_{f} = \sum_{f} (\Gamma \nabla \phi_{f}) \cdot A_{f} + S_{f} \Delta V$$  \hspace{1cm} (A.2)

where surface integrals are realized as a sum over all faces of a cell, volume integrals are approximated as $\int_{V} dV = \Delta V$, and a new variable, corresponding to the face flux $F_{f}$, is introduced and lagged by an iteration

$$\sum_{f} (u_{l} - u_{l-1} \cdot A_{f}) \phi_{f} = \sum_{f} F_{f} \phi_{f}$$  \hspace{1cm} (A.3)

The calculation of $F$ is based on weighted linear interpolation of nodal velocities $u$ between two neighboring cell centers ($P$ and $N$ in Fig. A.20). Although linear interpolation is second-order accurate [56], it is not bounded. Hence, using the same strategy for the calculation of $\phi_{f}$ results in non-physical oscillatory solutions for convection dominated flows. In order to ensure oscillation-free solutions, while still preserving second order accuracy, TVD (total variation diminishing) schemes are employed here. The convective term is written as [57]

$$F_{f} \phi_{f} = F \left[ \phi_{U} + \frac{\psi(r)}{2} (\phi_{D} - \phi_{U}) \right]$$  \hspace{1cm} (A.4)

where $r$ is the ratio of the upwind to the downwind gradient, $\psi(r)$ is a limiter function that resides in the TVD monotonicity region, and subscripts $U$ and $D$ represent upwind and downwind cells, respectively. Selection of these cells is done based on the direction of the flow (the sign of the face flux $F$) between two neighboring cells ($P$ and $N$ in Fig. A.20). The present work adopts a modified ratio $r$ for unstructured grids [58]

$$r = \frac{2 \nabla \phi \cdot d}{\phi_{D} - \phi_{U}} - 1$$  \hspace{1cm} (A.5)

and the SUPERBEE limiter [59] is utilized for the function $\psi(r)$ which reads

$$\psi(r) = \max[0, \min[1, 2r], \min[2, r]]$$  \hspace{1cm} (A.6)

It should be noted that, to improve numerical stability, the first term on the right hand side of Eq. (A.4) is treated implicitly, while the second term is calculated explicitly and added to the source in a deferred correction manner.

The calculation of the diffusive fluxes needs attention due the non-orthogonality of the cells. They are corrected with the help of the over-relaxed approach proposed by [60] to ensure second-order accuracy.

$$\Gamma \nabla \phi_{f} \cdot A = \Gamma \left[ A_{d} \frac{\phi_{U} - \phi_{P}}{|d|} + \Gamma A \cdot \nabla \phi_{f} \right]$$  \hspace{1cm} (A.7)

The orthogonal part is treated implicitly, whereas the non-orthogonal part is calculated explicitly from the previous iteration as a correction and added to the source. $A_{d}$ represents the parallel part of $A$ to $d$ which is given as

$$A_{d} = \frac{d}{d \cdot A} |A|^2$$  \hspace{1cm} (A.8)
The non-orthogonal part $A_r$ is defined as the difference between the area vector and the orthogonal contribution $A_d$: $A_r = A - A_d$. The explicit calculation of $\nabla \phi_f$ in the non-orthogonal correction is done by first approximating the gradient at the cell center through the Gauss theorem as

$$\nabla \phi_P = \frac{\sum_j \phi_f A}{\Delta V}$$  \hspace{1cm} (A.9)

The resulting cell center gradients are then interpolated to the cell faces through weighted linear interpolation.

The final discrete form of the transport equation can be written as

$$A_P \phi_P = \sum_N A_N \phi_N + S_P$$  \hspace{1cm} (A.10)

The implementation details for momentum, pressure correction, and turbulence model equations are presented in Appendix B.

Appendix B. Implementation details

The steady state incompressible RANS equations read

$$\nabla \cdot (u \otimes u) = \nabla \cdot T_v - \frac{1}{\rho} \nabla p + \nabla \cdot T_r$$  \hspace{1cm} (B.1)

where the viscous $T_v$ and Reynolds $T_r$ stress tensors are

$$T_v = 2 \nu S, \quad T_r = 2 \nu_t S - \frac{2}{3} k I, \quad S = \frac{1}{2} (\nabla u + \nabla u^T)$$  \hspace{1cm} (B.2)

The stress terms are combined, yielding an effective viscosity $\nu_{eff} = \nu + \nu_t$, as

$$T = 2 \nu_{eff} S - \frac{2}{3} k I = \nu_{eff} (\nabla u + \nabla u^T) - \frac{2}{3} k I$$  \hspace{1cm} (B.3)

Consequently, the total diffusion term in the RANS equations is treated as

$$\nabla \cdot T = \nabla \cdot \nu_{eff} \nabla u + \nabla \cdot \nu_{eff} \nabla u^T - \nabla \cdot \left( \frac{2}{3} k I \right)$$  \hspace{1cm} (B.4)

Utilizing the above procedure gives rise to the following discrete source contributions, due to both Reynolds stresses and pressure gradients:

$$b_P = \sum_f \left( \nu_{eff} \nabla u^T \right)_f \cdot A - \nabla \cdot \left( \frac{2}{3} k I \right) \Delta V - \sum_f p_f A$$  \hspace{1cm} (B.5)

The discretization techniques given in Appendix A can now be applied to the momentum equations to realize algebraic linear equations having the generic form:

$$A_P u_P = \sum_N A_N u_N + S_u, \quad S_u = S_P + b_P$$  \hspace{1cm} (B.6)

Here $S_P$ represents the source contributions, arising from the discretization of convective and diffusive terms (explicitly treated terms in Eqs. (A.4) and (A.7)). In order to improve the convergence properties and the diagonal dominance of the system matrix, implicit under-relaxation is applied to the solution of the momentum equations as

$$\frac{A_P}{\alpha_u} u_P = \sum_N A_N u_N + S_u, \quad S_u = S_P + b_P + \left[ (1 - \alpha_u) \frac{A_P}{\alpha_u} \right] u^{t-1}$$  \hspace{1cm} (B.7)

The discretized form of the continuity equation, given in Eq. (1), reads

$$\sum_f F = 0$$  \hspace{1cm} (B.8)
Due to the collocated storage of velocities and pressure at cell centers, Rhie–Chow interpolation [61] is applied on the face fluxes before deriving the pressure correction equation, which directly links the face fluxes to the driving pressure difference across faces.

\[
F^* = \mathbf{u}_f \cdot \mathbf{A} - \left( \frac{\Delta V}{A_P} \right)_f \left( \frac{p_N - p_P}{|d|} - \nabla p_f \cdot \mathbf{e} \right) |A_f| \quad (B.9)
\]

In the above \( \mathbf{e} = \frac{d}{|d|} \) is the unit vector in the direction of the central vector. It should be stressed that \( F^* \) is based on the solution of the momentum equations, and does not satisfy the continuity equation (B.8). Hence, it needs a correction to satisfy the divergence free condition. Thus, defining a flux correction in accordance with [62] results in the following discrete continuity equation

\[
\sum_f (F^* + F') = 0 \quad (B.10)
\]

where the flux correction \( F' \) is defined as [20]:

\[
F' = - \left( \frac{\Delta V}{A_P} \right)_f \left( \frac{p_N - p_P}{|d|} \right) |A_f| \quad (B.11)
\]

Substituting the flux correction \( F' \) into the discrete continuity equation, Eq. (B.10), yields the pressure correction equation with a source of mass imbalance, written here in generic form as

\[
a_P p'_P = \sum_N a_N p'_N + S_P - \sum_f F^* \quad (B.12)
\]

where \( S_P \) is the possible source contribution due to the diffusion discretization. The mass imbalance \( \sum_f F^* \) approaches zero at convergence. With the help of the pressure correction \( p' \), nodal velocities and pressures are obtained as

\[
\mathbf{u}_P = \mathbf{u}^*_P - \left( \frac{\Delta V}{A_P} \right) \nabla p'_P, \quad p_P = p^*_P + \alpha_P p'_P \quad (B.13)
\]

where \( \alpha_P \) is the under-relaxation factor for pressure. Continuity is strictly enforced on the face fluxes \( F \) at each SIMPLE iteration following the solution of the pressure correction

\[
F = F^* + F' \quad (B.14)
\]

Considering the two-equation \( k-\omega \) turbulence model, the terms on the right hand side of Eq. (B.15) require special attention

\[
\nabla \cdot (\mathbf{u} k) - \nabla \cdot \left[ \left( \nu + \frac{\sigma_k \Delta V}{\omega} \right) \nabla k \right] = T_t \nabla \mathbf{u} - \beta^* \omega k \quad (B.15)
\]

In order to preserve the positiveness of the solution and increase the numerical stability of RANS models, the positive terms (production) on the right hand side are treated explicitly, while the negative terms (dissipation) are treated implicitly. The total contribution to the central coefficient and source due to the production and dissipation terms in the \( k \) equation are given as

\[
\int_T T_t \nabla \mathbf{u} \, dV = 2
\]

\[
\int_T -\beta^* \omega k \, dV = -\beta^* \omega k \Delta V \quad \text{implicit} \quad (B.17)
\]

\[
S_k = 2\nu_t (S: \nabla \mathbf{u}) \Delta V - \frac{2}{3} (k: \nabla \mathbf{u}) \Delta V, \quad a_P(k) = \beta^* \omega k \Delta V \quad (B.18)
\]
Similarly, the transport equation for \( \omega \) is given as

\[
\nabla \cdot (\mathbf{u} \omega) - \nabla \cdot \left[ \left( v + \frac{\sigma_k}{\omega} \right) \nabla \omega \right] = \frac{\alpha_w}{k} \nabla \cdot \mathbf{u} - \frac{\beta}{\omega} + \frac{\sigma_\omega}{\alpha} \nabla k \cdot \nabla \omega \tag{B.19}
\]

the production term is handled in the same manner as above, where positiveness of the cross diffusion term is ensured through the closure parameter \( \sigma_\omega \). The dissipation term is discretized and linearized into the semi-implicit form \( \beta \omega \Delta V \). The term proportional to \( \omega^2 \) is added to the central coefficient.

The transport equation for the SA model is given as

\[
\nabla \cdot (\mathbf{u} \tilde{\omega}) - \frac{1}{\sigma} \nabla \cdot \left[ (v + \tilde{v}) \nabla \tilde{\omega} \right] = \tilde{c}_k \tilde{S}_k - \tilde{c}_{w1} f_w \left[ \tilde{\omega} \nabla \tilde{\omega} \right] + \frac{\tilde{c}_\omega}{\sigma} \tilde{\omega} \nabla \tilde{\omega} \cdot \nabla \tilde{\omega} \tag{B.20}
\]

Contributions to the central coefficient come from the linearization and implicit treatment of the dissipation term, whereas production and transport terms are added to the source. The overall contribution reads

\[
\int_{V} \tilde{c}_k \tilde{S}_k dV = \tilde{c}_k \tilde{S}_k \Delta V \quad \text{explicit}
\]

\[
\int_{V} \tilde{c}_{w1} f_w \left[ \tilde{\omega} \nabla \tilde{\omega} \right] dV = \tilde{c}_{w1} f_w \left[ \tilde{\omega} \nabla \tilde{\omega} \right] \Delta V \quad \text{explicit}
\]

\[
\int_{V} \frac{\tilde{c}_\omega}{\sigma} \tilde{\omega} \nabla \tilde{\omega} \cdot \nabla \tilde{\omega} dV = \frac{\tilde{c}_\omega}{\sigma} \tilde{\omega} \nabla \tilde{\omega} \cdot \nabla \tilde{\omega} \Delta V \quad \text{explicit}
\]

\[
S_v = \tilde{c}_k \tilde{S}_k \Delta V + \frac{\tilde{c}_\omega}{\sigma} \tilde{\omega} \nabla \tilde{\omega} \cdot \nabla \tilde{\omega} \Delta V, \quad \tilde{a}_{pv} = \tilde{c}_{w1} f_w \left[ \frac{\tilde{\omega}}{\tilde{y}} \right] \Delta V \tag{B.23}
\]

For the momentum equations and turbulence transport equations, residuals are checked against a prescribed tolerance \( \epsilon \) as:

\[
R_\phi = \left\| |S_\phi - \mathbf{M}_\phi^\phi|^{-1}| \right\|_\infty \leq \epsilon \tag{B.24}
\]

where \( \phi \) stands for any state variable, before solving the discrete system of equations. If the norm of the residual is smaller than the prescribed tolerance, then the solution from the previous iteration is considered to be sufficient for the discrete system defined by the newly updated coefficients. For the pressure correction \( \rho^* \), mass imbalance is considered for the convergence criteria (the source term of the pressure correction) (Eq. (B.12))

\[
R_p = \left\| \sum_f F^f \right\|_\infty \leq \epsilon \tag{B.25}
\]

Overall steps involved in the SIMPLE algorithm can be found in [20,56,57].

### Appendix C. Validation of the flow solver

The focus in this Appendix is on the simulation of turbulent flow in an asymmetric plane diffuser (Buice–Eaton diffuser [63]) for validation of the developed RANS solver. The general setup is shown in Fig. C.21. The dimensions are scaled with the channel height \( H \). The computational domain does not contain any sharp edges around the starting and ending sections of the diffuser ramp. A detailed description of the geometry can be found on the website provided by NASA [64].

Table C.12 presents the utilized relevant parameters for defining the simulation. In the experiment made by [63], the Reynolds number is defined using the upstream channel center line velocity (\( U_{cl} = 1.14U_{in} \)) and channel height \( H \), which results in \( Re_{cl} = 2 \times 10^5 \). The computational grid consists of 66,080 hexahedral cells. The mesh is clustered towards the walls such that the average value of the distance from the first cell center to the wall ensures that \( y^+ \approx 1 \) for both upper and lower walls.

Both turbulence models are tested, and both perform well near the inlet of the diffuser (location \( x/H = -6 \) in Fig. C.22), where a fully developed turbulent channel flow profile can be clearly observed. In the diffuser ramp
Fig. C.21. Illustrative schematic for the simulation of the asymmetric plane diffuser. The origin of the coordinate system is marked as \( o \) in the figure.

Fig. C.22. Computed velocity profiles from the simulation of the asymmetric (Buice–Eaton) plane diffuser, with \( Re = 2 \times 10^4 \). The blue solid lines indicate results from the \( k-\omega \) model, the red solid lines indicate results from the Spalart–Allmaras model, and the circles correspond to the measurement from [63]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table C.12

<table>
<thead>
<tr>
<th>( U_b ) [m/s]</th>
<th>( H ) [m]</th>
<th>( \nu ) [m²/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>19.812</td>
<td>0.015</td>
<td>( 1.695 \times 10^{-5} )</td>
</tr>
</tbody>
</table>

section (locations \( x/H = 6, 14, 20 \)) flow separation occurs due to adverse pressure gradients. The \( k-\omega \) model slightly outperforms the SA model, based on the measured mean velocity profiles. This result is expected, as the \( k-\omega \) model is known to perform well in adverse pressure gradient flow cases. In the outlet locations \( x/H = 30 \) and 40, both models predict similar velocity profiles, generally matching the measurements, though with small differences at location \( x/H = 40 \). Overall, the velocity profiles predicted with both models exhibit fine agreement with the experimental data at the presented locations of the diffuser.

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Publication P2

Density based topology optimization of turbulent flow heat transfer systems
Density based topology optimization of turbulent flow heat transfer systems

Sumer B. Dilgen 1 · Cetin B. Dilgen 2 · David R. Fuhrman 2 · Ole Sigmund 2 · Boyan S. Lazarov 2, 3, 4

1 Department of Electrical Engineering, Technical University of Denmark, Lyngby, Denmark
2 Department of Mechanical Engineering, Technical University of Denmark, Lyngby, Denmark
3 Lawrence Livermore National Laboratory, Livermore, CA, USA
4 School of Mechanical, Aerospace and Civil Engineering, The University of Manchester, Manchester, UK

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Abstract
The focus of this article is on topology optimization of heat sinks with turbulent forced convection. The goal is to demonstrate the extendibility, and the scalability of a previously developed fluid solver to coupled multi-physics and large 3D problems. The gradients of the objective and the constraints are obtained with the help of automatic differentiation applied on the discrete system without any simplifying assumptions. Thus, as demonstrated in earlier works of the authors, the sensitivities are exact to machine precision. The framework is applied to the optimization of 2D and 3D problems. Comparison between the simplified 2D setup and the full 3D optimized results is provided. A comparative study is also provided between designs optimized for laminar and turbulent flows. The comparisons highlight the importance and the benefits of full 3D optimization and including turbulence modeling in the optimization process, while also demonstrating extension of the methodology to include coupling of heat transfer with turbulent flows.

Keywords Topology optimization · Automatic differentiation · Turbulent flow · Thermal-fluid · Heat sink

1 Introduction
Forced convection is one of the most popular methods for cooling electronic devices and temperature sensitive equipment. The heat extraction process utilizes a heat sink built from highly conductive material, such as aluminum or copper, and a moving fluid which transports the heat away from the device. The performance depends on the amount of conductive material and its distribution, the contact area between the fluid and the sink, the fluid velocity distribution, temperature and thermal capacity. The fluid is accelerated using a pump or a small fan. A sink usually consists of plate or pin fins attached to a plate which is in contact with the heat source. The performance can be improved by parametric variations, e.g. changing the number and the positions of predefined fins; optimizing their shape; or changing completely in a non-uniform way the distribution of the conductive material to minimize the temperature of the device. The latter can be achieved by topology optimization and is the main subject of this article.

Topology optimization (Bendsøe and Sigmund 2003) is a design process which distributes material in a design domain by optimizing an objective function. For heat sinks, the objective is usually to minimize some performance measure, which is a function of the temperature on the surface or inside the heat source. In modern high-performance computing systems design, high density of the different components is necessary to increase the computational performance, and to decrease the cost and the space requirements for the installation. In such restricted space conditions the cooling is performed either in a closed loop fluid-cooling system or carefully guided air streams. In both cases, it is desirable to re-utilize the fluid for cooling
of more than one component which requires decreasing the energy dissipation or the pressure drop.

The material distribution in density based topology optimization is modeled with the help of an index function taking values of zero or one which, respectively, represent solid and fluid distributions in the selected design domain. Updates on the design are based on gradients of the objective and the constraints. Thus, the problem is relaxed, and the material distribution function is allowed to take intermediate values. Following a nested optimization approach, objective, constraints and gradient evaluations require the solution of a fluid state problem, resulting in fluid velocity and pressure distributions, and a subsequent temperature convective problem, which represents the heat conducted through the sink and transported through the fluid.

Topology optimization was originally introduced in solid mechanics problems where the methodology is well developed and utilized on a regular basis in industrial settings. In contrast, its development for mixed fluid-heat transfer problems is far from mature and requires further development and research. The first fluid mechanics applications for Stokes flow were reported in Borrvall and Petersson (2003). Large scale examples of Stokes flow problems have been demonstrated in Aage et al. (2008). Later applications to laminar flow can be found in Gersborg-Hansen et al. (2005), Olesen et al. (2006), Pingen et al. (2007). For general shape optimization, the derivation and the application of the topological sensitivities for Stokes and Navier-Stokes equations have been demonstrated in Guillaume and Idris (2004), Amstutz (2005). The fluid flow in forced convection is often turbulent which further complicates the optimization process. Topology optimization for such processes is applied in Othmer (2008) by using the so-called frozen turbulence assumption, i.e., the variation of the turbulence fields with respect to the design parametrization is neglected. In Zymaris et al. (2009) a continuous adjoint formulation is presented based on the Spalart-Allmaras (SA) turbulence model, and the solution of the -equation $k-\omega$ turbulence models (Wilcox 2008) have been presented only recently in Dilgen et al. (2018). This work provides the foundation of the current presentation, which is extended further to include heat transport, hence demonstrating the feasibility of the approach for large scale mixed thermo-fluidic topology optimization problems.

For topology optimization of coupled thermal-fluid problems, Koga et al. (2013) utilized Stokes flow and used a multi-objective function that combines pressure drop minimization and heat transfer maximization for the optimization. Heat sink optimization with laminar flow has been demonstrated in Matsumori et al. (2013), Yaji et al. (2015, 2016), Dede (2009) where Matsumori et al. (2013) carried out optimization of 2D heat exchangers for various input power formulations and Yaji et al. (2015) utilized the level set method for the topology optimization.

The extension to natural convection is described in Alexandersen et al. (2016). Regarding turbulent flow optimization of heat transfer systems, (Pietropaoli et al. 2017) utilizes the frozen turbulence assumption in the calculated sensitivities, and Kontoleonkos et al. (2013) presents continuous adjoint formulation. The present article demonstrates turbulent-flow heat-transfer topology optimization problems where the fluid flow is modeled by steady state incompressible Reynolds-averaged Navier-Stokes (RANS) equations. Turbulence closure is achieved utilizing the two-equation $k-\omega$ model, and the solution of the problem is obtained using an already developed 3D finite volume framework (Dilgen et al. 2018) which employs automatic differentiation (Griewank and Walther 2008) for calculating the adjoint equations and exact gradients consistent with the considered turbulence model. To the best of the authors’ knowledge, such topology optimization of coupled thermal-fluid problems with turbulent flows has not been previously demonstrated with exact sensitivities obtained within the discrete adjoint approach, and without any simplifying assumptions. Thus, demonstrating the ease of handling additional physics by adding heat transfer to the turbulent fluid solver is among the primary contributions of the present work.

The paper is organized as follows: Section 2 describes the governing equations along with the inclusion of the utilized penalization method to realize the effect of solid regions in the design domain. Section 3 introduces topology optimization. The exact form of the interpolation functions and the associated adjoint sensitivity analysis are also included. Finally, the optimization of heat sink devices with turbulent forced convection is demonstrated with several 2D and 3D optimization cases in Section 4.

### 2 Governing equations

The fluid flow is modeled with the help of the steady-state incompressible Reynolds-averaged Navier-Stokes (RANS) equations. In what follows, it is assumed that the temperature differences in the flow will be small enough that the variations of the fluid properties are neglected. Hence, temperature acts as a passive scalar and only one way coupling is considered in the system. The RANS equations are written as

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = \nabla \cdot (2\nu\mathbf{S}) - \frac{1}{\rho} \nabla p + \nabla \cdot \mathbf{T} - \lambda \chi(\gamma)\mathbf{u} \quad (2)$$
where \( \mathbf{u} \) is the mean velocity vector, \( p \) is the pressure, \( \nu \) is the kinematic viscosity of the fluid, \( \rho \) is the fluid density and the mean strain rate tensor is defined as \( \Omega = \frac{2}{3} ( \nabla \mathbf{u} + (\nabla \mathbf{u})^T ) \).

The Reynolds stress tensor is given as

\[
T_{ij} = -\mathbf{u} \otimes \mathbf{u}' = 2\nu t S_{ij} - \frac{2}{3} \delta_{ij} T
\]  

where \( \nu_t \) is the turbulent eddy viscosity and \( k = \frac{1}{2} \mathbf{u}' \cdot \mathbf{u}' \)

is the turbulent kinetic energy per unit mass, with \( \mathbf{u}' \) indicating turbulent fluctuating velocities.

The turbulent kinetic energy \( k \) has a well defined boundary at walls given as

\[
k_b = 0
\]

On the other hand, the specific dissipation rate \( \omega \) has a singular behavior near a wall. For smooth walls (as uniformly considered herein), the approximate (non-homogeneous Dirichlet type) boundary condition proposed by (Menter 1994) given as

\[
o_{rb} = \frac{60\nu}{\beta_1 y}\]  \( \beta_1 = 0.075 \)  

is utilized in the computations. The value of \( y_1 \) represents the distance from the wall to the cell center nearest the wall.

The physical meaning of the wall boundary condition \( o_{rb} \) (10) is related to the length scale \( l = \sqrt{k/\omega} \) of turbulent eddies where \( o_{rb} \) ensures that turbulent eddies become infinitesimally small as a wall is approached. During the optimization process, both \( k \) and \( \omega \) are penalized to their values at the wall boundary conditions in the solidified regions (Dilgen et al. 2018). Since a regular mesh is used in the design domain, \( y_1 \) does not vary and is defined by the half cell length for penalization of the wall boundary condition \( o_{rb} \) inside the design domain.

For detailed explanation of all equations and coefficients presented above, interested readers are referred to Wilcox (2006).

\section{Heat transfer}

The temperature variations in the fluid and the solid regions, are captured using the conjugate heat transfer equation

\[
\chi_t(\gamma) \nabla \cdot (\mathbf{u}_f T) = \nabla \cdot [\alpha(\gamma) \nabla T] + Q(\gamma)
\]

where \( T \) is the temperature (in Kelvin), \( Q(\gamma) \) is the volumetric heat source, \( \chi_t(\gamma) \) is a non-dimensional function to turn on and off the convection term in fluid \( \chi_t(\gamma) = 1 \) and solid regions \( \chi_t(\gamma) = 0 \), and \( \alpha(\gamma) \) interpolates.
between thermal diffusivity of the fluid and the solid according to

\[ \alpha_f = \frac{\nu}{\text{Pr}_f} \]

\[ \alpha_s = \frac{k_s}{c_s \rho_s} \]

(12)
(13)

Here $\text{Pr}_f$ and $\text{Pr}_s$ are the laminar and the turbulent Prandtl numbers, $k_s$ is the thermal conductivity and $c_s$ is the specific heat capacity. The considered interpolation functions for the conjugate heat transfer are presented in Section 3.

2.2 Discretization

The above system of PDEs is discretized using the finite volume method on a non-uniform computational grid (Versteeg and Malalasekera 2007; Ferziger and Peric 2001). The discrete set of algebraic equations is solved using a segregated approach for the pressure-velocity coupling, with the help of the SIMPLE (semi-implicit method for pressure-linked equations) algorithm (Patankar 1980). The SIMPLE algorithm is one of the most attractive schemes for solving problems in computational fluid dynamics due to its low memory requirements and the ability to simulate both steady and unsteady flows. The present implementation is based on the PETSc library (Balay et al. 1997, 2017a, b), which is utilized mainly for its efficient parallel sparse solvers. A verification of the implemented fluid dynamics solvers and the source term coefficients in (11) are computed as

\[ \alpha_f = \alpha_s + \left( a_f - a_s \right) \gamma_i^n \]  
\[ \beta_i = \left( 1 - \gamma_i^n \right) \frac{q}{c_s \rho_s} \]

(22)
(23)

where $q$ is the volumetric heat source which is only active in the intermediate and the solid regions ($\gamma_i < 1.0$), and $n$ is the parameter which controls the curvature of the interpolation function (see Fig. 1). The updating of the design variables $\gamma$ is determined using the method of moving asymptotes (MMA) (Svanberg 1987), with a parallel PETSc implementation presented in Aage and Lazarov (2013), Aage et al. (2015).

3 Topology optimization

The topology optimization problem is defined as

\[ \min_{\gamma} C(\gamma, U(\gamma), T(\gamma)) \]

(14)
\[ \text{s.t. } R_U(\gamma, U(\gamma)) = 0 \]
(15)
\[ R_T(\gamma, T(\gamma), U(\gamma)) = 0 \]
(16)
\[ g_i(\gamma) \leq 0, \quad \forall i = 1, \ldots, N \]
(17)
\[ 0 \leq \gamma \leq 1 \]
(18)

where $C(\gamma)$ is the objective function, $U$ and $T$ are vectors with discrete state variables representing flow (velocity, pressure and turbulence quantities) and temperature, respectively, $R_U$ and $R_T$ are residual vector functions obtained from the discretization of the governing equations of velocity, pressure, turbulence quantities and temperature fields. The set $g_i(\gamma), i = 1 \ldots N$ represents additional inequality constraints and the vector $\gamma$ the material (fluid/solid) distribution in the design domain. The interpolation between solid and fluid is realized with the help of the function $\chi(\gamma)$, which is defined as

\[ \chi(\gamma) = \frac{1 - \gamma_i^n}{q + \beta_i} \]

(19)

where the parameter $q$ controls the curvature of the function. The physical design field $\chi$ is obtained using regularized Heaviside projection (Wang et al. 2011), controlled by a sharpness parameter $\beta$ and a threshold $\eta = 0.5$. The projection is applied on a filtered density field (Bourdin 2001). Gradients of the objective and constraints with respect to the original design field $\gamma$ are subsequently obtained by applying the chain rule.

To model the impermeable solid regions, the Brinkman penalization parameter $\lambda$ must be sufficiently high. The choice of $\lambda$ is based on the dimensionless Darcy number defined as

\[ Da = \frac{vU/L}{\lambda L U} = \frac{v}{\lambda L^2} \]

(20)

which represents the ratio of viscous forces to Darcy damping forces, where $U$ and $L$ are, respectively, characteristic velocity and length scales defining a given flow problem. To capture the temperature variations, the coefficients of the heat equation are interpolated. The convection, the diffusion and the source term coefficients in (11) are computed as

\[ x_i(\gamma) = \gamma_i^n \]
(21)
\[ a(\gamma) = a_s + \left( a_f - a_s \right) \gamma_i^n \]
(22)
\[ Q(\gamma) = \left( 1 - \gamma_i^n \right) \frac{q}{c_s \rho_s} \]
(23)

3.1 Discrete adjoint

Obtaining the gradients and more precisely the discrete adjoint equations for finite volume discretization of fluid flow problems represents one of the main challenges in the current work. The primary issue is that the Jacobian of the residual system of equations is never formed explicitly.
The state solution is obtained using the SIMPLE algorithm in a matrix free fashion. The complexity of forming the exact Jacobian for the discrete adjoint equation comes from the large number of fully coupled physical fields (three velocity components, the pressure, the turbulent kinetic energy and the specific dissipation rate) in the governing system of equations. Furthermore, due to the iterative nature of the forward solution algorithm, an additional set of state variables representing the fluxes for every finite volume element is added to the original set of physical fields. The complete details are described in Dilgen et al. (2018).

The Jacobian of such a complex set of fully coupled equations is obtained with the help of Automatic Differentiation (AD) (Griewank and Walther 2008). AD represents a set of software techniques for evaluating derivatives of functions implemented as a computer code. The general idea is to apply the chain rule automatically for every complex function by representing it as a set of simple function evaluations with well-known derivatives. In modern object oriented languages like C++, such functionality is achieved using operator overloading techniques (Hogan 2014; CoDiPack 2016). The obtained gradients are exact to the machine precision. General discussion with examples on the applicability to topology optimization are presented in Nørgaard et al. (2017). Here, AD (Hogan 2014) is applied for evaluating the Jacobian of the residual form. The gradients of the objective and the constraints are computed using standard adjoint analysis presented below. As discussed in Dilgen et al. (2018), Nørgaard et al. (2017) such an approach saves a significant amount of memory. The slow down regarding computational time is negligible compared to the speed-up of the actual implementation process.

The objective is augmented with two sets of Lagrange multipliers and the residuals for the fluid and the heat transfer problems as

\[
\mathcal{L} = C(\gamma, U(\gamma), T(\gamma)) + \lambda_T^T R_T(\gamma, U(\gamma)) \\
+ \lambda_U^T R_U(\gamma, U(\gamma)) \tag{24}
\]

For zero residuals the Lagrangian function coincides with the objective/constraint function. The derivative with respect to the design parametrization can be written as

\[
\begin{split}
\frac{d\mathcal{L}}{dy} &= \frac{\partial C}{\partial y} + \lambda_T^T \frac{\partial R_T}{\partial y} + \lambda_U^T \frac{\partial R_U}{\partial y} \\
+ \lambda_T^T \frac{\partial R_T}{\partial U} + \frac{\partial R_T}{\partial y} + \lambda_U^T \frac{\partial R_U}{\partial U} + \frac{\partial R_U}{\partial y} \tag{25}
\end{split}
\]

To avoid computation of derivatives of the state variables, which are expensive to evaluate, all terms containing these derivatives are collected and required to be equal to zero. This requirement provides the adjoint equations for the optimization problem:

\[
\begin{align*}
\frac{\partial C}{\partial y} + \lambda_T^T \frac{\partial R_T}{\partial y} &= 0 \\
\frac{\partial C}{\partial y} + \lambda_U^T \frac{\partial R_U}{\partial y} + \lambda_T^T \frac{\partial R_T}{\partial y} &= 0 \tag{26}
\end{align*}
\]

The temperature and flow adjoint problems are, respectively, written as

\[
\begin{align*}
\left( \frac{\partial R_T}{\partial T} \right)^T \lambda_T &= -\frac{\partial C}{\partial T} \\
\left( \frac{\partial R_U}{\partial U} \right)^T \lambda_U &= -\frac{\partial C}{\partial U} \left( \frac{\partial R_T}{\partial U} \right)^T \lambda_T \tag{27, 28}
\end{align*}
\]

and the final vector of gradients is evaluated as

\[
\begin{align*}
\frac{\partial C}{\partial y} &= \frac{\partial C}{\partial y} + \left( \frac{\partial R_T}{\partial y} \right)^T \lambda_U + \left( \frac{\partial R_T}{\partial y} \right)^T \lambda_T \tag{29}
\end{align*}
\]

The gradient evaluation procedure described above is applied to the already-discretized governing equations and a selected objective function. As this approach operates at the discrete level, where the boundary conditions are already accounted for, it can handle any cost function and governing equation in a robust manner. Most importantly, calculated sensitivities are always exact for the considered discretization. The two Jacobians \( \left( \frac{\partial C}{\partial y} \right)^T \), \( \left( \frac{\partial R_T}{\partial y} \right)^T \), and all partial derivative terms involved in the adjoint analysis are computed and assembled cell-wise using AD as described in Dilgen et al. (2018).
3.2 Objective and constraint functions

In this work, the objective function is to minimize the average temperature in solid domains. In 2D the considered objective function is defined as

$$\mathcal{C} = \frac{\int V (1 - \gamma) T dV}{\int V (1 - \gamma)}$$

(30)

where $\gamma$ denotes the volume fraction of fluid in the design domain. The main idea is that the 2D setup represents a horizontal cut through the actual 3D model shown in Fig. 7. Due to the high conductivity of the sink material, the heat propagates through the solid material and later is extracted and transported by the fluid. In 3D, the domain in which the average temperature is minimized is passive (not depending on design) and hence the objective function is

$$\mathcal{C} = \frac{\int V T dV}{\int V dV}$$

(31)

The fluid volume is bounded from above and the constraint is given as

$$g_i(\mathbf{x}) = \frac{\Delta V_i}{V_i} - 1 \leq 0, \quad i = 1, \ldots, N_e$$

(32)

The above constraint ensures that the heat input to the system is bounded from below. In addition to the above objective and constraint, the power dissipation of the system is controlled using a reference power dissipation value $g_r$. The power dissipation between inlet and outlet boundaries is given as

$$g_r(\mathbf{x}) = \int \left( u \cdot \mathbf{n} \left( \frac{1}{2} u^2 + p \right) - 2 \nu_{eff} (\mathbf{S} \cdot \mathbf{n}) \right) dV$$

(33)

Here, $\mathbf{n}$ is the normal vector, $\mathbf{S}$ is the mean strain rate tensor which is defined in Section 2 and $\nu_{eff}$ is the effective viscosity given as $\nu_{eff} = \nu_1 + \nu$. With the above definitions, the power dissipation is constrained as follows

$$g_r(\mathbf{x}) = \frac{\mathcal{J}}{w \cdot \mathcal{J}_{eff}} - 1 \leq 0$$

(34)

where $\mathcal{J}_{eff}$ is the reference value.

In the considered optimization cases $\mathcal{J}_{eff}$ is calculated starting with the design domain comprised only of the fluid region ($\gamma = 1$). The parameter $w$ is considered to be larger than one in the presented examples, i.e. $w > 1$. It should be noted that the above power dissipation constraint is a function of the state fields of the RANS equations, i.e., velocities, pressure, fluxes and turbulence quantities. Hence, for each optimization step, an additional adjoint equation has to be solved in order to calculate the gradient of the constraint with respect to the design parameters.

4 Optimization of cooling systems

The procedure will now be demonstrated on several topology optimization examples dealing with coupled thermal-fluid problems. The first study deals with 2D heat sink design, where the effect of the power dissipation constraint on the optimized designs is studied in detail. Following this, 3D heat sink examples will demonstrate the advantages of optimizing design without reducing the number of dimensions and including turbulence modeling in the optimization process.

Throughout the present work, air and aluminum are chosen as materials for fluid and solid, respectively. The flow properties considered for the cooling system cases are given in Table 1. The geometry is scaled with half the inlet channel height $H$. The Reynolds number in the considered optimization problems is computed as $Re = U_b H / \nu = 5 \times 10^5$ where $U_b$ is the bulk inlet velocity. The solid material properties used throughout are listed in Table 2. Considering the listed material properties, the thermal diffusivity ratio of the solid and the fluid is approximately $a_s/a_f \approx 4.5$.

The Brinkman penalization parameter is set to $\lambda = 400 \ \text{s}^{-1}$ which is sufficient to yield nearly impermeable solidified regions ($Da_a \sim 10^{-4}$, taking $U_b$ and $H$ as the characteristic velocity and length scales, respectively) without adversely affecting the convergence of the optimization process. The sharpness parameter of the regularized Heaviside projection is taken as $\beta = 6$.

It has been found that the formulated optimization approach is somewhat sensitive to the choice of parameter $q$ which controls the interpolation function that is utilized in the penalization of fluid flow. To this end, a continuation strategy is performed for the curvature parameters $q$ and $n$ of the interpolation functions (19) and (21)-(23) to avoid convergence to poorly performing locally optimal solutions.

| $U_b$ [m/s] | $H$ [m] | $\nu$ [m$^2$/s] | $Pr$ | $Pr_s$
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.75</td>
<td>0.1</td>
<td>$1.5 \times 10^{-5}$</td>
<td>0.7</td>
<td>0.9</td>
</tr>
</tbody>
</table>

Table 1 Flow (air) properties considered for the cooling system optimization

<table>
<thead>
<tr>
<th>$k_s$ [W/m K]</th>
<th>$c_v$ [kJ/kg K]</th>
<th>$\rho_s$ [kg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>237</td>
<td>900</td>
<td>2700</td>
</tr>
</tbody>
</table>

Table 2 Thermo-physical properties of the solid (aluminum) considered for the cooling system optimization
The parameter \( q \) is initially set to 0.01 for which the flow ignores a large section of the gray scale and diffuses into solidified regions, enhancing the sensitivities, which in turn provides a “smart” initial guess for the optimization problem (Borrvall and Petersson 2003). Hereafter, it is increased in a step-wise manner to 0.1, 1.0 and 10. Similarly, the parameter \( n \) which controls the interpolation in the heat transfer equation takes values of 3 and 4 leading up to its final value of \( n = 5 \).

The 2D and 3D optimization cases utilize a mesh resolution which roughly keeps a distance in wall coordinates \( y^+ = yU_f/\nu \approx 10 \) when calculated from the inlet channels, where \( U_f \) is the friction velocity. Since the location of the wall along with the flow solution can not be known a priori, \( y^+ \) values are not necessarily ensured to stay within an acceptable range during the optimization, though the inlet conditions provide simple and generally useful scales. Presently, it is not computationally feasible to use mesh size comparable to \( y^+ \approx 1 \).

### 4.1 2D heat sink

The first example demonstrates the optimization of a 2D heat sink, subject to a constraint on the power dissipation. The objective is the minimization of the integral of the temperature in the solid parts of the design domain \( \Omega_d \) as defined in the (30). The fluid volume is limited to 55% of the whole computational domain. The problem setup can be seen in Fig. 2. The temperature is set to 300 K at the inlet and zero gradient boundary condition is utilized at the outlet. All other boundary conditions are realized as adiabatic walls. Fully developed turbulent channel flow profiles are mapped to the flow and the turbulence model variables at the inlet. These values are obtained using preliminary simulations of the inlet channel. Due to the symmetry, only half of the domain is considered in the optimization process. Following the assumption of infinitely long channels, heat generation is only considered in the solid regions with \( q = 175 \text{ kW/m}^2 \) and the heat source is evaluated using (23).

Figure 3 shows optimized designs for increasing value of the power dissipation constraint. The complexity of the design increases with the allowed power dissipation, which results in a better cooling performance. The increased cooling performance is evident from the objective values of the end designs, shown in Fig. 3, as well as from the temperature fields, shown in Fig. 4. The best performing heat sink (lowest temperature rise) is obtained for 10 times increased power dissipation compared to the initial reference state. The velocity magnitude contours for each optimized design are shown in Fig. 5. For larger power dissipation the size of the main channel is decreased allowing higher velocity in the secondary channels, thus providing better cooling performance.

In order to further investigate the validity of the followed optimization approach, the 2D heat sink design that is obtained for \( w = 10 \) (Fig. 3c) is simulated with a body-fitted mesh. The body-fitted profile is obtained using a sharp threshold of \( \eta = 0.5 \) on the optimized porosity field. The boundary layer is fully resolved in the fluid channels by keeping the distance (in dimensionless wall units) from the first cell center to the wall well below unity. Figure 6 shows the results from the body-fitted mesh analysis on the optimized design in which the calculated objective function \( C = 300.58 \) agrees well with the objective value obtained from the penalized model (Fig. 3c). From the investigation...
of the velocity magnitude contour predicted with the body-fitted mesh (Fig. 6a), it can be deduced that the fixed-grid optimization model over-estimates the velocity in the lowest secondary channel (Fig. 5c). This can be seen as a shortcoming of the Brinkman penalization where the solid regions still contain pressure gradients which affect the velocity distribution in thin channels. The remedy can be found in increasing the mesh resolution along the transition region of the thin channels or increasing the Brinkman penalization parameter $\lambda$. On the other hand, the predicted temperature field in the penalized model (Fig. 4c) compares well with the temperature distribution obtained from the body-fitted mesh (Fig. 6c). Furthermore, Fig. 6b shows the resulting turbulent kinetic energy in the fluid channels of the optimized heat sink. Overall, a reasonable agreement is found between the penalized and the body-fitted models.

4.2 3D heat sink with two heat sources

The 2D setup is a simplification of a real 3D problem. Thus, to compare the performance of the 2D designs a full-scale 3D model is considered as a second example. The 3D problem setup is shown in Fig. 7. Due to symmetry in both $y$ and $z$ directions only a quarter of the domain is considered for the optimization process. Blue color marks fixed fluid inlet and outlet channels. Similar to the 2D case, fully developed turbulent channel flow profiles are mapped to the flow and turbulence model variables at the inlet, now also accounting for the presence of the side wall. The design domain $\Omega_d$ is colored green in the provided sketch. Heat to the system is provided from the bottom and the top boundary of a fixed solid region (a thin heated plate) which is fixed as solid throughout the optimization. The heat source is colored with red. The heat enters the system through the boundary. The heat source term utilized in the previous section is changed in this case to a non-homogeneous Neumann boundary condition

$$ \frac{\partial T}{\partial n} = \frac{\dot{q}}{k_v} $$

where the heat influx is set to $\dot{q} = 175 \text{ kW/m}^2$.

The objective in this case is the minimization of the integral of the temperature in the heated plate $\Omega_p$ (31).

A power dissipation constraint with parameter $w = 10$
The calculated objective value is $C = 300.58$ (34) is utilized in the optimization process. The allowed volume fraction for the fluid is the same as in the 2D case. The temperature is set to 300 K at the inlet and a zero gradient boundary condition is utilized at the outlet. All other boundaries (excluding the heated boundaries) are realized as adiabatic walls.

Figure 8 shows the optimized flow channels where the shaded red areas illustrate the location of the heated plates. The design consists of rather flat and thin channels parallel to the heated plates. The half cut of the optimized design shown in Fig. 8b demonstrates parts of the channel that provide the required speed up of the flow for more efficient cooling. The resulted streamlines of the flow are shown in Fig. 9 and are colored with the temperature and the velocity magnitude. The fluid is heated almost uniformly toward the outlet region.

Due to the symmetry, only a quarter of the domain is utilized for the optimization. Blue color represents the fixed fluid regions for inlet and outlet, green color shows the design domain $\Omega_1$ and the red color specifies the fixed solid region $\Omega_p$ (heated thin plate).
The design domain consists of 216,000 hex cells which result in 2.5M DOFs for the fluid problem and 216K DOFs for the heat transfer problem. The number of optimization iterations is 300 which takes around 10 h of computational time on 100 Intel Xeon e5-2680v2 CPU cores.

4.3 Comparison between the 2D and 3D designs

To compare the 3D optimized heat sink to the 2D design shown in Fig. 3c, the 2D topology is extruded. The heat source is set in the same manner as for the 3D optimization case. Figure 10 compares the streamlines of the flows from the extruded 2D design and the 3D design, colored with the temperature field. It is apparent from Fig. 10a that the flow in the extruded 2D design is heated unevenly and the heated lower part of the fluid cannot transfer the heat to the mid parts of the domain. Hence, the large bulk of the fluid cannot extract heat from the plate, in contrast to the 3D optimized heat sink where the flow gets heated almost uniformly (Fig. 10b). The actual performance depends on the fluid-solid contact surface, the velocity and the temperature of the fluid close to the heated plate and on the temperature difference between the solid and the fluid.

Figure 11 compares the temperature distributions in the solid regions of the extruded and the 3D optimized design. The superior cooling performance of the 3D optimized design can be observed. For the 2D extruded design the fluid heats up in thin channels close to the plate, and cannot extract more heat from the source toward the outlet. This effect is strongly pronounced in the thinner outer channels. The mid channel performs reasonably well, however, due to the limited contact area the fluid cannot extract more heat. On the other hand, the 3D optimized design provides larger contact surface area. Hence, a more uniform temperature distribution is realized both in the solid and the fluid regions, and the temperature gradient between the heated solid and the fluid remains large even close to the outlet of the sink. This effect allows the fluid to extract more heat which explains the better performance of the 3D optimized design and demonstrates the benefits of full 3D optimization.

Another possibility for a simplified 2D model is to take a vertical cut through the middle of the 3D design domain. The constraint of the fluid volume is not enforced as the
heat input is supplied from the bottom and the top plates. In this case, the optimizer distributes a thin layer of solid on top of the heated plate. This distribution accelerates the flow and increases the heat transport. However, due to the strict constraint on the pressure drop, the amount of distributed material is limited. The temperature in the plates increases significantly in this case and the 3D objective is $C = 348$. This 2D design is not shown for the sake of brevity.

4.4 3D heat sink with one heat source

Performance improvement due to increased design freedom is further demonstrated in this section. To assess the effect of including turbulence modeling in the optimization framework, the section also provides a comparative study with a heat sink design that is optimized for laminar flow.

The full length of the 3D model is utilized for optimization. The setup considers a heat influx ($\frac{\partial T}{\partial n} = \dot{q} k_s$ with $\dot{q} = 175$ kW/m$^2$) from the bottom boundary of the heated plate and the top boundary is considered as an adiabatic wall. The case utilizes the symmetry only in the $z$ direction and rest of the computational domain is the same as presented in Fig. 7. The computational mesh consists of 400,000 hex cells which results in 4.8M DOFs for the fluid problem and 400K DOFs for the heat transfer problem. The number of optimization iterations is 300 which takes around 16 h of computational time on 120 Intel Xeon e5-2680v2 CPU cores. The initial design consists of a porous material, with a value of 0.5, distributed everywhere in the design domain. The allowed volume fraction for the fluid and power dissipation constraint parameter $w$ (34) are the same as in the previous 3D case (Section 4.2).

The optimized heat sink design with turbulent flow of $Re = 5000$ is shown in Fig. 12a and c with different iso-views. As can be seen from Fig. 12e, the additional freedom allows the optimizer to accelerate the fluid close to the heat source resulting in lower maximal temperature. The design is much more sophisticated than the one presented in...
Fig. 12. Topology optimized design of 3D heat sink device for $Re = 5000$ with $k-\omega$ model (left column) and $Re = 50$ with a laminar model (right column).

Fig. 8. The additional channels mix heated and colder fluid streams, thus, keeping high-temperature gradient between the plate and the cooler toward the sink outlet.

The same flow and solid properties are utilized for the laminar flow optimization (as shown in Tables 1 and 2) where the only difference is the lowered bulk velocity of
the inlet flow which is taken to be $U_b = 0.0075 \, \text{m/s}$, and the Reynolds number of the flow is tailored to be $Re = 50$. A laminar channel flow profile is used as the inlet flow. The resulting optimized channels for the laminar flow can be seen with different iso-views in Fig. 12a and c. Although the heat sink is optimized for the given Reynolds number of $Re = 50$, an immense rise in temperature can be observed from the temperature distribution of the flow field given in Fig. 12f. This is mainly due to the laminar nature of the fluid with lowered diffusivity where an effective cooling to the plate can not be realized considering the chosen material properties. To further investigate the effect of introducing turbulence modeling to the optimization process and to compare the designs obtained with turbulent and laminar flow, the resulting designs are run for various Reynolds numbers ranging from $Re = 50$ to $Re = 5000$. For simulations, the RANS $k-\omega$ model is utilized for $Re \geq 1000$. Figure 13 shows the calculated objective values of both designs in the given range of Reynolds numbers. As expected, both designs outperform the other at the Reynolds number which they are optimized for. This also confirms that the turbulence model is correctly embedded in the optimization process. Both the laminar and turbulent designs achieve quite similar performance trends. However, after a Reynolds number of $Re \approx 200$ the design obtained with turbulent flow optimization exhibits better cooling performance than the laminar design as expected. Further investigations regarding the behavior and comparison of the two designs for higher Reynolds numbers must be based on body-fitted meshes that resolve the boundary layer accurately.

![Figure 13](image_url)  

**Figure 13** Objective values of the optimized 3D heat sink designs computed for different values of Reynolds numbers where turbulent design is shown in Fig. 12a and the laminar design is given in Fig. 12b

### 5 Conclusions

The article demonstrates the advantages of optimizing realistic 3D designs compared to 2D simplified models. The additional dimension provides extra freedom to the optimizer for better material distribution. A comparative study is provided between the designs optimized for laminar and turbulent flows confirming that improved designs can be obtained by including turbulence modeling in the optimization process. For forced convection and similar pressure drop, the larger design space leads to lower device temperature. The inclusion of turbulence models introduces additional complexity in the state and the adjoint solvers, however, allows for higher fluid velocities. The complexity is managed with the help of automatic differentiation. The additional temperature field is introduced in the simulation using the same techniques applied to the turbulent fluid solver presented earlier in Dilgen et al. (2018). Additional transport processes are handled without significant changes to the code, thus demonstrating the extendability and the feasibility of the approach for large-scale optimization problems, and opening the possibility of obtaining optimized topologies of even more complicated multi-physics problems.

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Publication P3

Topology optimization of acoustic mechanical interaction problems: a comparative review
Abstract

The pursuit for design improvements by geometry modifications can easily become prohibitive using a trial and error process. This holds especially when dealing with multi-physics problems—such as acoustic-structure interaction—where it is difficult to realize design improvements intuitively due to the complexity of the coupled physics. Compared to classical shape optimization, where a near optimal shape has to be supplied as an initial guess, topology optimization allows for innovative designs through a completely free material distribution, such that the topology can change during the optimization process. The goal of this article is to provide a comprehensive critical review of the proposed strategies for topology optimization of coupled acoustic-structure interaction problems. The work includes a comparison of topology optimization formulations with density, level set, and evolutionary-based methods and discusses the corresponding strengths and weaknesses through the considered application examples. The review concludes with recommendations for future research directions.

Keywords Vibro-acoustics · Topology optimization · Density methods · Level set methods

1 Introduction

Since its introduction in the late 1980s, gradient-based topology optimization has diversified significantly both in terms of application areas, but also with emerging variants of the original design parameterization. The initial homogenization approach (Bendsøe and Kikuchi 1988) laid the foundation for the so-called density method, often referred to as the SIMP method (Bendsøe 1989). Here, a pixel (or in 3D: voxel)-based design description is used with continuous element-wise design variables representing a relative “element density” (not to be confused with the mass density of the involved material). Elimination of intermediate-valued (grey) design variables with the penalization approach combined with appropriate regularization of the optimization problem using filtering techniques and length-scale control (Bourdin 2001; Bruns and Tortorelli 2001; Guest et al. 2004; Wang et al. 2011) led to a breakthrough regarding generation of well defined (black-white) pixelized structures. The result is that only limited post-processing (if any, e.g., Christiansen et al. 2015) is needed before fabrication. Combined with efficient adjoint sensitivity analysis and the use of robust and versatile mathematical programming tools, e.g., The Method of Moving Asymptotes (MMA) (Svanberg 1987), this has paved the way for the tremendous popularity of this approach. Recently, a milestone has been reached with the report of giga-scale design of a full aircraft wing with more than one billion 3D elements and corresponding design variables (Aage et al. 2017). Moreover, the method has also proven its worth for a number of other applications, ranging from material design (Larsen et al. 1997), acoustics (Park and Wang 2008), optics (Jensen and Sigmund 2011), and microfluidics (Alexandersen et al. 2016) as well as coupled multi-physics problems such as thermo-electro-mechanical devices (MEMS) (Sigmund 2001), turbulent...
flow heat transfer systems (Dilgen et al. 2018), and many other application areas.

As an inherent feature of the density-based approach, the structural boundary is constantly evolving during the optimization procedure. That is, boundaries may appear and disappear in a seamless fashion due to the continuous design variables. The corresponding structural appearance with gray scale at intermediate design stages can, however, cause uncertainty and ambiguity in identifying well defined boundaries. This poses a challenge when dealing with structures affected by, e.g., pressure boundary loads and calls for specialized schemes to be developed (Olhoff et al. 1991; Sigmund and Clausen 2007).

The quest for a well-defined boundary has partly motivated the use of level set methods (Osher and Sethian 1988; Sethian and Wiegmann 2000) for structural optimization. With the aim of keeping the full design flexibility from the density approach and combining this with the well-defined boundaries known from shape optimization methods, a level set function implicitly defines the structural boundary through its zero level iso-curve. The level set function is evolved via design sensitivities and holes may merge or new holes may appear, partially thanks to the introduction of topological derivatives (Novotny and Sokolowski 2013). Several variants of the method has appeared using the original version based on a boundary-fitted mesh and design updates based on the solution of a Hamilton-Jacobi equation. Since then, many alternative versions have been introduced, of which the one based on fixed meshes, curfem methods (Hansbo and Hansbo 2004) and the use of level set functions has been reported well-suited for complex interface problems cf. (Villanueva and Maute 2017). Moreover, variants of the level set methods such as phase field methods and implicit functions have also appeared, which share theoretical and implementation details with the mentioned approaches. It should be mentioned that the numerical implementation of level set methods share many of same issues as the density method, and we refer to the review paper by (Sigmund and Maute 2013) for a thorough review and comparison of the two methods for structural optimization applications.

When considering coupled multi-physics problems like electro-thermo-elastic or elasto-optical, the density and level set methods can be applied with only minor adaptation and usually without altering the basic parameterization scheme. However, a challenge arises when considering coupled problems where different physical fields couple at the structural boundary. Examples include fluid-structure and acoustic-structure interaction. In this paper, we focus exclusively on the acoustic-structure interaction problem, where the fluctuating acoustic pressure field acts as a boundary load on the structure and the structural vibrations act as acoustic sources. In standard solution procedures, it is thus imperative to know the location of this boundary. The level set methods operate with a well-defined boundary and in both Shu et al. (2014) and Desai et al. (2018), the authors adapted the re-meshing-based level set approach to the acoustic-structure interaction problem where the zero level set is now used to separate the structural and the acoustic domains. That is, one solves the standard structural vibration problem where the level set is positive and the acoustic Helmholtz equation is solved in regions where the level set function is negative. Instead of using re-meshing, the level set method has also been used in combination with the density parametrization, i.e., using an erstatz material model and phase field approach to drive the design evolution. In this approach, the level set field is mapped to an indicator function which in turn used to interpolate the material properties of the acoustic and elastic mediums, thus preventing the challenges of tracking the boundary changes throughout the optimization. Using this technique, Noguchi et al. (2015) employed the unified multiphase (UMP) technique based on Biot’s theory for poroelastic waves (Lee et al. 2012). In Noguchi et al. (2016), the authors derived a topological derivative for a vibro-acoustic system modeled by a two-phase material model. Using topological derivatives and the same modeling approach, Noguchi et al. (2017) and Miyata et al. (2018) carried out level set–based topology optimization. The UMP technique has also been used in context of density-based topology optimization of acoustic-mechanical-septa distribution by (Lee et al. 2015). The vibro-acoustic systems have also been studied with a combined Boundary Element (BEM) and FE formulation to take advantage of the high capabilities of the BEM for modeling the unbounded acoustic domains, while relying on FEM for the structural part. Isakari et al. (2017) studied the level set– based topology optimization of an elastic sound scatterer using such a BEM-FEM solver.

As argued, the density method does not naturally provide knowledge of the location of the acoustic-structural interface. However, the mixed FE formulation has been used to circumvent this problem and facilitate a monolithic density-based parametrization approach. This formulation was also used in Sigmund and Clausen (2007) to treat the static pressure-load problem. With this formulation, the pressure is introduced as an auxiliary variable in addition to the displacements which allows one to transfer pressure loads without explicit indication of the boundary location. This formulation was used in the seminal work on acoustic-structure topology optimization presented in Yoon et al. (2007) and has later been applied to design a porous microstructures for increased loss factor (Kook and Jensen 2017).

In addition to these main methods, we will briefly review acoustic-structure interaction problems solved by the bi-directional evolutionary topology optimization (BESO)
method as presented in Picelli et al. (2015), Vicente et al. (2015), and Chen et al. (2017). It should be noted also that a number of topology optimization problems have been studied for which the topological changes do not involve a change in the boundary between the structural and acoustic domains. For most problems, the in-plane material distribution involving two material constituents is optimized (Yamamoto et al. 2008; Du and Olhoff 2010; Yang and Du 2013), but also optimal distribution of thin damping layers has been considered (Zhang and Kang 2013) in addition to optimal plate thickness distribution (Akl et al. 2009), laminated composites (Niu et al. 2010), and piezoelectric structures (Yoon et al. 2018). Also, a few studies have appeared where the optimization problem has been defined so as to circumvent the need for modifying the structural boundaries and thus enables the use of standard parameterization schemes (see, e.g., Søndergaard and Pedersen 2014).

In the present paper, we will conduct a review of the methods that have appeared which allows for introducing topological changes in the distribution of acoustic and structural domains, i.e., the level set method, the density-based method using the mixed FE formulation, and the BESO method as a special variant of the density-based method. The computational framework for the density and level set methods will be outlined and results for a series of test problems will be critically examined. All results presented will be based on the authors’ implementation of the optimization algorithm. Based on this comparative review, recommendations for future research will be provided.

2 Topology optimization approaches

The general goal of an acoustic-structure topology optimization problem is to determine the optimal layout of the structural and acoustic domains, such that a given performance measure, that we may denote \( \Phi(u(x,t), p(x,t)) \), is minimized. This formulation indicates that the performance measure may depend both on both the structural vibration level (the vibration amplitude \( u \)) as well as the acoustic pressure amplitude \( p \).

Figure 1a shows an illustration of the initial configuration for a typical acoustic-structure optimization problem. Here, a mechanical structure has two internal acoustic cavities and is surrounded by an external acoustic medium. The structure is excited by a time-harmonic mechanical load \( f(t) \) and also a time-harmonic acoustic load \( q(t) \). The loads generate vibrations of the structure and also acoustic pressure fluctuation in the acoustic medium. The aim of the optimization problem is now to minimize the prescribed objective function

\[
\min \Phi(u(x,t), p(x,t))
\]  

which in the hypothetical scenario illustrated in Fig. 1 results in the optimized distribution of structural and acoustic domains shown in Fig. 1b. During the optimization process, the structural domain has been reshaped and one of the internal acoustic cavities has been removed. Acoustic-structure optimization problems will most often involve additional constraints on the allowable performance or its configuration. A typical constraint in topology optimization is to enforce a maximum allowable volume of the structure, which we can formulate as

\[
\int_{\Omega_s} d\Omega \leq V^*
\]

where \( \Omega_s \) is the domain occupied by the structure, \( \Omega \) is the total domain under consideration, and \( V^* \) is the allowable volume fraction.

In order to solve this optimization problem, the following key points should be addressed:

– **Design parametrization.** The methods reviewed apply parametrization based on the density or the level set approach.
– **Analysis method.** All strategies reviewed rely on finite element analysis of the underlying structural and acoustic problems. The formulations used depend on the choice of parametrization applying either a standard segregated analysis combined with a body-fitted and adaptive FE mesh (level set approach) or a mixed
The methods reviewed are gradient-based (the BESO method only to a certain extend) and apply sensitivity analysis based on the FE analysis.

- Design updates. The choice of design update method is also linked to the choice of parametrization scheme: The works using the level set approach use an update scheme based on a solution to the Hamilton-Jacobi transport equation. The density approach uses mathematical programming, e.g., MMA, while the BESO uses a heuristic update scheme.

In the following, the strategies outlined in the four key points will be described in details including implementation considerations.

### 2.1 Design parametrization

Existing approaches for topology optimization of acoustic-structure interaction problems can, as previously stated, be split into two main groups depending on the choice of design parametrization. Note, however, that although the design representations used for the density and level set approaches are conceptually very different, it can be argued that when it comes to a numerical implementation, the similarities actually outweigh the differences as reported for the case of structural optimization in Sigmund and Maute (2013).

#### 2.1.1 The density approach

The basic idea of density-based structural optimization is to describe the topology by a spatially varying design field, here $\gamma(x)$. In the discretized setting, this is achieved by assigning a design variable to each of the computational domain pixels (2D) or voxels (3D). For the case of acoustic-structure interaction, this means that a pixel with $\gamma = 1$ is interpreted as being structure, while $\gamma = 0$ corresponds to an acoustic medium. The only difference to classical structural topology optimization is that $\gamma = 0$ corresponds to void in that case. Also, it is worth noting that in the density method, the same mesh is often used for both analysis and design and the mesh is usually kept fixed throughout the optimization process. Furthermore, the mesh is often regular which means that elaborate mesh generation or re-meshing is avoided. In order to apply gradient-based optimization methods, the design variable field is represented as continuous, i.e.,

$$0 \leq \gamma_i \leq 1 \quad (3)$$

where $i$ indicates the pixel (element) number.

A schematic of the entire density-based optimization process is illustrated in Fig. 2. Figure 2a shows a possible initial structure modeled by setting the appropriate design variables to either 1 (black) or 0 (white). However, one of the greatest strengths of the density approach is that initial designs are often not needed. In fact, more often, a uniform distribution of the design variables is applied.
as illustrated in Fig. 2b. The choice of the initial design distribution is in general arbitrary, but could be chosen to match the volume constraint $\gamma = V^*$, if such a constraint is present. Naturally, a random distribution of the densities can be applied as well. As the optimization process progresses, the topology of the design evolves and often grey regions appear as shown in Fig. 2c. Through different filtering and projection methods, the intermediate design variables are slowly suppressed until the design converges to a completely black (1) or white (0) configuration. The optimized design is illustrated in Fig. 2d which also shows how the pixel-based representation leads to the so-called staircasing phenomena. This might pose problems in multiphysics settings, which is why it is sometimes beneficial to allow the interface to be smeared over a couple of pixels.

2.1.2 The level set approach

In level set–based topology optimization, the design representation is most often separated from the underlying analysis mesh. This is achieved by representing the topology by a scalar function $\phi$, and by defining the different material phases and interface based on the following rule:

$$
\begin{align*}
\phi(x) > 0, & \quad x \in \Omega_s \text{ (structural domain)} \\
\phi(x) = 0, & \quad x \in \partial \Omega \text{ (interface)} \\
\phi(x) < 0, & \quad x \in \Omega_a \text{ (acoustic domain)}
\end{align*}
$$

(4)

Figure 3a illustrates an example of a level set function and how it can be used to define structural and acoustic domains as well as their common interface. This definition is a straightforward extension of the approach usually used for structural topology optimization where $\phi < 0$ then corresponds to void.

The level set function is usually discretized on a regular grid, similar to that for the design variables in the density-based method. However, the level set values are most often assigned to nodal points instead of element centers.

Figure 4a shows a representative level set function discretized on a regular grid, whereas Fig. 4b shows the corresponding design configuration described by the the zero-level contour. During the optimization process, the level set function evolves into a new configuration. This is illustrated in Fig. 4c and d which shows the grid-based level set function and its geometric interpretation, respectively.

The mapping of the level set function to the mesh used for analysis can be done in several ways. The method most often used in structural optimization is to apply an ersatz material model and in this case the level set method and the density-based method are very similar with only minor differences. To the author’s knowledge, this approach has not yet been applied to acoustic-structure interaction problems. Instead, the approach used in the existing works is to perform a complete remeshing-based on the zero level contour, which ensures a crisp and well-defined interface. However, we should note that recent work on level set–based topology optimization applies novel immersed boundary methods such as cut finite elements or finite cell representations. These methods allow the analysis and level meshes to coincide, while still maintaining the crisp interface by using elaborate integration schemes (see, e.g., Hansbo and Hansbo (2004) and Düster et al. (2008) for more details).

Implicit representation of the interface using the values of the level set function $\phi(x)$ also allows for easy calculation of the geometric properties such as the unit normal vector and the mean curvature, not only on the design interface $\partial \Omega$, but everywhere in the domain $D$. The unit normal vector
Fig. 4 Illustration of the discretized level set function. 
(a) Grid values of the initial level set function. 
(b) Initial design described by the the zero-level iso-curve. 
(c) Grid values of the optimized level set function. 
(d) Final design described by the zero-level iso-curve.

\[ \mathbf{n}_s = \frac{\nabla \phi}{|\nabla \phi|} \]  
\[ \mathbf{n}_a \] pointing out from the acoustic domain is calculated as

\[ \kappa = \nabla \cdot \mathbf{n}_s = \nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right) \]  

2.2 Finite element analysis of acoustic-structural interaction (ASI)

Discretizing and meshing the analysis domain based on the zero-level contour of the scalar level set function makes it possible to employ standard segregated analysis. That is, the structural equation is solved only in the solid region and the acoustic wave equation is solved only in the acoustic region. Thus, this approach is analogous to standard simulation of acoustic-mechanical interaction problems as used in most commercial and open source numerical tool boxes. In the following section, we will describe how to perform the segregated analysis using standard finite elements.

2.2.1 Segregated analysis

The governing equations for the time-harmonic motion of a linear elastic body \( \Omega_s \) can be written as

\[ \nabla^T \sigma + \omega^2 \rho_s \mathbf{u} = 0 \quad \text{in} \quad \Omega_s \]  
\[ \sigma = C \epsilon \]  
\[ \epsilon = \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ 2 \epsilon_{12} \end{bmatrix}^T \]  
\[ \epsilon_{11} = \frac{\partial u_1}{\partial x}, \quad \epsilon_{22} = \frac{\partial u_2}{\partial y}, \quad \epsilon_{12} = \frac{1}{2} \left( \frac{\partial u_1}{\partial y} + \frac{\partial u_2}{\partial x} \right) \]  

where body forces have been neglected, \( \rho_s \) is the density of the solid, and \( \omega \) is the radial frequency. Moreover, \( \sigma \) is the Cauchy stress vector, \( C \) is the constitutive matrix, and the \( \epsilon \) is the strain vector. We consider the body to be subjected to standard boundary conditions as well as being adjacent to an acoustic medium in part of the boundary. The boundary conditions read

\[ \mathbf{u} = \mathbf{u}_0 \quad \text{in} \quad \Gamma_{sd} \]  
\[ \mathbf{n}_s^T \sigma = \mathbf{f} \quad \text{in} \quad \Gamma_{sn} \]  
\[ \mathbf{n}_a^T \sigma = \rho n_a \mathbf{u} \quad \text{in} \quad \Gamma_{as} \]  

where \( \mathbf{n}_s \) is the normal vector of the acoustic boundary pointing outward from the acoustic domain defined in (5) and \( \mathbf{n}_a \) is the normal vector of the structural boundary pointing to the acoustic domain. The vector \( \mathbf{f} \) is the traction load.
which is zero for the hard wall boundaries. The following weak form of the elasticity equation is the finite element discretization of the governing equations, and is the density, \( k \) is the wave number, \( i \) is the imaginary unit and \( \alpha \) is the prescribed Neumann boundary condition which is zero for the hard wall boundaries.

Similarly, the strong form of the Helmholtz equation describing the pressure fluctuations in the acoustic domain is written as

\[
\nabla^2 \overline{p} + \left( \frac{\omega}{c_a} \right)^2 \overline{p} = 0 \quad \text{in} \quad \Omega_a
\]

along with the following common boundary conditions:

\[
\begin{align*}
\overline{p} &= p_0 \quad \text{in} \quad \Gamma_{ad} \quad \text{(15)} \\
\mathbf{n} \cdot \nabla \overline{p} &= a_n \quad \text{in} \quad \Gamma_{ae} \quad \text{(16)} \\
\mathbf{n} \cdot \nabla \mathbf{u} &= -\omega^2 \rho_a \mathbf{n} \cdot \mathbf{u} \quad \text{in} \quad \Gamma_{as} \quad \text{(17)} \\
\mathbf{n} \cdot \mathbf{v} + i k \overline{p} &= 2ik p_{in} \quad \text{in} \quad \Gamma_{ar} \quad \text{(18)}
\end{align*}
\]

where \( c_a \) is the speed of sound in the acoustic medium, \( p_0 \) is the density, \( k = \frac{\omega}{c_a} \) is the wave number, \( i \) is the imaginary unit and \( a_n \) is the prescribed Neumann boundary condition which is zero for the hard wall boundaries.

Applying the standard Galerkin procedure to carry out the finite element discretization of the governing equations, the following weak form of the elasticity equation is obtained

\[
\int_{\Omega_s} \delta \varepsilon : \mathbf{C} \varepsilon \, d\Omega - \omega^2 \rho_s \int_{\Gamma_{as}} \delta \mathbf{u} \cdot \mathbf{n} \, d\Gamma = \int_{\Omega_s} \delta \mathbf{u} \cdot \mathbf{f} \, d\Omega
\]

Similarly, the weak form of the acoustic domain reads

\[
\begin{align*}
\int_{\Omega_a} (\nabla \varphi)^T \nabla \varphi \, d\Omega - \omega^2 \rho_a \int_{\Gamma_{as}} \delta \mathbf{u} \cdot \mathbf{n} \, d\Gamma &= \int_{\Omega_a} \delta \mathbf{u} \cdot \mathbf{f} \, d\Omega \\
-\omega^2 \rho_a \int_{\Gamma_{as}} \delta \mathbf{p} \cdot \mathbf{n} \, d\Gamma &= \int_{\Gamma_{as}} \delta \mathbf{p} \cdot \mathbf{n} \, d\Gamma
\end{align*}
\]

where the radiation boundary condition in (18) is excluded from the derivation for brevity. Here, \( \delta \varepsilon \) is the virtual strain, \( \delta \mathbf{u} \) and \( \delta \mathbf{p} \) are the test functions for displacements and the pressure field, respectively. In order to carry out the discretization, the continuous variables \( \mathbf{u} \) and \( \mathbf{p} \) are approximated using linear iso-parametric shape functions

\[
\begin{align*}
\mathbf{u} &= N_i \mathbf{u} \\
\mathbf{p} &= N_j \mathbf{p}
\end{align*}
\]

where \( \delta \) is the differential operator and \( \mathbf{B} \) is the linear strain-displacement matrix. The discretized matrix system of the weak form is then

\[
\begin{bmatrix}
\mathbf{K} - \omega^2 \mathbf{M} & -\mathbf{C} \\
-\rho_a \omega^2 \mathbf{C}^T & (\mathbf{K}_a - \omega^2 \mathbf{M}_a)
\end{bmatrix}
\begin{bmatrix}
\mathbf{u} \\
\mathbf{p}
\end{bmatrix} =
\begin{bmatrix}
\mathbf{f} \\
\mathbf{g}
\end{bmatrix}
\]

with the matrices and vectors being

\[
\begin{align*}
\mathbf{K}_s &= \int_{\Omega_s} \mathbf{B}_s^T \mathbf{C} \mathbf{B}_s \, d\Omega_s \\
\mathbf{M}_s &= \int_{\Omega_s} \rho_s \mathbf{N}_s^T \mathbf{N}_s \, d\Omega_s \\
\mathbf{T} &= \int_{\Gamma_{as}} \mathbf{N}_s^T \mathbf{f} \, d\Gamma_{as} \\
\mathbf{K}_a &= \int_{\Omega_a} \mathbf{B}_a^T \mathbf{C} \mathbf{B}_a \, d\Omega_a \\
\mathbf{M}_a &= \int_{\Omega_a} \frac{1}{2} \mathbf{N}_a^T \mathbf{N}_a \, d\Omega_a \\
\mathbf{g} &= \int_{\Gamma_{as}} \mathbf{N}_a^T \mathbf{n} \, d\Gamma_{as}
\end{align*}
\]

for the acoustic domain where the matrix \( \mathbf{B}_p = \partial \mathbf{N}_p \). The coupling matrix is found as:

\[
\mathbf{C} = \int_{\Gamma_{as}} \mathbf{N}_a^T \mathbf{n} \mathbf{n}^T \, d\Gamma_{as}
\]

As previously mentioned, the mesh is usually adapted to the acoustic-structural boundary in each step of the optimization algorithm. Figure 6 shows an example of a such finite element grid where the the boundary curve is obtained utilizing the marching square algorithm and the curve is fitted to the mesh using simple triangulation.

### 2.2.2 Mixed formulation

In the case of a density-based parametrization, it is no longer possible to clearly define the acoustic and structural parts of the domain due to the possible appearance of "grey" pixels in the design. Therefore, a single monolithic formulation governing both physics and their coupling is needed. The mixed formulation has been proposed to do exactly this, that is, to model the acoustic-mechanical interaction problems without having an explicit boundary representation. The mixed finite element formulation, also called the \( \mathbf{u}/p \) (displacement/pressure) formulation, can be found in many references (see, e.g., Zienkiewicz and Taylor (2000)). In Wang and Bathe (1997), the formulation...
was proposed to model acoustic-mechanical interaction problems. In Sigmund and Clausen (2007), the static mixed FE-formulation was used to solve pressure load problems in density-based topology optimization and in Yoon et al. (2007), the formulation was used for the first time for topology optimization of acoustic-structure interaction problems.

In the following, we present and motivate the use of the mixed formulation for density-based topology optimization. The mixed formulation is derived by first defining a pressure variable using the bulk modulus as follows:

$$p = -\frac{K}{m} \mathbf{T} \epsilon$$  \hspace{1cm} (29)

which is valid for small strains. Here, \(K\) is the bulk modulus and \(m = \{1, 1, 0\}^T\) is the vector formulation for the Kronecker’s delta considering two-dimensional analysis. The stress-strain relationship can then be stated as

$$\sigma = 2Ge - m\mathbf{p}$$  \hspace{1cm} (30)

where \(G\) is the shear modulus and the deviatoric strain vector \(\epsilon\) reads

$$\epsilon = (I_0 - \frac{1}{2}m) \mathbf{e}$$  \hspace{1cm} (2D)

with \(I_0\) defined as a diagonal matrix \(I_0 = \text{diag}(1, 1, 0.5)\). Moreover, the bulk and shear moduli are defined from the Young’s modulus \(E\) and the Poisson’s ratio \(\nu\) as

$$K = \frac{E}{2(1-\nu)}, \quad G = \frac{E}{2(1+\nu)}$$  \hspace{1cm} (32)

in the case of 2D plane stress conditions. The coupled equations derived from the mixed formulation can now be written as

$$\nabla^T (2Ge - m\mathbf{p}) + \omega^2 \rho \mathbf{p} = 0$$  \hspace{1cm} (33)

$$\frac{\mathbf{p}}{K} + m^T \epsilon = 0$$  \hspace{1cm} (34)

which can be viewed as an alternative formulation of the original structural equations (with the advantage that it can be applied to perfectly incompressible materials as well).

However, it can also be shown that the Helmholtz equation governing the acoustic pressure can be recovered from this equation by substituting \(\mathbf{u}\) into (33) into (34) and setting the shear modulus to zero \((G = 0)\). Thus, using the mixed formulation, structural \(\Omega_s\) and acoustic \(\Omega_a\) parts of the domain \(\Omega\) can be realized by defining the bulk modulus \(K\), shear modulus \(G\) and density \(\rho\) as

\[
\begin{aligned}
K &= K_s, & G &= G_s, & \rho &= \rho_s & \text{on } \Omega_s \\
K &= K_a, & G &= 0, & \rho &= \rho_a & \text{on } \Omega_a
\end{aligned}
\]  \hspace{1cm} (35)

In regions with intermediate values of \(\gamma\), thus not belonging to neither \(\Omega_s\) nor \(\Omega_a\), it is proposed to interpolate the values of \(K\), \(G\), and \(\rho\) between the structural and acoustic values in (35). Such an interpolation is found in Yoon et al. (2007):

\[
\begin{aligned}
K(\gamma) &= K_s \gamma + (1 - \gamma) K_a \\
G(\gamma) &= G_s \gamma + (1 - \gamma) G_a \\
\rho(\gamma) &= \rho_s \gamma + \rho_a (1 - \gamma)
\end{aligned}
\]  \hspace{1cm} (36-38)

in which the interpolation of \(K\) and \(G\) is based on a two material RAMP interpolation scheme (Stolpe and Svanberg 2001) used to avoid the artificial vibration modes in low-density areas reported for the more standard SIMP interpolation function (Pedersen 2000). Here, the parameter \(n\) is a positive number that controls the curvature of the interpolation function. As seen from the (38), the mass density \(\rho\) is interpolated linearly between the acoustic and the structural domains.

Acoustic boundary conditions for the mixed formulation are derived using that

$$\nabla^T \mathbf{p} = \omega^2 \rho_s \mathbf{u}$$  \hspace{1cm} (39)

Figure 7 illustrates the most commonly used boundary conditions for the mixed formulation in the acoustic domain. Boundary conditions...
In order to realize a stable finite element solution to the mixed \( u/p \) formulation, displacement variables should use higher order interpolations than the auxiliary pressure variable (Zienkiewicz and Taylor 2000; Wang and Bathe 1997). To this end, displacement variables are discretized with second order Lagrangian shape functions whereas the pressure field is represented using first order Lagrangian shape function. For triangular and quadrilateral elements, this corresponds to using \( T6/3 \) and \( Q8/4 \) elements, respectively.

### 2.3 Sensitivity analysis

A gradient-based optimization approach requires computation of the sensitivities of the objective function and constraints with respect to the design variables. In the following, we will outline the basic procedure followed when using the density and the level set approaches.

#### 2.3.1 Density-based parametrization

In order to carry out the adjoint analysis, firstly the Lagrangian is formed

\[
\mathcal{L} = \Phi(y, v|y) + \lambda^T r(y, v|y)
\]

where \( r = Sv - h = 0 \) defines the residual vector, \( v = (u, p)^T \) is the vector of state variables, \( h = \{f, g\}^T \) is the source vector, \( S \) is the system matrix found from (43), and \( \lambda \) is a vector of Lagrange multipliers. For zero residual, the Lagrangian coincides with the objective function. The derivative with respect to the design variable can be written following the chain rule as

\[
\frac{d\mathcal{L}}{y'} = \frac{\partial \mathcal{L}}{\partial y'} + \lambda^T r_y = \frac{\partial \mathcal{L}}{\partial y'} + \lambda^T \left( \frac{\partial r}{\partial y} + \frac{\partial r}{\partial y} \right) = \frac{\partial \Phi}{\partial y'} + \lambda^T \frac{\partial r}{\partial y} + \frac{\partial \Phi}{\partial y} \frac{\partial y}{\partial y}
\]

Since the Lagrange multiplier can be freely chosen, it is selected such that the underlined part of the equation becomes zero to avoid the computationally expensive evaluation of the term \( \frac{\partial r}{\partial y} \). The adjoint equation then becomes

\[
S^T \lambda = -\left( \frac{\partial \Phi}{\partial y} \right)^T
\]

Here, it is noted that, the state variables can be complex variables if, e.g., the radiation condition given in Fig. 7 is utilized. In this case, the term \( \frac{\partial r}{\partial y} \) on the right hand side of the adjoint equation in (50) is realized as Dühring et al. (2008)

\[
\frac{\partial \Phi}{\partial y} = -\frac{\partial \Phi}{\partial y} - i\frac{\partial \Phi}{\partial y}
\]
where the subscripts $r$ and $i$ denote the real and the imaginary parts of a complex number. Having calculated the Lagrange multipliers that satisfy (50), the sensitivity of the objective function is then calculated as

$$\frac{d\Phi}{d\gamma} = \frac{d\Phi}{d\gamma} + \Re \left( \lambda^T \frac{dS}{d\gamma} \right) \text{ (52)}$$

where $\Re(\cdot)$ denotes the real part of a complex quantity. The $\Re(\cdot)$ operator is used to compress the sensitivity equation into a simplified form and details of this derivation can be extracted from the results in Jensen (2007).

It should be emphasized that the adjoint approach presented here is especially efficient for a very high number of design variables and a low number of constraint functions. The main cost is associated with solving the adjoint equation (50)—a step that is particularly cheap if the original FE equation is solved using a direct solver since the stiffness matrix is then already factorized.

### 2.3.2 Level set parametrization

Level set sensitivity analysis differs significantly from the density-based analysis presented in Section 2.3.1 where the differentiation was carried out with respect to an element design variable $\gamma$. Instead, the derivatives are here handled by treating the domain $\Omega$ as a continuous medium and examining what happens when the boundary $\partial\Omega$ is perturbed; i.e., the sensitivities take the form of shape derivatives. However, there are also similarities, since the adjoint method is employed for efficient computation. An in-depth introduction to shape derivatives can be found in Choi and Kim (2005). Here, it is noted that we have left out the overbar notation for the continuous variables to keep the notation clean for the reminder of this work.

We will assume, without loss of generality, that the objective function to be minimized can be written on the following form:

$$J = \int_{\Omega_{\text{obj}}} \Phi(u, p) \, d\Omega \text{ (53)}$$

The shape derivative of the objective function $J$ is now computed as

$$\delta J = \int_{\Omega_{\text{obj}}} \frac{\partial \Phi}{\partial \gamma} \, d\Omega + \int_{\partial \Omega_{\text{obj}}} \frac{\partial \Phi}{\partial u} u \, d\Gamma + \int_{\partial \Omega_{\text{obj}}} \Phi \, d\Gamma \text{ (54)}$$

where the prime superscript specifies a derivative with respect to a pseudo-time, $\partial \Omega$ is the boundary variation and $\Gamma$ represents a normal (or design) velocity of the boundary. For simplicity, we will assume that $\Omega_{\text{obj}}$ is a fixed domain and separate from the design domain. Hence, the third term in (54) vanishes because $\Gamma = 0$ for $\partial \Omega_{\text{obj}}$ since there is no overlap between the design and objective domains.

In a similar way as for the density-based sensitivity analysis, we will construct an adjoint problem in order to avoid explicit computation of the terms $p'$ and $u'$. For this purpose, a weak form of the governing equations is constructed, where the test functions are replaced by Lagrange’s multipliers $\lambda_p$ and $\lambda_u$, corresponding to the pressure and displacement fields, respectively. Furthermore, the two weak forms are added into one single equation:

$$\int_{\Omega_{\text{a}}} \lambda_p^T \epsilon(u) \, d\Omega - \alpha^2 \rho_a \int_{\Gamma_{\text{a}}} \lambda_p^T u \, d\Gamma + \int_{\Omega_{\text{a}}} (\nabla \lambda_p)^T \nabla p \, d\Omega - \alpha^2 \rho_a \int_{\Gamma_{\text{a}}} \lambda_p p \, d\Gamma - \int_{\Gamma_{\text{a}}} \lambda_u^T n_a p \, d\Gamma - \alpha^2 \rho_a \int_{\Gamma_{\text{a}}} \lambda_p n_a u \, d\Gamma = 0 \text{ (55)}$$

where $\lambda_p$ has also been introduced as an adjoint strain field which is calculated as $\lambda_p = \mathbf{B} \lambda_s$. In (55), the radiation boundary $\Gamma_{\text{r}}$ is not included and the Neumann boundaries for both acoustic and structural domains ($\Gamma_{\text{as}}$ and $\Gamma_{\text{sn}}$) are considered to be zero for clarity.

For use in the subsequent derivation, we now take the shape derivative of (55). Terms containing the pseudo-time derivative of the adjoint fields recover the state equation of the coupled system and sum to zero. This leaves us with the following expression

$$\int_{\Omega_{\text{a}}} \lambda_p^T \epsilon(u) \, d\Omega - \alpha^2 \rho_a \int_{\Gamma_{\text{a}}} \lambda_p^T u \, d\Gamma + \int_{\Omega_{\text{a}}} (\nabla \lambda_p)^T \nabla p \, d\Omega - \alpha^2 \rho_a \int_{\Gamma_{\text{a}}} \lambda_p p \, d\Gamma - \int_{\Gamma_{\text{a}}} \lambda_u^T n_a p \, d\Gamma + \int_{\Gamma_{\text{a}}} \mathbf{G}_a V_a \, d\Gamma + \int_{\Gamma_{\text{a}}} \mathbf{G}_e V_a \, d\Gamma + \int_{\Gamma_{\text{a}}} \mathbf{G}_{\text{as}} V_a \, d\Gamma = 0 \text{ (56)}$$

where the $\mathbf{G}$ functions collect the boundary terms in (56) that are the coefficients of the normal velocity $V_n$: $\mathbf{G}_a = \lambda_p^T \mathbf{B} \epsilon(u)$, $\mathbf{G}_e = (\nabla \lambda_p)^T \nabla p - \alpha^2 \rho_a \lambda_p p$, and $\mathbf{G}_{\text{as}} = -\nabla \left( \lambda_u^T n_a p \right)^T n_a - \kappa \left( \lambda_u^T n_a p \right)$

$$- \alpha^2 \rho_a \left( \nabla \left( \lambda_p n_a u \right)^T n_a - \kappa \left( \lambda_p n_a u \right) \right) \text{ (57)}$$

and $\kappa$ is the mean curvature defined in (6).

In order to construct the adjoint equation, the differentiated weak form in (56) is added to (54) and the terms containing $p'$ and $u'$ are collected together. The adjoint
variables are now chosen so that the following adjoint equation is fulfilled

\[
\int_{\Omega} \lambda^T \nabla \psi \, d\Omega + \frac{\alpha^2}{c_s^2} \int_{\Omega} \lambda^T u \, d\Omega \\
+ \int_{\Gamma_a} (\nabla \lambda \rho)^T \nabla p' \, d\Gamma - \frac{\alpha^2}{c_s^2} \int_{\Gamma_a} \lambda \rho \, d\Gamma \\
- \int_{\Gamma_a} \frac{\partial \Phi}{\partial p} \rho' \, d\Gamma = 0
\]

Using the discretization approach outlined in (42), the discrete form of the (58) takes the form

\[
\begin{bmatrix}
(K_s - \alpha^2 M_s) & -C_s \\
-p_s \alpha^2 C_f & (K_a - \alpha^2 M_a)
\end{bmatrix}
\begin{bmatrix}
\lambda_s \\
\lambda_a
\end{bmatrix}
= \begin{bmatrix}
\frac{\partial \Phi}{\partial \psi_i} \\
\frac{\partial \Phi}{\partial \psi_i}
\end{bmatrix}
\]

Considering optimization problems where the parts of the acoustic boundary \( \partial \Omega_a \) and structural boundary \( \partial \Omega_s \) subjected to design changes are equal to the boundary of the coupled surface \( \Gamma_{as} \) and having a set of Lagrange multipliers that satisfies the adjoint equation (58), the expression for the shape derivative of the objective function \( J \) becomes

\[
\dot{J} = \int_{\Gamma_{as}} \mathcal{G}_{\Gamma_{as}} V_a \, d\Gamma
\]

where

\[
\mathcal{G}_{\Gamma_{as}} = \lambda^T \nabla \psi_i + \frac{\alpha^2}{c_s^2} \lambda_a + \left( \nabla \lambda_a \rho_a \right)^T \frac{\partial \Phi}{\partial \psi_i}
\]

We note that, if the radiation boundary condition is included in the acoustic domain, i.e., (18), the derivation remains the same. However, the state and adjoint variables become complex variables, in which case the shape derivative of the objective function should be replaced by

\[
\dot{J} = \int_{\Gamma_{as}} \Re \left( \mathcal{G}_{\Gamma_{as}} \right) V_a \, d\Gamma
\]

In order to convert the optimization problem with an inequality volume constraint to an unconstrained optimization problem (Nocedal and Wright 2006), the following augmented Lagrange function is proposed:

\[
\mathcal{L} = J + \lambda \left[ \int_{\Omega} d\Omega - V_0 \right] + \frac{1}{2\lambda} \left[ \int_{\Omega} d\Omega - V_0 \right]^2
\]

where \( \lambda \) is the Lagrangian multiplier and \( \Lambda \) is a penalization parameter. The updating scheme is

\[
\lambda^{l+1} = \lambda^l + \frac{1}{\lambda^l} \left[ \int_{\Omega} d\Omega - V_0 \right], \\
\Lambda^{l+1} = \eta \Lambda^l
\]

where \( l \) is the number of the current iteration of the algorithm and \( \eta \) is a small positive number (\( \eta > 1 \)) which slowly increases the value of the penalization parameter \( \Lambda \). Thus, the shape derivative of the augmented Lagrange function reads

\[
\dot{\mathcal{L}} = \int_{\Gamma_{as}} \Re \left( \mathcal{G}_{\Gamma_{as}} \right) + \lambda^l \left[ \int_{\Omega} d\Omega - V_0 \right] \right] V_a \, d\Gamma
\]

Using the steepest decent method in which the decent direction satisfies \( \dot{\mathcal{L}} < 0 \), the design velocity \( V_a \) is chosen as

\[
V_a = -\mathcal{G}_{\text{tot}}
\]

which will be used in the update scheme presented later.

### 2.4 Design update methods

Before proceeding, we note that all reviewed methods are based on an optimization cycle that consists of FE analysis, sensitivity analysis, and design updates repeated in an iterative fashion until a convergence criteria is met. The procedures applied for the design updates for the density methods and the level set method will be outlined in the following.

#### 2.4.1 Non-linear mathematical programming

The topology optimization problem can be posed by first defining a real valued cost function \( \Phi \). The minimization of this function with respect to the design variables \( \gamma \) is sought while satisfying the given constraints \( \psi_i \). Mathematically, the problem is stated as

\[
\min_{\gamma} \Phi(\gamma, \psi(\gamma)) \\
\text{s.t.} \: \psi(\gamma) = 0 \quad (67)
\]

\[
\psi_i \leq 0 \quad (68)
\]

The solution to the above stated optimization problem ((67) to (70)) is solved using nonlinear programming tools. A popular choice among the topology optimization community is the method of moving asymptotes (MMA) algorithm (Svanberg 1987, 2001). The algorithm requires the derivatives of both the cost function \( \Phi \) and the constraints \( \psi_i \) with respect to the design variable \( \gamma \). The problem is solved in a nested manner, such that the state-problem is left out of the optimization problem. It should be noted that topology optimization problems are often
characterized by a large number of design variables and few constraints.

To introduce mesh independence and to avoid checkerboard problems, regulation techniques should be applied on the design parametrization. For this purpose, either the convolution type density filtering (Bruns and Tortorelli 2001) or the density filtering based on the solution of a Helmholtz type equation (Lazarov and Sigmund 2011) is applied on the design variable field. Also to achieve crisp designs, projection schemes on the filtered design variable can be applied (Guest et al. 2004; Wang et al. 2011). Additionally, a continuation scheme is applied on the penalization parameter \( \eta \) in the interpolation scheme in (36)–(36) which reduces the risk for the optimization algorithm to get stuck in a local minimum.

The overall algorithm for density-based topology optimization of acoustic-structure interaction problems can be stated as follows.

1. Initialize the design variable field. This can be either uniform, random or a specified design.
2. Apply filtering operation to obtain the physical design.
3. Solve the mixed state equation, (43).
4. Solve the adjoint equation, (50).
5. Calculate the sensitivity, (52), and apply chain rule to take filtering operation into account.
6. Update the design using MMA.
7. Stop iterations when the change in design variables is below a user defined tolerance or continue from the step 2.

2.4.2 BESO

As an alternative to using mathematical programming for the design updates in density-based topology optimization, the BESO formulation is also included in this work. The overall optimization algorithm is identical to the one presented in the previous section except for step 6 which is replaced by:

1. [6.] Heuristic design updates based on the sensitivities evaluated at the discrete design (without any intermediate densities and following a “soft-kill” approach where only structural and acoustic elements are allowed).

   This means that at all stages throughout the optimization procedure the design will be fully discrete, meaning that the removed structural elements are replaced with acoustic elements and vice versa. The corresponding material properties of both media are still calculated through the interpolation functions given in the (35) to (38). Various heuristic update schemes have been introduced for the BESO approach (see, e.g., Huang and Xie (2007), (2009), (2010); Huang et al. (2010)). Here, we use the BESO update scheme presented in Huang and Xie (2009) and Huang et al. (2010).

   The BESO formulation has previously been presented in Vicente et al. (2015) for acoustic-mechanical interaction problems. However, it should be noted that our BESO implementation is based on the mixed finite element formulation (Section 2.2.2), hence the sensitivities are calculated in the same fashion as presented in Section 2.3.1. This means that our BESO approach differs from the one in Vicente et al. (2015) where a segregated finite element model is used to solve the acoustic-mechanical interaction problem and only the structural part of the domain is included in the sensitivity analysis.

2.4.3 Boundary shape evolution

When using the level set approach, the normal “design” velocity \( V_\phi \), computed such that \( \bar{J} < 0 \), is used to update the design. A Hamilton-Jacobi type of equation (Osher and Fedkiw 2003) is obtained by defining a “time derivative” of the level set function \( \phi (x) \):

\[
\frac{\partial \phi}{\partial t} - V_n |\nabla \phi| = 0 \quad \text{in } \Omega, \quad \phi(x,0) = \phi_0(x) \quad (71)
\]

As seen from the Hamilton-Jacobi equation, the design \( \partial \Omega \) is updated by moving the zero level set \( \phi = 0 \) with the normal velocity \( V_n \) of the moving boundaries.

Solution of the Hamilton-Jacobi, i.e., (71), is most commonly realized by employing the finite difference method. A number of different explicit upwind finite difference schemes can be found in the literature (Sethian 1999; Osher and Fedkiw 2003), which provide a robust and stable solution to (71). In a finite element framework, Xing et al. (2010) realized the solution of the Hamilton-Jacobi equation by adding stabilizing diffusion in the streamline direction, whereas (Liu et al. 2003) solved a reaction-diffusion equation obtained by adding an artificial diffusion term.

In our implementation, we make use of the finite volume method and hence solve the following form of the Hamilton-Jacobi equation

\[
\frac{\partial \phi}{\partial t} - v_n \cdot \nabla \phi = 0 \quad (72)
\]

where \( v_n = V_\phi \left( \frac{\nabla \phi}{|\nabla \phi|} \right) \) and the discretization is done on the equivalent divergent form of (72), which reads

\[
\frac{\partial \phi}{\partial t} - [\nabla \cdot (v_n \phi) - \phi \nabla \cdot v_n] = 0 \quad (73)
\]

First-order upwind scheme is utilized for the discretization of the convective term and the temporal term is discretized by the finite difference method using the first order
forward Euler scheme. Stable time evaluation is realized by satisfying the CFL stability condition

$$\Delta t \leq \frac{h}{\max |V_n|}$$

where $h$ is the grid size in the level set mesh.

Furthermore, after a few design iterations, too steep or flat regions can occur in the level set function which can lead to inaccurate representation of the boundaries. In order to regularize the optimization, the level set function is thus periodically re-initialized into a signed distance function by solving the re-initialization equation (Osher and Fedkiw 2003). We remark that many alternative regularization methods exist. For example, Yamada et al. (2010) proposed a level set method from the concept of the phase field model which provides a perimeter constraint method to regularize the optimization problem and does not require solving the reinitialization equation throughout the optimization. The following equation is used for reinitialization of the level set function $\phi$

$$\frac{\partial \phi}{\partial t} + s \cdot \nabla \phi = S(\phi)$$

where $s = S(\phi) \left( \frac{\nabla \phi}{|\nabla \phi|} \right)$ and the sign function $S(\phi)$ is approximated as Peng et al. (1999)

$$S(\phi) = \frac{\phi}{\sqrt{\phi^2 + |\nabla \phi|^2}}$$

(76)

Here, it is noted that $S(\phi)$ is updated at every time-step. For the finite volume discretization of the reinitialization equation, the second term on the left hand side of (76) is also written in its equivalent divergent form as

$$\frac{\partial \phi}{\partial t} + [V \cdot (s \phi) - \phi \nabla \cdot s] = S(\phi)$$

(77)

For the examples considered in this work, the reinitialization equation is discretized with a first-order upwind scheme for the convective term and a first order forward Euler scheme for the temporal term. Selection of the utilized time step $\Delta t$ is again based on the CFL stability condition given in the (74) where $V_n$ is replaced by $|s|.$

The overall algorithm for the level set–based topology optimization of acoustic-structure interaction problems is then

1. Initialize the level set function to represent the initial design and update the mesh in the structural and acoustic domains either by marching-squares algorithm or by total re-meshing the both domains.
2. Solve the state equation (21).
3. Solve the adjoint equation (58).
4. Update the Lagrange multiplier according to 64.
5. Calculate the design velocity $V_n$ (66) and extrapolate it to the level set mesh.
6. Solve the Hamilton-Jacobi equation (73) to evolve the shape. (See Section 2.4.3)
7. Re-initialize the level set function (77). (See Section 2.4.3)
8. Update the mesh from the new level set function.
9. Stop iterations when the change in the objective function is below a user defined tolerance or continue from the step 2.

### 3 Comparison of methods

In the following sections, we use our implementations of the density-based and level set topology optimization methods to solve two representative topology optimization problems in vibro-acoustics. Both problems concern the minimization of the sound pressure in a prescribed objective domain, i.e.,

$$J(p) = \int_{\Omega_{obj}} |p| \, d\Omega$$

subject to a volume constraint.
Table 1 Material properties considered for the structure

<table>
<thead>
<tr>
<th>E [Pa]</th>
<th>ν</th>
<th>ρs [kg/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000.0</td>
<td>0.3</td>
<td>1.0</td>
</tr>
</tbody>
</table>

3.1 Example 1

The first example is adopted from Yoon et al. (2007) and a schematic illustration of the design problem, including boundary conditions, is given in Fig. 8. The design problem concerns the design of a flexible partition which minimizes the downstream sound pressure in a duct. The model is excited by an incoming plane wave with amplitude $p_{in} = 1$ kPa to the left and the right most boundary is modelled as open using an absorbing boundary condition. The optimization is carried out for a single frequency of $f = 1.0/\pi$ Hz. The allowed volume fraction is set to 55% of the design domain. The material properties of the considered structure and the acoustic fields are listed in the Tables 1 and 2. To allow for a fair comparison, the same background mesh is used for both density-based and level set topology optimization methods, i.e., an uniform mesh with an element size of $2 \times 10^{-2}$ m.

The problem is first solved using the density-based formulation. To regularize the problem, a Helmholtz-type density filtering (Lazarov and Sigmund 2011) with a filtering radius of $r = 0.015$ m is used. Regularized Heaviside projection (Wang et al. 2011) with a threshold $\eta = 0$ is employed where the sharpness parameter is taken as $\beta = 3$ at the start of the optimization. To avoid getting stuck in a low-quality local minima, we apply a continuation strategy on the convexity parameter $n$ in the RAMP interpolation functions (36) to (38) and the sharpness parameter $\beta$. The process is started with $n = 3$ and at every 50th design cycle the value is increased by one until it reaches $n = 6$. After this $n$ takes the values of 7 and then 14 in the subsequent 50 design iterations. The initial material distribution is a uniform design with $\gamma = 0.5$.

The optimized design obtained using the density method with the mixed formulation is shown in Fig. 9. There result is the well-known structure from the literature and it closely resembles the structure reported by Yoon et al. (2007). We note that the problem closely corresponds to the maximization of the clamped beam’s first natural frequency.

The example problem is then solved using the level set formulation. In order to avoid too large or too small gradients of the level set function, we re-initialize it as a signed distance function at every 6th iteration. Also, since the level set method is known to be highly dependent on the initial topology (Villanueva and Maute 2014), we use two different initial configurations. First, the design domain is initialized with a straight beam with holes distributed periodically (Fig. 10a). Secondly, the design obtained from the density-based optimization is considered as a “smart” initial guess for the level set optimization. This is included to investigate if the level set optimization keeps and/or improves the structure obtained using the density method.

The optimized designs are given in Fig. 10 where the displacement magnitude of the structures is included for qualitative comparison. The corresponding level set surface for the optimized design in Fig. 10c is shown in Fig. 11. We note that the design obtained using the density-based result as initial guess performs significantly better than the design obtained with an initial configuration based on a beam with holes. Qualitatively, the design obtained using the density-based method is unaltered when used as input for the level set method. However, interestingly, it is found that the objective of the level set design in Fig. 10c constitutes a 28.6% reduction in objective value compared to the density based result evaluated using the mixed formulation, c.f. Fig. 9. To investigate this discrepancy further, we perform a body-fitted mesh analyses of all three designs using the segregated formulation. The density-based design is thresholded at $\gamma = 0.5$ using the marching square algorithm and the resulting frequency responses are collected in Fig. 12. From the plot, it is clear that the performance of the density-based design is practically identical to the best result obtained using the level set method. Hence, the discrepancy...
in objective value is due to the mixed formulation requiring a finer mesh than the segregated analysis (Zienkiewicz and Taylor 2000).

Figure 13 shows the sound pressure level (SPL) of the acoustic domain. The plots confirm by visual inspection that the designs obtained by both initial guesses indeed lower the sound pressure level in the objective domain when compared to initial beam structure with holes. It is also clear that the lowest pressure level is obtained for the optimized design using the density-based result as an initial guess.
It is important to mention that the objective evolution of any initial guess for the level set method is relatively smooth (c.f. Fig. 14). This means that the design update scheme for the level set function is likely to result in a local mimima, which is similar to solving the density-based problem without a continuation scheme, i.e., using a constant high value for the penalization parameter. However, there is no obvious way to introduce the same convexification in the level set method using the Hamilton-Jacobi equation, and hence, great care must be exerted when designing the initial guess for the level set method.

3.2 Example 2

In Example 2, the design of a dome structure is considered. The problem is adopted from Shu et al. (2014) and Vicente et al. (2015) and a schematic illustration of the model problem can be seen in the Fig. 15 along with the dimensions of the computational domain. The boundary condition for the bottom of the computational domain is clamped for the structure and zero Dirichlet for the acoustic domain. All other boundary conditions for the acoustic problem are hard wall conditions. The system is excited with a point pressure load in the acoustic domain inside the dome and the objective is to minimize the absolute pressure over the prescribed objective domain near the top boundary. The design domain is fixed to the dome area shown at the Fig. 15 and 80% of the design domain is allowed to be filled with material. This example is solved for three frequencies, i.e., 4 Hz, 5.3 Hz, and 6 Hz, and the sum of the absolute pressures constitutes the objective function.

The material properties of the structure and the acoustic field are listed in the Tables 3 and 4. We construct a uniform mesh with an element size of $1.5 \times 10^{-2}$ m for the computational domain and carry out the optimization using...
Fig. 15 Schematic illustration of example 2 showing the boundary conditions of the optimization problem. Gray color shows the design domain, blue color illustrates the region where the objective function is evaluated. The coordinates of the lower left and upper right corners of the objective domain are (0.06, 1.44) and (2.94, 1.485), respectively.

The same mesh resolution for both the density-based and the level set–based methods.

The density-based topology optimization approach utilizes a similar continuation strategy for the convexity parameter $n$ and the sharpness parameter $\beta$ as used in Example 1 (c.f. Section 3.1). In this case, the parameter $n$ is increased at every 100th design cycle and after the final value of $n = 6$, the parameter $\beta$ takes the values of 7, 14, and 28 for the subsequent 50 design iterations. The filtering radius and the initial material distribution are taken to be the same as in the previous example.

Figure 16 shows the optimized design obtained using the density-based method. The structure contains one partial hole at the top and the profile of the dome gets thinner towards the sides of the dome. The structure is as thick as the diameter of the prescribed design domain around the top partial hole.

The problem is then solved using the level set formulation. Similar to the first example, the level set function is re-initialized as a signed distance function every 8th iteration. In Fig. 17, the level set surface of the optimized design is shown. The optimized design contains no holes and looks very similar to the structure reported in Shu et al. (2014). Although in Shu et al. (2014), the dome structure is optimized for a distributed load applied at the outer edge of the dome compared to the initial dome structure with equally spaced holes. Considering the objective values of the end designs listed in Fig. 18, we note that the optimized design using the density method performs approximately 40% percent better than the structure optimized with the level set method.

Finally, the frequency responses of the dome structures are shown in Fig. 20. We note that the plot consists of the three designs, i.e., the initial beam with holes and two optimization results as well as an extra design consisting of the design domain fully filled with material. Firstly, it is clear that both optimized designs outperforms the initial design and the fully filled dome. Secondly, it is noted that the optimization results in a minimization of the first resonance frequency and maximization of the second. Third and lastly, it is observed that the density-based method has a better performance for two target frequencies, i.e., $f = 4$ Hz and $f = 6$ Hz. However, from visual inspection of the

| Table 3 Material properties considered for the structure |
|--------------------------------------|------------------|
| $E$ (Pa)                             | $\nu$            | $\rho_s$ (kg/m$^3$) |
| $100 \times 10^3$                    | 0.3              | 100                  |

| Table 4 Material properties considered for the acoustic domain |
|---------------------------------------------------------------|------------------|
| $c_a$ (m/s)                                                   | $\rho_a$ (kg/m$^3$) |
| 343                                                           | 1.21             |
frequency response, it is clear that the level set method has the lowest response around the target frequency $f = 5.3 \ Hz$. This advocates the use of a finer frequency range discretization though this is deemed outside the scope of the current review paper.

3.2.1 BESO

The comparative study is concluded with a single design obtained using the BESO formulation. The optimized design is shown in Fig. 21 along with the sound pressure level contour for a frequency of 4Hz. The resulting topology is found to be in good agreement with the result presented in Vicente et al. (2015).

The performance of the BESO design shows a similar reduction of the acoustic pressure outside the optimized dome compared to the level set and density method results given in Fig. 19. The frequency response of the BESO optimized dome is shown in the Fig. 22 which also includes the response for the density-based design, both evaluated using a body fitted mesh and a segregated analysis. The difference in response in the vicinity of the three optimization frequencies are clearly observed, showing that the density-based design has superior performance for the target frequencies of 4 Hz and 6 Hz, whereas the BESO design exhibits better performance around the second target frequency 5.3 Hz similar to the level set design. It is noted that for all methods, the reduction in the sound pressure level in the specified frequency range is obtained by reducing the first resonance frequency and increasing the second resonance frequency of the coupled system. Here, it is noted that, even though the BESO approach provides a crisp design without any gray scale, the calculated objective value of the final design shows a significant discrepancy in the objective value compared to a body fitted analysis of the design, c.f. Fig. 21. This further underlines the previously mentioned inherent limitations of the standard $u-p$ mixed formulation wrt. modelling accuracy.

4 Conclusions and recommendations

The aim of this review paper has been to provide an overview and comparison of the different approaches that have currently been applied for solving topology optimization problems in vibro-acoustics. In the following, we summarize the most significant findings, highlight the challenges, and conclude with recommendations for future directions within the field of acoustic-mechanical topology optimization.

For all studied examples, the density-based method was shown to provide the best performing designs from an arbitrary initial guess. We mainly ascribe this to the possibility of designing a continuation scheme on the penalization parameter that effectively and consistently results in better local minima. On the contrary, the level set approach does not facilitate such a continuation scheme making the results more prone to stuck in local minima and highly dependent on the initial design. Also, though not presented here, we emphasize that the use of rigorous mathematics such as non-linear programming methods easily facilitates the inclusion of additional constraints on both physics and geometry (Sigmund and Maute 2013).

However, this should not be interpreted as a rejection of the level set-based methods. On the contrary, problems having a multiphysical nature is often highly dependent on the interface representation, i.e., the coupling conditions. The examples presented here clearly demonstrated the issues arising from intermediate density regions and thus a poor interface representation. That is, poor accuracy in the modeling using mixed formulation makes the density-based optimization approach challenging and problematic for problems which are strongly coupled and sensitive to design
Fig. 18 Displacement magnitude $|u| \, [m]$ contours for the frequency $f = 6 \, [Hz]$ showing a initial structure for the level set method, b optimized design obtained with the level set method, the objective value of the end design $C = 0.0026 \, N$, and c body-fitted analysis of optimized design obtained with the density method resulting in an objective value of $C = 0.0015 \, N$. The analysis in c is performed on a thresholded design at $\gamma = 0.5$ using the marching squares algorithm.

Fig. 19 Sound pressure level [dB] contours for the frequency $f = 4 \, [Hz]$ showing a initial structure for the level set method, b optimized design obtained with the level set method, and c body fitted analysis of the optimized design obtained with the density method, thresholded at $\gamma = 0.5$ using the marching squares algorithm.
Fig. 20 Frequency response of the objective function for example 2. The blue line is the optimized design using the level set method, the red line is the initial design with holes, the yellow line is the design domain fully filled with material and the purple line is the optimized design using the density method.

Fig. 21 Optimized design obtained from the BESO method with mixed FE formulation showing (a) final optimized design field and (b) sound pressure level [dB] contour for the frequency \( f = 4 \) Hz. The objective value of the end design evaluated with mixed formulation, \( C = 0.0029N \) and body fitted analysis of optimized design obtained with BESO resulting in an objective value of \( C = 0.0019N \).

Fig. 22 Frequency response of the objective function. Black line is the optimized design obtained from BESO approach with mixed formulation, and purple line is the optimized design with the density method.
changes at the interface. Another significant challenge for the density-based methods is that the optimized designs require a postprocessing step and a subsequent body fitted analysis to verify its performance. This step can be completely avoided when using the level set methods with a crisp interface representation, which together with the possibility to easily enforce complicated coupling conditions advocates the continued use and development of level set methods.

Finally, it was shown that the BESO method provided comparable results in the second example. While the method generally yields very good results for pure static structural optimization where the design sensitivities are of equal sign (more material is always better), its application to more complicated problems involving dynamics and/or multi-physics appears to be more problematic. Throughout the work, the BESO method is found to be the least stable of the considered methods and in some cases it leads to lack of convergence. This we ascribe to the heuristic BESO update algorithm that is not well suited for handling problems with both positive and negative design sensitivities. However, the BESO method also has its justification. That is, the method is very easy to implement in commercial black-box codes without the need to access element integration routines and does not require expensive re-meshing schemes. In fact, for many problems one can use energy expression to get sensitivity information which makes it even simpler to adopt into existing codes.

4.1 Recommendations

Firstly, we recommend that subsequent work on vibro-acoustic optimization always includes a benchmark against previous work as shown in this paper. That is, solving old problems with new methods can only be justified if the new method provides an improvement compared to existing methods. In the following, we provide recommendations for the density and level set method, separately.

For the density-based methods, we have the following recommendations. Firstly, we note that the mixed formulation is an expensive modeling tool since it can lead to poor accuracy on coarse meshes, even with crisp designs, and that the intermediate densities at the interface lack a physical explanation. The mixed formulation is also prone to numerical instabilities arising from the choice of interpolation functions (Wang and Bathe 1997), which means that for a stable solution high order elements must be used which in turn increases the computational complexity even further. Therefore, we suggest that more work should go into new interpolation schemes that, potentially, could alleviate the need for the mixed formulation. On the other hand, a monolithic formulation have many desirable properties and hence another path to follow is to modify, or expand, the standard $u-p$ mixed formulation such that it is better at capturing the sharp jumps in state fields that arise when performing topology optimization.

For the level set-based methods, we have the following recommendations. The main issue with level set methods using the Hamilton-Jacobi update scheme is the problem of adding more constraints. We therefore suggest that focus is put on methods that ensure crisp interfaces, e.g., xFEM (Gerschenberger and Wall 2008) or CutFEM methods (Hansbo and Hansbo 2004; Burman et al. 2014), together with mathematical programming tools. This latter would allow the optimization analyst to include more constraints whereas the first means that tedious post processing can be avoided.

5 Replication of results

All results presented in this work are in fact reproductions of already published and developed methods. For replicating the presented examples, the readers can find the relevant information in the corresponding sections.

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Compliance with ethical standards

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References


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Generalized shape optimization of transient vibroacoustic problems using cut elements
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Generalized shape optimization of transient vibroacoustic problems using cut elements

Cetin B. Dilgen | Niels Aage

Centre for Acoustic-Mechanical Micro Systems (CAMM), Department of Mechanical Engineering, Technical University of Denmark, Denmark

Correspondence
Cetin B. Dilgen, Technical University of Denmark, Nils Koppel's Allé, Building 404, DK-2800, Denmark
Email: cedil@mek.dtu.dk

Abstract
This paper propose a generalized shape optimization method for transient coupled acoustic-mechanical interaction problems. The transient problem formulation allows to optimize for a broadband frequency content and the possibility to investigate transient phenomena such as pulse shaping. Throughout the work, the geometry is defined with the help of a nodal based design field, for which its zero level contour describes the interface between acoustic and structural domains. The approach utilizes a fixed background mesh to represent the geometry and a cut element immersed boundary method for the physical modelling. This provides accurate solutions to the strongly coupled governing equations based on a special integration scheme. The optimization problem is solved using a gradient based optimizer and employs a fully discrete adjoint approach for calculating the sensitivity information. A numerical examination on the accuracy of the sensitivity analysis compares the fully discrete gradients to the commonly used semi-discrete adjoint approach for transient optimization revealing the importance of consistent sensitivities. The transient design formulation is validated on a 2D benchmark problem concerning the design of a time-harmonic acoustic partitioner. The developed framework is then applied for the design of vibroacoustic pulse shaping devices to demonstrate control of a transient phenomena.

KEYWORDS:
Vibroacoustics, Transients, Generalized shape optimization, Cut elements, Gradients, Level set methods

1 | INTRODUCTION

Shape and topology optimization have become widely popular in engineering design with ever widening application areas of in both academia and industry. One of the most popular approaches is density based topology optimization, which is a method to determine optimized material distributions that minimizes a given objective function. The key to the success of the density method is to relax the material representation by introducing intermediate densities, meaning that the material properties are commonly interpolated between solid and void phases. This approach readily facilitates the use of efficient gradient based optimizers such as the method of moving asymptotes (MMA). However, for certain problem types in which the interface plays a crucial role in the modelling, the physical interpretation of intermediate material realizations can pose severe and limiting issues. This can, for some problems, be mitigated through image processing filters and projection filters that serves to
eliminate intermediate densities. These methods have paved the way for giga-scale structural optimization\textsuperscript{8} and made the density approach a commonly used tool in industrial design. Although primarily used for structural optimization, the method has gained popularity in many other applications and different physics including fluid dynamics\textsuperscript{9,10}, acoustics\textsuperscript{11,12,13}, transient wave propagation problems\textsuperscript{14,15,16}, space-time methods\textsuperscript{17,18}, optics\textsuperscript{19} and as well as multi-physics applications\textsuperscript{20,21,22}.

However, the presence of the intermediate densities in the optimized design (including those appearing during the optimization stage) can cause issues due to the lack of a clear boundary definition. Furthermore, for multi-physics problems coupled through an interface it is often crucial to have a smooth boundary definition due to an inherent sensitivity to sharp boundary variations, e.g. kinks. To this end, the so called staircase (pixelated) boundary representation introduces issues for density based topology optimization when it is used for coupled multi-physics problems\textsuperscript{1,2,21}. Another issue for interface dependent design problems occurs after the optimization process. For example, for strongly coupled vibroacoustic problems, the final design’s performance can be adversely affected after post-processing, especially for high frequency applications, due to a lack of physical interpretation of small regions of gray material or the smoothing of jagged edges. So although density based methods have been successfully applied to low frequency vibroacoustic design problems using a mixed finite element formulation\textsuperscript{24}, the potential drawbacks as mentioned above advocates the use of design and modelling approaches capable of a clear and crisp interface representation.

An often used alternative to the density design methodology is the level set method\textsuperscript{25,26}. Such approaches implicitly defines the geometry from the zero contour of a level set function which in turn facilitates a crisp representation of the design with well-defined boundaries. However, it is important to remark that an accurate representation of the state fields at the interface is not given by the level set method itself, but is completely dependent on the underlying numerical model. Nonetheless, multiple variations of the level set approach has been used in the context of structural optimization for vibroacoustic problems including those that employ ertsatz-type material models\textsuperscript{27}, those that depends on extensive remeshing\textsuperscript{28} and those that use an advection-diffusion equation for the design update\textsuperscript{29,30}. For a detailed comparison of density, level set and evolutionary based topology optimization methods for vibroacoustic problems the reader is referred to the recent review paper\textsuperscript{31}.

This work presents a level set based generalized shape optimization framework for transient vibroacoustic problems. The transient formulation of the vibroacoustic systems enables the optimization to be carried out for a broad frequency content while also allowing the possibility to investigate transient phenomena. The developed design method is based on the cut element topology optimization approach presented in\textsuperscript{32} which is extended to accommodate the coupled vibroacoustic state problem. The cut element method can, to some extend, be seen as a special case of the finite cell method\textsuperscript{33} or X-FEM without enrichments\textsuperscript{34,35} in which the entire background mesh in maintained at all times. To the best of the authors’ knowledge, transient shape optimization of vibroacoustic problems using a cut element method combined with a fully discrete adjoint approach has not been demonstrated before. The thorough explanations of the level set parameterization, the utilized immersed boundary method and the discrete temporal adjoint method that is applicable to any time integration scheme are also among the contributions of the present work. The remainder of the paper is organized as follows: The governing equations with spatial and temporal discretization of the coupled physics are introduced in section 2. Section 3 describes the employed level set parameterization used for the optimization. The cut element method used for the accurate modelling of the coupling of structural and acoustic domains is explained in section 4. Section 5 introduces the optimization problem and implementation aspects of the discrete adjoint method for the sensitivity analysis. In section 6 the discrete sensitivities are compared to the semi-discrete approach and the optimization setup for the develop framework is validated on a benchmark problem. The transient shape optimization for vibroacoustics problems are then demonstrated on acoustic pulse shaping examples, after which the findings are discussed and summarized.

\section{GOVERNING EQUATIONS}

In this section, the governing equations that are used throughout the work considering the structural displacements and acoustic pressure are introduced. Since the cut element method is utilized for the modeling of the coupled system and the subsequent optimization, both the structural and acoustic fields are embedded in the domain $\Omega$ which consists of the entire computational domain as

$\Omega = \Omega_s \cup \Omega_e$ \hspace{1cm} (1)

where $\Omega_s$ denotes the current acoustic region and $\Omega_e$ is the embedded structure. Similar to other fictitious domain approaches, such as density methods, both physics are solved in $\Omega$ which allows for an automated evolution of the structure throughout the optimization. Both physics are coupled through the interface $\Gamma_{e,s}$ between $\Omega_s$ and $\Omega_e$. Hence the correct definition of the
boundaries and the coupling conditions are important for the modeling accuracy. The specifics of the cut element approach is described in section 4.

The governing equations for linear elasticity considering a time dependent motion without the presence of a body force can be written as

\[
\rho_s \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \mathbf{\sigma} + \rho_s \frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \left( \beta_p \frac{\partial \mathbf{p}}{\partial t} \right) = 0 \quad \text{in} \quad \Omega \tag{2}
\]

\[
\mathbf{u} = 0 \quad \text{in} \quad \Gamma_{ad} \tag{3}
\]

\[
\mathbf{n}_s \cdot \mathbf{\sigma} = 0 \quad \text{in} \quad \Gamma_{m} \tag{4}
\]

\[
\mathbf{n}_s \cdot \mathbf{\sigma} = \rho \mathbf{n}_s \quad \text{in} \quad \Gamma_{es} \tag{5}
\]

where \(\rho_s\) is the density of the solid material, \(\mathbf{u}\) is the displacement vector, \(p\) is the acoustic pressure, \(\mathbf{n}_s\) is the normal vector defined at the interface pointing outwards from the structural boundary, \(\mathbf{n}_s\) is the normal vector pointing outwards from the acoustic domain into the structural region. In order to approximately reflect the loss mechanism of the real world, the Rayleigh damping is considered (the last two terms on the right hand side of the Eq. 2) in which \(\alpha_p\) and \(\beta_p\) are the Rayleigh damping parameters. Moreover, \(\mathbf{\sigma}\) is the Cauchy stress vector which is defined as

\[
\mathbf{\sigma} = \mathbf{C} (E_s, \nu) \mathbf{\varepsilon} \tag{6}
\]

Here, \(\mathbf{C} (E_s, \nu)\) is the plane stress constitutive matrix, \(E_s\) is the Young’s modulus, \(\nu\) is the Poisson’s ratio and the strain vector \(\mathbf{\varepsilon}\) is defined as

\[
\mathbf{\varepsilon} = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix} \tag{7}
\]

For the structural domain, coupling from the acoustic domain is realized through the boundary condition written in Equation 5 which means that the acoustic pressure \(p\) applies a pressure load onto the structural boundary.

The solution to the elasticity equation follows the cut element fictitious approach of\(^{12}\). That is, the solution of the displacements in the fictitious domain, which is the void phase in \(\Omega_s\) for the structure, is obtained by altering the material properties of the considered solid as

\[
E_s = a E_s', \quad \rho_s = a \rho_s \tag{8}
\]

where \(a\) is a dimensionless contrast parameter and the tilde superscript is used to specify the original material properties of the solid. Throughout the work, \(a\) takes the values of unity for the structure domain and \(10^{-8}\) for the void phase of the structure.

The acoustic pressure is governed by the Helmholtz equation

\[
\frac{1}{K_p} \frac{\partial^2 p}{\partial t^2} - \frac{1}{\rho_p} \nabla^2 p = 0 \quad \text{in} \quad \Omega \tag{9}
\]

\[
\mathbf{n}_s \cdot \nabla p = 0 \quad \text{in} \quad \Gamma_{ad} \tag{10}
\]

\[
\mathbf{n}_s \cdot \nabla p = \frac{\partial^2 (\mathbf{n}_s \cdot \mathbf{u})}{\partial t^2} \quad \text{in} \quad \Gamma_{m} \tag{11}
\]

\[
\mathbf{n}_s \cdot \nabla p + \frac{1}{c_s} \frac{\partial p}{\partial t} = \frac{2 \rho_p}{c_s^3} \frac{\partial^2 p}{\partial t^2} \quad \text{in} \quad \Gamma_{es} \tag{12}
\]

Here \(c_s\) is the speed of sound in the acoustic medium, \(\rho_p\) is the density of the fluid, \(K_p\) is the bulk modulus for the acoustic medium defined as \(K_p = \rho_p c_s^2\). Hard-wall boundary condition is given in the Equation 10 and the coupling to the structural domain is given in Equation 11 which represents an acceleration boundary condition into the acoustic domain. Equation 12 describes an absorbing boundary condition with plane wave radiation where \(p_m\) denotes the transient incoming pressure wave.

Similarly to the elasticity problem, the acoustic pressure solution in the fictitious domain, which is the rigid phase for the acoustic pressure defined in \(\Omega_s\), is obtained by changing the material properties of the acoustic medium as

\[
K_p = \tilde{K}_s \frac{a}{\alpha}, \quad \rho_p = \tilde{\rho}_s \frac{a}{\alpha} \tag{13}
\]

Again, the \(\alpha\) takes the values of unity for the acoustic domain and \(10^{-8}\) for the rigid phase of the acoustic solution.
2.1 Spatial discretization

The finite element discretization of the vibroacoustic system is obtained by a standard Galerkin procedure. However, note in the following that the continuous state variables have been replaced by $\vec{u}$ and $\vec{p}$ such that the resulting discrete system can be written without overbars. The resulting weak form can be stated as the following integral expression

$$
\int_{\Omega} \rho \frac{\partial \vec{u}}{\partial t} \frac{\partial \vec{u}}{\partial t} d\Omega + \int_{\Omega} \frac{\partial \vec{e}}{\partial t} \mathbf{C} \vec{e} d\Omega + \int_{\Gamma} \mathbf{p} \mathbf{P} \frac{\partial \vec{u}}{\partial t} d\Gamma - \int_{\Gamma} \frac{\partial \vec{e}}{\partial t} \mathbf{C} \vec{e} d\Omega = 0 \tag{14}
$$

where $\rho$ is the density, $\vec{u}$ is the displacement vector, $\mathbf{C}$ is the linear strain-displacement matrix, and $\mathbf{P}$ is the damping matrix.

Employing the standard Galerkin procedure

$$
\mathbf{M} \frac{\partial^2 \vec{u}}{\partial t^2} + \mathbf{C} \frac{\partial \vec{u}}{\partial t} + \mathbf{K} \vec{u} = \mathbf{F} \tag{18}
$$

where the test functions are replaced by the shape functions of the variables, the discretized finite element matrices are identified as

$$
\mathbf{K} = \int_{\Gamma} \mathbf{B}^T \mathbf{C} \mathbf{B} d\Gamma, \quad \mathbf{M} = \rho \int_{\Gamma} \mathbf{N}^T \mathbf{N} d\Gamma, \quad \mathbf{S} = \int_{\Gamma} \mathbf{N}^T \mathbf{n} \mathbf{N} d\Gamma, \quad \mathbf{C} = \int_{\Gamma} \mathbf{N}^T \mathbf{C} \mathbf{N} d\Gamma \tag{19}
$$

$$
\mathbf{K}_x = \frac{1}{\rho_e} \int_{\Gamma} \mathbf{N}_x^T \mathbf{N}_x d\Gamma, \quad \mathbf{C}_x = \frac{\omega_s}{\rho_e} \int_{\Gamma} \mathbf{N}_x^T \mathbf{C} \mathbf{N}_x d\Gamma \tag{20}
$$

$$
\mathbf{K}_y = \frac{1}{\rho_e} \int_{\Gamma} \mathbf{N}_y^T \mathbf{N}_y d\Gamma, \quad \mathbf{C}_y = \frac{\omega_s}{\rho_e} \int_{\Gamma} \mathbf{N}_y^T \mathbf{C} \mathbf{N}_y d\Gamma \tag{21}
$$

$$
\mathbf{K}_z = \frac{1}{\rho_e} \int_{\Gamma} \mathbf{N}_z^T \mathbf{N}_z d\Gamma, \quad \mathbf{C}_z = \frac{\omega_s}{\rho_e} \int_{\Gamma} \mathbf{N}_z^T \mathbf{C} \mathbf{N}_z d\Gamma \tag{22}
$$

2.2 Time integration

After the spatial discretization the coupled system has the following semi discrete form

$$
\mathbf{M} \frac{\partial^2 \vec{v}}{\partial t^2} + \mathbf{C} \frac{\partial \vec{v}}{\partial t} + \mathbf{K} \vec{v} = \mathbf{h} \tag{23}
$$

where the contents of the combined mass matrix $\mathbf{M}$, damping matrix $\mathbf{C}$ and stiffness matrix $\mathbf{K}$ are given in Equation 18. Here, the superscript $n$ denotes current time, the vector $\vec{v}$ is the solution vector $\vec{v} = [\vec{u} \; \vec{p}]^T$ and the vector $\vec{h} = [0 \; \vec{g}]^T$ is the load vector for the given dynamic system. Throughout the presented work a Newmark algorithm is, i.e. an implicit time-stepping scheme.
is used for the temporal discretization. Here the first and the second time derivatives of the solution vector $v$ are expressed as

$$
\dot{v}^n = a_1 \dot{v}^{n-1} + a_2 v^{n-1} + a_3 (v^n - v^{n-1})
$$

\hspace{1cm}
$$
\ddot{v}^n = -a_4 \ddot{v}^{n-1} - a_5 v^{n-1} + a_6 (v^n - v^{n-1})
$$

where the parameters $a_1$ to $a_6$ are the Newmark parameters. Substituting the above definitions (Eqs. 24 and 25) into the semi discrete coupled system given in Equation 23, leads to the following fully discrete linear system of equations to be solved for $v^n$ for the current time $n$

$$
\hat{K} v^n = \hat{h}^n
$$

where $\hat{K}$ and $\hat{h}^n$ are the so called effective stiffness matrix and load vector, respectively. $\hat{K}$ and $\hat{h}^n$ are defined as

$$
\hat{K} = K + a_4 M + a_4 C
$$

$$
\hat{h}^n = h^n + M (a_4 \dot{v}^{n-1} + a_5 v^{n-1}) + C (-a_4 \ddot{v}^{n-1} - a_5 v^{n-1} + a_6 v^n)
$$

Moreover, the Newmark parameters are given as

$$
a_1 = 1 - \frac{\bar{\gamma}}{\bar{\beta}}, \quad a_2 = \left(1 - \frac{\bar{\gamma}}{2\bar{\beta}} \right) \Delta t, \quad a_3 = \frac{\bar{\gamma}}{\bar{\beta} \Delta t}
$$

$$
a_4 = \frac{1}{\bar{\beta} \Delta t}, \quad a_5 = \frac{1}{2\bar{\beta}} - 1, \quad a_6 = \frac{1}{\bar{\beta} \Delta t^2}
$$

where $\Delta t$ is the time step size. Following $^{39,40,41}$, $\bar{\beta}$ and $\bar{\gamma}$ are chosen such that the utilized time-stepping scheme is unconditionally stable which are given as

$$
\bar{\beta} = \frac{1}{4}, \quad \bar{\gamma} = \frac{1}{2}
$$

Throughout the work, the initial conditions $v^0$ and $\phi^0$ are assumed to be zero and the initial condition for the second time derivative of the solution vector $\ddot{v}^0$ is found by solving

$$
M \ddot{v}^0 = h^0
$$

The numerical model presented here is implemented in C++ where the PETSc library $^{39,40,41}$ is utilized for its parallel data arrangement. The solution of equation 26 is obtained using the parallel direct solver MUMPS $^{42,43}$.

### 3 | DESIGN PARAMETERIZATION

The design parameterization used in the presented work follows the level set approach based on density methods presented in $^{32}$. That is, a continuous mathematical nodal design field $s$ is introduced similar to that of classical density methods, i.e.

$$
0 \leq s \leq 1
$$

This choice of bounds for the design field means that standard optimizers such as the Methods of Moving Asymptotes can readily be applied $^2$. However, to ensure that the interface does not progress to fast during the optimization process, a mesh dependent mapping is used to introduce the element size to the parameterization as

$$
-0.5 h_e \leq \delta(s) \leq 0.5 h_e
$$

where $h_e$ is the average element side length. The last step before feeding the design field to the finite element analysis is to regularize the problem with a convolution filter. This is included to regularize the problem by increasing the zone of influence of the design variables, and hence also the sensitivities, which stabilizes and speeds up the design process. The filter, which is applied on $\delta(s)$, is realized using a Helmholtz type differential equation $^{44}$. Here it is noted that, for stability, the filter equation is implemented employing the finite volume method in which the variables are stored in cell centers and represented as piece-wise constants. Hence the field $\delta(s)$ is first interpolated to cell centers. The filter equation reads

$$
-\nu \Delta^2 \delta_{c} + \delta_{c} = \delta_{c}
$$

where the subscript $c$ specifies variables that are defined in cell centers and $r$ is the filtering radius. Utilizing finite volume method for the filter equation allows us to use any filter size $r$. After filtering, the cell centered field $\delta_{c}$ is interpolated back to the
nodes leading to the physical design field $\bar{z}$. It is noted that the two interpolation operations (from nodes to the element centers and from element centers to the nodes) provide extra implicit filtering that is always active even when the filtering radius $r$ is set to zero.

The physical design field, $\bar{z}$, can now be used as a level set field to determine if a given part of $\Omega$ is either acoustic, structural or the interface based on the following rule

\[
\begin{align*}
\bar{z}(x) > 0, & \quad x \in \Omega_s \text{ (structural domain)} \\
\bar{z}(x) = 0, & \quad x \in \Gamma_{\text{int}} \text{ (interface)} \\
\bar{z}(x) < 0, & \quad x \in \Omega_a \text{ (acoustic domain)}
\end{align*}
\] (36)

An illustrative example of the function $\bar{z}$ can be seen in Figure 1 where the embedded structural and acoustic domains are identified along with the shared interface between the two domains. Figure 1 also shows the projection of $\bar{z}$ onto a fixed background finite element mesh.

As shown in figure 1 b, since both $z$ and $\bar{z}$ use linear shape functions, the resulted non-conforming boundary is represented by linear straight curves inside cut elements. We note that a 2D level set method cannot introduce holes without an auxiliary hole generation scheme, e.g. topological derivatives, but that a 3D version of the presented approach could. Therefore the proposed 2D method is termed a generalized shape optimization method. Finally, we remark that the proposed design parameterization does not introduce a minimum length scale to the design problem. Although this could be included following the robust approach e.g. 7,32, this is deemed outside the scope of this manuscript since the focus is on the numerical methodology allowing for transient vibroacoustic generalized shape optimization optimization.

4 | CUT ELEMENT INTEGRATION

Having introduced the design parameterization, this section describes the modeling of non-conforming boundaries through a simple cut element method. That is, instead of re-meshing with conforming elements along the interface, which is expensive and difficult to parallelize, the cut element method realizes the exact boundary representation (piecewise linear) by special integration of the elements cut by the zero contour of the level set field. The utilized method does not enrich the shape functions or add additional degrees of freedom to the system. Hence, it is easily parallelizable as the integration that is done in the cut elements are only local operations.

The cut element procedure can be summarized as follows. Firstly the cut elements are identified by looping through all elements and checking for a sign change in the nodal level set field. Then, a triangulation algorithm is employed to sub-divide the intersected element into triangles with respecting the partial interface inside the element. The present work utilizes the marching
squares algorithm in which the nodal physical level set values are used to determine the location of the zero level contour (intersecting boundary) along the edges of the element. The subsequent triangulation is done from a pre-generated look-up table since in marching squares algorithm there are only 16 unique cases a Quad element can be intersected. Figure 2 illustrates the cut element identification process.

**FIGURE 2** An example finite element mesh where white color shows the uncut elements in the acoustic domain, gray color shows the uncut elements in the solid region and the blue color shows the cut elements. Figure also shows an example of identifying a cut element from its nodal level set values.

### 4.1 Sub-integration
This section describes the sub-element integration which is carried out for the elements that are cut by a non-conforming boundary. Cut elements utilize the Gaussian quadrature rule for capturing the effect of the boundary description through weighted integration. As such, it is important to correctly place the integration points in the sub-elements of the parent cut element. Here it is noted that the triangulation in the cut elements are only carried out in order to correctly place the integration points in the sub-elements and the interface line inside the parent cut element.

Figure 3 a shows an example of a cut element where the sub-elements are obtained through triangulation. Figures 3 b to 3 c illustrates mapping the Gauss points defined at the reference domain of the sub-triangle element to the reference domain of the parent element where the integration is carried out. The reader is referred to for details regarding the mapping of integration

**FIGURE 3** Illustration of a sub-cell integration in a cut element. (a) physical domains are identified for the triangulated cut elements where white color is the acoustic domain, gray color is the structural domain and the blue line is the interface. (b) Gauss points are inserted in an iso-parametric triangle sub-element in local coordinates. (c) Gauss points of the iso-parametric triangle sub-element are mapped to the reference domain of the parent element for integration.
points. Following the nomenclature of Figure 3, the element matrix contribution for the stiffness part of linear system becomes

\[
K_i = \sum_{j=1}^{m_i} B_j(\xi_{i,j}, \eta_{i,j}) C(E_{i,j}) B_j(\xi_{i,j}, \eta_{i,j}) W_{i,j} \|J(\xi_{i,j}, \eta_{i,j})\| \tag{37}
\]

Where the weight \(W_{i,j}\) is modified to take into account the area scaling between sub-triangle and parent element. Since the vibroacoustic system also needs to include the coupling at the material interface, a similar procedure is applied to the line integrals. The process is illustrated in Figure 4 and the subsequent integration over the quadrilateral is performed as

\[
S = \sum_{j=1}^{m_i} N_j(\xi_{i,j}, \eta_{i,j}) n_j N_j(\xi_{i,j}, \eta_{i,j}) W_{i,j} \frac{l}{2} \tag{38}
\]

where \(l\) is the length of the coupling boundary. Again, it should be emphasized that the contribution from the integration goes to the original degrees of freedoms of the parent element.

5 | OPTIMIZATION PROBLEM

In this section a generic optimization problem for a transient optimization is given where an objective function is sought to be minimized while satisfying the considered constraints. The optimization problem is written as

\[
\min_{\mathbf{s}} \Phi(\mathbf{s}, \mathbf{U}^0(\mathbf{s}), \ldots, \mathbf{U}^N(\mathbf{s})) = \sum_{n=0}^{N} \phi_n(\mathbf{s}, \mathbf{U}^n(\mathbf{s})) \tag{39}\]

s.t. \( \mathbf{R}^n(\mathbf{s}, \mathbf{U}^n(\mathbf{s})) = 0, \quad \text{for} \quad n = 0, 1, \ldots, N \)

\( \psi_i(\mathbf{s}, \mathbf{U}^0(\mathbf{s}), \ldots, \mathbf{U}^N(\mathbf{s})) \leq 0, \quad \text{for} \quad i = 0, 1, \ldots, m \)

\( s_{\text{min}} \leq \mathbf{s} \leq s_{\text{max}} \) \tag{42}

where \(\mathbf{s}\) is the vector of design variables, \(\Phi\) is the objective function, \(\mathbf{U}^n\) is the vector of state variables, the residual vector \(\mathbf{R}^n\) is obtained from the discretization of the governing equations (sections 2.1 and 2.2). \(N\) denotes the total number of time steps considered in the optimization, \(\psi_i\) are the \(m\) possible inequality constraints, \(s_{\text{min}} = 0\) and \(s_{\text{max}} = 1\) are the bounds for the design variables.

As a consequence of using Newmark algorithm for temporal discretization, the vector \(\mathbf{U}^n\) contains the state variables and their first and the second time derivatives. Likewise, the residual vector \(\mathbf{R}^n\) contains the corresponding residuals which are written as
where the individual residual vectors can be identified from the temporal discretization using the equations 24 to 28 as
\[
\begin{align*}
\mathbf{r}^n &= [\mathbf{K} + a_1 \mathbf{M} + a_2 \mathbf{C}] \mathbf{v}^n - [a_1 \mathbf{M} + a_2 \mathbf{C}] \mathbf{v}^{n-1} - [a_2 \mathbf{M} - a_1 \mathbf{C}] \mathbf{\psi}^{n-1} + [a_1 \mathbf{C} - a_2 \mathbf{M}] \mathbf{\psi}^{n-1} - \mathbf{h}^n \\
\mathbf{r}^n &= \mathbf{v}^n - a_1 \mathbf{v}^{n-1} - a_2 \mathbf{\psi}^{n-1} - a_3 \mathbf{\psi}^{n-1} \\
\mathbf{r}^n &= \mathbf{v}^n + a_1 \mathbf{v}^{n-1} + a_2 \mathbf{\psi}^{n-1} - a_3 \mathbf{\psi}^{n-1}
\end{align*}
\]

The optimization problem (Eqs. 39 to 42) is solved using the Method of Moving Asymptotes (MMA)\(^2\). The present work uses a parallel PETSc implementation of the optimizer, c.f.\(^16,17\).

5.1 Sensitivity analysis

The sensitivity analysis needed for the application of a gradient based optimizer is here presented considering the generic objective function stated in Eq. 39. To this end a fully discrete sensitivity analysis is employed rather than the commonly used semi-discrete sensitivities for transient optimization\(^14,17\). This approach is similar to that presented in\(^16\), however, here the derivation is written in a general matrix form to ease the implementation and extension by others. The result is valid for any objective function and the use of a fully discrete sensitivity analysis ensures that the sensitivities always are consistent. Moreover, the quality of the calculated gradients does not depend on the utilized time step size or the time integration scheme since there is no time integration for the adjoint equation. The process of obtaining the sensitivity expression follows the standard engineering approach. That is, first the objective function is augmented using a vector of Lagrange multiplier \(\mathbf{\Lambda}\) and the resulted Lagrangian function \(\mathcal{L}\) is written as
\[
\mathcal{L} = \sum_{n=0}^{N} \phi^n(\mathbf{S}, \mathbf{U}(\mathbf{S})) + \mathbf{\Lambda}^T \mathbf{R}^n(\mathbf{S}, \mathbf{U}(\mathbf{S}))
\]

Here it is used that the residual is always satisfied, i.e. \(\mathbf{R}^n = 0\), for any given time step \(n\). As with the state variable \(\mathbf{U}\), the Lagrange multiplier vector consists of three fields as
\[
\mathbf{\Lambda}^n = \begin{bmatrix} \lambda_1^n \\ \ldots \\ \lambda_3^n \end{bmatrix}
\]

The derivative of the Lagrangian function with respect to the physical level set field \(\mathbf{S}\) can be written as
\[
\frac{d\mathcal{L}}{d\mathbf{S}} = \sum_{n=0}^{N} \frac{d\phi}{d\mathbf{S}} + \frac{d\phi}{d\mathbf{U}} \frac{d\mathbf{U}}{d\mathbf{S}} + \mathbf{\Lambda}^T \left[ \frac{d\mathbf{R}^n}{d\mathbf{S}} + \frac{d\mathbf{R}^n}{d\mathbf{U}} \frac{d\mathbf{U}}{d\mathbf{S}} \right]
\]
\[
= \sum_{n=0}^{N} \frac{d\phi}{d\mathbf{S}} + \mathbf{\Lambda}^T \frac{d\mathbf{R}^n}{d\mathbf{S}} + \frac{d\phi}{d\mathbf{U}} \frac{d\mathbf{U}}{d\mathbf{S}} \left[ \frac{d\mathbf{U}}{d\mathbf{U}} \right]_{\mathbf{U}=0}
\]

Since the Lagrangian vector can be freely chosen the calculation of the partial derivative \(\frac{d\mathcal{L}}{d\mathbf{S}}\) can be avoided if the underlined part of the above equation 50 is set to zero. This gives rise to the following set of adjoint equations for each time step
\[
\left( \frac{d\mathbf{R}^n}{d\mathbf{U}} \right)^T \mathbf{\Lambda}^n = -\frac{d\phi}{d\mathbf{U}} \quad \text{for} \quad n = 0, 1, \ldots, N
\]

or more compactly written
\[
\frac{d\mathbf{R}^T}{d\mathbf{U}} \mathbf{\Lambda} = -\frac{d\phi}{d\mathbf{U}}
\]

where the superscript \(n\) is dropped to indicate that Eq. 52 now contains all time steps used in the optimization. The partial derivative of the residual vector with respect to the state variables \(\frac{d\mathbf{R}}{d\mathbf{U}}\) then has the following form
where the subscripts denote the current time step and the superscripts show the corresponding state variables for the sub-matrices in $\partial \mathbf{R}/\partial \mathbf{U}$. Here, the sub-matrices $\mathbf{A}$ and $\mathbf{B}$ are written in general form and will vary depending on the employed time integration scheme. Considering the Newmark algorithm, the $\mathbf{A}$ and $\mathbf{B}$ sub-matrices are identified from the residuals written in equations 44 to 46. For a time step greater than zero, i.e. $n > 0$, these are constant and can be written as

\[
\mathbf{A} = \begin{bmatrix} \mathbf{K} + \alpha_2 \mathbf{M} + \alpha_1 \mathbf{C} \\ -\alpha_1 \mathbf{I} & \mathbf{I} \\ -\alpha_1 \mathbf{I} & \mathbf{I} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} -\alpha_0 \mathbf{M} - \alpha_1 \mathbf{C} & -\alpha_0 \mathbf{M} + \alpha_1 \mathbf{C} \\ \alpha_0 \mathbf{I} & -\alpha_1 \mathbf{I} \\ \alpha_0 \mathbf{I} & \alpha_1 \mathbf{I} \end{bmatrix}
\]

(54)

Since these are constant the can be assembled once and reused throughout the optimization cycle. Considering the initial conditions of the state equations where $\mathbf{v}_0^t$ and $\mathbf{v}_0^\theta$ are assumed to be zero and the initial condition of $\mathbf{v}_0^\theta$ is found by solving the equation 32, the matrix $\mathbf{A}_0$ is written as

\[
\mathbf{A}_0 = \begin{bmatrix} \mathbf{I} \\ \mathbf{I} \\ \mathbf{M} \end{bmatrix}
\]

(55)

(56)

As a consequence of the transpose operation on $\partial \mathbf{R}/\partial \mathbf{U}$ in the adjoint equation (Eq. 52), the adjoint equation is decomposed into reverse pseudo time steps as

\[
\begin{align*}
\langle \mathbf{A} \rangle^T \mathbf{A}^N &= \frac{\partial \phi^N}{\partial \mathbf{U}} \\
\langle \mathbf{A} \rangle^T \mathbf{A}^{N-1} &= \frac{\partial \phi^{N-1}}{\partial \mathbf{U}} - \langle \mathbf{B} \rangle^T \mathbf{A}^N \\
&\vdots \\
\langle \mathbf{A}_0 \rangle^T \mathbf{A}^0 &= -\frac{\partial \phi^0}{\partial \mathbf{U}} - \langle \mathbf{B} \rangle^T \mathbf{A}^1
\end{align*}
\]

(57)

(58)

(59)

(60)

This is the same type of reversal in time that is seen for the usual semi-discrete temporal adjoint approach. Now, having found the Lagrange multiplier $\mathbf{A}$ which satisfies the adjoint equation (Eq. 52), the final sensitivity of the objective function is calculated as follows

\[
\frac{\partial \mathbf{F}}{\partial \mathbf{K}} = \alpha_0^T \mathbf{A}^1 \frac{\partial \mathbf{K}}{\partial \mathbf{R}} + \sum_{n=1}^{N} \alpha_0^T \mathbf{A}^n \left[ \frac{\partial \mathbf{A}_n}{\partial \mathbf{U}} \mathbf{U}_n^T + \frac{\partial \mathbf{B}_n}{\partial \mathbf{U}} \mathbf{U}_n^{n-1} \right]
\]

(61)

As it can be seen from the final sensitivity expression, the state variables calculated from the solution of the forward problem needs to be stored in order complete the summation. This is potentially extremely memory consuming, but for the 2D problems considered in this work this has been possible. However, we remark that one could also write the forward solution to disc and then load it as necessary when solving the adjoint problem. Or one could employ a check-pointing scheme, which is both memory and disc-space efficient, although it comes at the cost of having to solve the forward problem twice.

The derivatives $\frac{\partial \mathbf{A}_n}{\partial \mathbf{R}}$, $\frac{\partial \mathbf{A}_n}{\partial \mathbf{K}}$ and $\frac{\partial \mathbf{B}_n}{\partial \mathbf{R}}$ contain the partial derivatives of the finite element matrices ($\mathbf{K}$, $\mathbf{M}$ and $\mathbf{C}$) with respect to the physical level set field $\mathbf{K}$. For simplicity, these partial derivatives are approximated by a finite difference method using a central difference scheme.
It is also noted that the sensitivity calculation in equation 61 is only done in the cut elements, since the terms \( \frac{\partial A}{\partial x}, \frac{\partial A}{\partial y} \) and \( \frac{\partial A}{\partial z} \) are zero elsewhere. For completeness, the matrices \( \frac{\partial A}{\partial x}, \frac{\partial A}{\partial y} \) and \( \frac{\partial A}{\partial z} \) are written here as

\[
\frac{\partial A}{\partial \delta s} = \begin{bmatrix}
\frac{\partial a}{\partial x} + \frac{a_y a}{\partial x} + \frac{a_z a}{\partial x} \\
0 & 0 \\
0 & 0
\end{bmatrix}, \quad \frac{\partial \phi_A}{\partial \delta s} = \begin{bmatrix}
0 \\
0 \\
\frac{\partial a}{\partial s}
\end{bmatrix}
\] (62)

\[
\frac{\partial B}{\partial \delta s} = \begin{bmatrix}
-\alpha_0 \frac{\partial a}{\partial s} - \frac{\partial a}{\partial s} & -\alpha_1 \frac{\partial a}{\partial s} + \frac{\partial a}{\partial s} \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\] (63)

After calculating the sensitivities \( \frac{\partial \phi}{\partial a} \), the gradient with respect to the design variable \( s \) is obtained from the following chain rule

\[
\frac{\partial \Phi}{\partial s} = \frac{\partial \Phi}{\partial \delta s} \frac{\partial \delta s}{\partial \delta s} \frac{\partial \delta s}{\partial \delta s} \frac{\partial \delta s}{\partial \delta s} \frac{\partial \delta s}{\partial \delta s}
\] (64)

Above partial derivatives describe the operations involved in linking the physical level set \( s \) to the design variable \( s \) in which they are applied in reverse order to obtain the gradient of the objective with respect to the design variable \( \frac{\partial \phi}{\partial s} \). Here the partial derivatives \( \frac{\partial x}{\partial s} \) and \( \frac{\partial y}{\partial s} \) are easily calculated since they describe interpolating the variables from element centers to nodes and from nodes to element centers, respectively. The term \( \frac{\partial a}{\partial s} \) deals with the utilized PDE filter and its implementation is thoroughly described in \( \text{a}^{41} \). Finally, the partial derivative \( \frac{\partial a}{\partial s} \) is readily available since it describes changing the bounds on the level set field, c.f. \( \text{a}^{52} \).

### 6 NUMERICAL EXAMPLES

The numerical investigations are conducted on the DTU Sophia cluster made up of 555 compute nodes each equipped with two AMD EPYC 7351 16 core CPUs and 128GB RAM. A maximum of two nodes, i.e. 64 cores, are used since the MPI parallelized direct solver MUMPS \( \text{c}^{42,43} \) is used for the solution to the state problem i.e. because direct solution methods are inherently sequential and cannot scale indefinitely. For all the presented optimization examples the code was allowed to run for 1500 design iterations which took no more than 5 hours to complete. We remark that the convergence of the objective function for all examples was monotone with small and insignificant oscillations towards the end. The settings for the MMA algorithm is for all examples: an MMA asymptote initialization of 0.5, an MMA asymptote increase of 1.2, an MMA asymptote decrease of 0.7, an MMA constraint penalization parameter of \( c = 1000 \) and an outer move limit of 0.5%.

#### 6.1 Gradient validation

This first numerical example concerns a validation study for the implemented discrete adjoint approach. Furthermore, in order to motivate the discrete adjoint approach for transient optimization, the section also compares the method against the sensitivities that are obtained with the commonly used semi-discrete approach \( \text{c}^{44} \). In the semi-discrete approach derivation for the adjoint equation is done analytically in time, i.e. before the temporal discretization, using an already spatially discretized system of equations. This means the utilized time integration scheme does not play a role in the derivation of the adjoint equation, i.e. the residual form of the chosen time stepping scheme is not considered. The derived adjoint equation therefore only has the same form as the spatially distretized forward problem (Eq. 23). This means that one is free to use a different time stepping algorithm for the adjoint problem, although the common practise is to reuse the one chosen for the forward problem.

This section considers a straightforward problem setup to validate and compare the calculated sensitivities in which the objective function is simply the summation of the absolute downstream acoustic pressure in the objective region over all time.
steps given as

$$\Phi = \sum_{k=1}^{N} \int_{\Omega_{k}} |p|^2 \, d\Omega$$

Figure 5 shows a schematic illustration of the design problem. The left most boundary is excited with an incoming sinusoidal acoustic plane wave with an amplitude of $p_{i} = 1kPa$. The top and the bottom boundaries are set as hard-walls while the right most boundary realizes an open boundary. The location where the objective function is evaluated is highlighted in the illustration with blue. A simple circular shaped structure is placed in the middle of the domain for which the calculated sensitivities at its interface will be investigated.

Table 1 lists the material properties for the structural and acoustic domains, respectively. Regular quad elements having the edge length of $0.02m$ is utilized for the computational mesh and the time step size is set to $\Delta t = 0.05s$ for the calculations.

<table>
<thead>
<tr>
<th></th>
<th>$E$ [Pa]</th>
<th>$\nu$</th>
<th>$\rho_s$ [kg/m$^3$]</th>
<th>$c_s$ [m/s]</th>
<th>$\rho_a$ [kg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>0.3</td>
<td>15</td>
<td>1.0</td>
<td>1.0</td>
<td></td>
</tr>
</tbody>
</table>

TABLE 1 Material properties considered for the structural and acoustic media.

For the first comparison, the calculated sensitivities using both methods are checked against a backward finite difference calculation. To this end, a random design variable contained in a cut element is chosen for investigation. The time step size $\Delta t$ is then held constant and a different number of time steps are utilized to illustrate the effect of the number of time steps on the quality of the calculated sensitivities.

Figure 6 presents the result of the finite difference check comparison for semi and fully discrete adjoint methods. As it can be seen from the figure, the finite difference check for the discrete adjoint method demonstrates the correct first order convergence as the step size for finite difference is decreased. This result was expected since the discrete sensitivity analysis always produces consistent sensitivities where the quality of the gradients does not depend on the utilized time step size or the number of time steps. The correct convergence behavior for the sensitivities calculated using the semi discrete approach on the other hand approached the first order convergence with an increasing the number of time steps.

In addition to finite difference comparison, the sensitivities that are calculated using both methods are numerically compared to each other. To this end, the calculated sensitivities for the design variables located on the lower half of the circular structure are extracted and compared to each other.
FIGURE 6 Finite difference check for validating the calculated sensitivities. Blue color specifies the semi-discrete adjoint method and the black color is the discrete adjoint method. For both methods, dashed lines are 50 time steps, solid lines are 100 time steps and dash-dot lines are 200 time steps.

FIGURE 7 Calculated sensitivities $\frac{d}{du} \Phi$ on the nodes of the mesh which are cut by the zero level set. Blue markers show the semi-discrete sensitivity calculation and black markers illustrate the discrete sensitivity calculation.

The calculation considers 50 time steps for both methods and the result is presented in the figure 7. It can be seen from the figure that sensitivities follow the same trend in magnitude. However, difference becomes more critical at the locations where the calculated gradients change sign. It is seen that the inconsistent gradients produced with semi-discrete approach result in wrong signed sensitivities which would drive the design update in optimization towards the opposite direction. These findings motivate the use of the fully discrete adjoint approach for calculating consistent gradients.

6.2 Benchmark problem comparison

The second example concerns the solution to a benchmark design problem taken from the seminal paper on vibroacoustic topology optimization[24]. The problem deals with the design of an elastic partitioner placed in an acoustic duct under a steady state assumption. The loading is through an incoming plane wave from the left and the duct is terminated with an open boundary to the right, c.f. Figure 8. The goal is to minimize the radiated acoustic pressure in the blue domain shown in the problem sketch. The amplitude of the incident wave is set to $P_{in} = 1$ kPa and a single frequency of $f = 1/\pi$ Hz is used to generate the input signal. The material properties of both structure and acoustic medium can be seen in table 1 and the problem is solved
for a total of 90 s using a time step of $\Delta t = 0.006$ s, i.e. a total of 1500 time steps. The objective function can be written in terms of the absolute acoustic pressure over the considered time span as

$$\Phi = \sum_{n=0}^{N} \left[ \int_{\Omega} |p| \, d\Omega \right] \Delta t$$  \hspace{1cm} (66)

Note, that since the original benchmark problem is posed under a steady state assumption, the initial transient effects are omitted from this example by only summing over the final part of the time span. That is, the objective function calculation starts at the time step $n_0$ corresponding the time 70 s. After this time the system response gets into an approximate steady state region, c.f. the interval between the two red lines in Fig. 9. Moreover, a volume constraint of 65% of the design domain is considered for the optimization. The computational domain is meshed with regular quad elements having the edge length of 0.02 m and the filter radius is set to $\tau = 0.06$ m throughout the optimization.

**FIGURE 8** Schematic illustration of the benchmark example showing the boundary conditions of the optimization problem. Gray color shows the design domain and blue color illustrates the region where the objective function is evaluated.

**FIGURE 9** Averaged transmitted acoustic pressure calculated at the objective region. Blue lines is the initial design, black line is the optimized design, the vertical red lines illustrate the time span where the objective is calculated.

Figures 10 a and 10 b present the initial guess supplied to the optimization and the optimized design, respectively. As it can be seen from the figure, the optimized design realizes approximately 53.4% performance increase compared to the initial guess where the previously reported “hour glass” shape is obtained.
Figure 9 compares the transient response of the volume averaged acoustic pressure over the objective calculation domain for the initial guess and the optimized design. The reported performance increase is also apparent from the figure in which the peaks of the transmitted acoustic pressure are approximately halved for the optimized design throughout the considered time span.

Moreover, Figure 11 shows the transient acoustic pressure response (figure 11 a) given in sound pressure level (SPL) [dB], and the corresponding scaled structural deformation (figure 11 b) at the last time step. Here, the SPL is calculated as

\[
\text{SPL} = 20 \log_{10} \left[ \frac{|p(t)|}{2 \times 10^{-5}} \right] \quad \text{[dB]}
\]  

As it can be seen from Figure 11 b the structure is designed such that only the left-most bar is excited by the plane wave and hence the majority of the acoustic signal is reflected towards to inlet in order to minimize the transmitted downstream acoustic pressure.
6.3 | Acoustic pulse shaping

Having verified both sensitivities and the proposed transient optimization framework on a benchmark problem, the remainder of
the paper is devoted to the design of vibroacoustic devices that utilizes the temporal problem formulation. To this end, a pulse
shaping design problem inspired by the 1D counterpart from\textsuperscript{15} is employed and extended to 2D using both point and averaged
line objectives.

6.3.1 | Pulse shaping at a point

The first example considers the design of a structure where the transmitted acoustic pressure pulse at a specified point is to be
fitted to a desired pulse shape after passing through a structural partitioner. Since the present case deals with the shape of the
acoustic pulse rather than the specific pressure oscillations, the calculation of the pulse shape has been done through an envelope
extraction of the recorded signal.

![Image of an example acoustic pulse showing the original signal, its Hilbert transform and the extracted envelope.]

**FIGURE 12** An example acoustic pulse showing the original signal, its Hilbert transform and the extracted envelope.

![Image of a schematic illustration of the optimization case for acoustic pulse shaping at a point showing the boundary conditions of the optimization problem. Top red line specifies the symmetry plane and gray color shows the design domain. Input acoustic pulse and the desired pulse shape at the specified point are also shown.]

**FIGURE 13** Schematic illustration of the optimization case for acoustic pulse shaping at a point showing the boundary conditions of the optimization problem. Top red line specifies the symmetry plane and gray color shows the design domain. Input acoustic pulse and the desired pulse shape at the specified point are also shown.

For a single frequency modulated signal, extracting the envelope information in topology optimization has been done in\textsuperscript{48}. However, the current work utilizes the approach presented in\textsuperscript{15} in which the Hilbert is applied to transform and extract the envelope information. This way, the envelope of any signal containing a broad range of frequencies can be calculated. Figure
design configurations (14 a and 14 c, respectively) shows that the optimization only changes the shape of the cavities present in the acoustic pulse. Comparing the initial and the optimized designs, it is clear that the acoustic pulse shape follows closely the desired envelope shape. The poor performance is also evident from the objective measure which is very low, i.e., \( \Phi^* = 0.00448\% \).

The overall calculation is chosen as \( 2 \times 10^{-3} \) s. The Rayleigh parameters are assumed to be \( \alpha_1 = 1600 \pi \text{ rad/s} \) and \( \omega_2 = 2200 \pi \text{ rad/s} \). For modeling and the subsequent optimization, the time step size is set to \( \Delta t = 2 \times 10^{-5} \) s. The material and its first and second time derivatives due to the Newmark algorithm. The derivation of adjoint source term \( \Phi^{-\Delta} \) is described in details in Table 2.

The objective function uses a least squares type formulation in order to minimize the difference between the calculated and the desired pulse shape as:

\[
\Phi = \sum_{i=1}^{N} \left[ (e^*)_i^2 - (f^*)_i^2 \right] \Delta t
\]

where \( f(t) \) is the desired envelope shape. The above terms are squared in order to avoid division by zero when calculating the adjoint source \( \Phi^{-\Delta} \) which is due to \( \Phi^{-\Delta} = 0 \) at the start of the calculations. Here the vector \( \mathbf{U} \) in \( \Phi^{-\Delta} \) is given in the Eq. 43 which contains the solution vector \( \mathbf{v} = [\mathbf{u}, \mathbf{p}]^T \) and its first and second time derivatives due to the Newmark algorithm. The derivation of \( \Phi^{-\Delta} \) is described in details in Table 2.

The reported objective values are given in a normalized form in order to better assess the performance of the designs as:

\[
\Phi^* = \frac{\Phi}{\sum_{i=1}^{N} (f^*)_i^2 \Delta t}
\]

Figures 14 a and 14 c shows the initial guess and the optimized designs, respectively. It can be seen from Figure 14 b that the incoming acoustic pulse is completely smeared out after passing through the initial design configuration. The transmitted signal can be seen to have an almost constant envelope shape, although slowly attenuating, after it first hits the measurement point. The poor performance is also evident from the objective measure which very low, i.e., \( \Phi^* = 0.9258 \).

The table shows the material properties considered for the structural and acoustic domains.

<table>
<thead>
<tr>
<th>( E ) [Pa]</th>
<th>( \nu )</th>
<th>( \rho_s ) [kg/m(^2)]</th>
<th>( c_s ) [m/s]</th>
<th>( \rho_a ) [kg/m(^2)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 \times 10^6</td>
<td>0.4</td>
<td>1000</td>
<td>1.21</td>
<td>343</td>
</tr>
</tbody>
</table>

The optimized design, on the other hand, realizes an objective of \( \Phi^* = 0.00448\% \) and by visual inspection of figure 14 d, it is clear that the acoustic pulse shape follows closely the desired envelope shape. Comparing the initial and the optimized design configurations (14 a and 14 c, respectively) shows that the optimization only changes the shape of the cavities present.
in the initial design which clearly illustrates a strong initial guess dependency of the level set based shape optimization method. The limited design change throughout the optimization and the resulting performance increase for the optimized design, also indicates that the coupled vibroacoustic performance in a point is quite sensitive to small design variations. This also points to the fact that tailoring the response in a point seems to be an easy optimization problem as well.

In summary, the result in Figure 14 shows that the proposed optimization setup can successfully tailor the transient response of the coupled system in a point. Furthermore, inspecting a snapshot of the acoustic SPL at time 0.007s, as shown in Figure 15, reveals that the vibroacoustic interaction caused by the shape of the optimized design, focuses the transmitted acoustic wave towards to middle of the channel where the acoustic response is measured. Note that the selected snapshot corresponds to the time of the second peak of the desired envelope shape.

It should be noted that if the optimized design is analyzed using a stiffer material, the envelope fitting is completely lost and hence that the chosen structure indeed utilizes the vibroacoustic coupling to achieve the desired performance. Finally, it is important to stress that the optimized design is quite sensitive to boundary variations, or defects, and hence that a geometric robust approach should be included when considering fabrication. This could, as already mentioned, be done by e.g. the robust level set approach of [32], but is deemed outside the scope of this manuscript.
6.3.2 Pulse shaping over a line

The last numerical example extends the pulse shaping problem from a point objective to an objective given as the average over a line. This is considered to be a harder optimization problem as the optimizer can no longer focus the acoustic energy at a point, but must match the target shape over the entire line in question. Hence, the envelope calculation has to be modified to accommodate the new objective, i.e.

\[ e(t) = \sqrt{\langle p \rangle_{\text{out}}^2 + \langle \hat{p} \rangle_{\text{out}}^2} \]

where \( \langle p \rangle_{\text{out}} \) is the acoustic pressure signal averaged over the outlet boundary for at each time step and \( \langle \hat{p} \rangle_{\text{out}} \) is its Hilbert transformed counterpart. The averaging is simply calculated as

\[ \langle p \rangle_{\text{out}} = \frac{\int_{\Gamma_{\text{out}}} p(t) \, d\Gamma}{\int_{\Gamma_{\text{out}}} \, d\Gamma} \]

\[ \langle \hat{p} \rangle_{\text{out}} = \frac{\int_{\Gamma_{\text{out}}} \hat{p}(t) \, d\Gamma}{\int_{\Gamma_{\text{out}}} \, d\Gamma} \]

FIGURE 15 Sound pressure level [dB] contours of the optimized design for the first pulse shaping example. The given pressure field is from the time 0.007 s.

FIGURE 16 Schematic illustration of the optimization case for acoustic pulse shaping at the outlet showing the boundary conditions of the optimization problem. Top red line specifies the symmetry plane and gray color shows the design domain. Input acoustic pulse and the desired pulse shape at the outlet are also shown.
The modified pulse shaping design problem is illustrated in Figure 16 in which the line used for the pressure averaging has been highlighted. The pulse excitation, number of time steps, total time, discretization, material and damping parameters, as well as the boundary conditions remain the same as those used in the previous design case.

This also goes for the objective function, however, in order to account for the pressure averaging, the adjoint source term is modified as

$$\frac{\partial \Phi}{\partial U} = \frac{\partial \Phi}{\partial (U)}$$

(75)

where the first term on the right hand side concerns the derivative of the Hilbert transform operation wrt the averaged acoustic pressure and second the term, i.e. $\frac{\partial (U)}{\partial \Phi}$, deals with the averaging operation.

The initial configuration together with the optimized design can be seen in Figures 17 a and 17 c, respectively. Inspecting the initial configuration and its corresponding envelope measured at the outlet boundary, c.f. Figure 17 b, makes it clear that the signal is almost killed (in an average sense) when reaching the outlet after the initial pulse has passed. This is contrary to that observed for the point objective and is due to internal reflections in the initial structure resulting in highly non-uniform

FIGURE 17 Optimization for acoustic pulse shaping at the outlet. (a) Initial configuration $\Phi^* = 0.9945$. (b) Calculated acoustic pulse shape with the initial configuration, black line is the desired pulse shape and blue line is the calculated pulse shape. (c) Optimized design $\Phi^* = 0.0045$. (d) Calculated acoustic pulse shape with the optimized design, black line is the desired pulse shape and blue line is the calculated pulse shape.

The initial configuration together with the optimized design can be seen in Figures 17 a and 17 c, respectively. Inspecting the initial configuration and its corresponding envelope measured at the outlet boundary, c.f. Figure 17 b, makes it clear that the signal is almost killed (in an average sense) when reaching the outlet after the initial pulse has passed. This is contrary to that observed for the point objective and is due to internal reflections in the initial structure resulting in highly non-uniform
wave pattern reaching the outlet boundary. This is also evident in the initial objective value which is \( \Phi^* = 0.9945 \). Again, the optimization process is capable of producing a design with a good fit to the desired pulse, c.f. Figure 17 d. This is also clear from the objective value of the optimized design which reaches \( \Phi^* = 0.0045 \). More surprisingly is the topological change observed in the optimized design compared to the initial configuration. That is, the initial configuration has a total of 45 holes including those that touch the top and bottom boundary. On the other hand, the optimized has a total of 47 holes and has in general undergone a more noticeable topological change compared to that of the point objective problem. As no hole generation scheme is included in the presented work, the new holes are a consequence of the existing holes having merged at an early point in the process to form large holes. The boundaries of these larger holes then subsequently meet at multiple points which leads to the topological change. It is also worth to mention that the central half-circular holes at the top and bottom boundary has moved away from the interface and thus also resulted in a topology change. Finally, it also seen that two very small holes remain in the optimized design. However, by inspecting the SPL field plot in Figure 18 it is seen that the intensity in these holes are negligible and hence, they have no significant influence on the performance of the pulse shaping device.

A couple of common observation are valid for both point and line objective formulations of the pulse shaping problem. First, it is clear from the results that neither of the designs are capable of delaying the pulse impact on measurement point/line. That is, from the transmission graphs in Figures 14 b, 14 d 17 b and 17 d it is seen that the initial impact of the acoustic pressure occurs at the same time for both initial and optimized configurations. Based on the findings of\(^15\) it is expected that a significantly wider design domain capable of representing multiple repeated Bragg gratings would be able to delay the impact of the pulse. However, this would require a much larger numerical model for which more efficient solution strategies have to be employed for an efficient solution. Secondly, it is also clear that the used objective measure favours to match the target envelope at the peaks and not at the side lobes. This can again be related to the design domain size in the sense that multiple reflecting surfaces would be necessary to efficiently reflect the input signal such that the transmitted signal would die out after desired target envelope time has passed.

![FIGURE 18](image_url) Sound pressure level [dB] contours of the optimized design for the second pulse shaping example. The given pressure field is from the time 0.007 [s].

### 7 CONCLUSIONS

The article presents a generalized shape optimization problem for transient vibroacoustic problems. The work utilizes an explicit level set approach where the nodal level set values are directly linked to the mathematical design variables to allow for the use of efficient nonlinear programming tools e.g. the (MMA) algorithm. Instead of following the classical level set approach in which the re-meshing is commonly done to capture the design for carrying out the analysis, the current work employs an
immersed boundary cut element method which operates on a fixed background mesh. Using this method, complex geometries can be accurately modelled for strongly coupled physics such as acoustic mechanical interaction problems. To accurately model the coupling interface between the two physics, the cut element method uses a special integration scheme without adding extra degrees of freedom to the system. Therefore the method can be included into existing parallel FEM frameworks with minimal effort on the development. For the optimization, the discrete adjoint method is utilized for calculating the gradients of the objective and constraint functions. Overall the derivation of the discrete adjoint method has been done considering the utilized time integration scheme which is the Newmark algorithm. However, the approach can readily be applied for any other time integration scheme since the derivation is given in discrete residual form. The considered numerical examples starts with the validation of the calculated sensitivities within the discrete adjoint approach. The example compares the calculated sensitivities considering a test problem where the discrete and commonly used semi-discrete methods are compared. It is illustrated that the quality of the calculated gradients using the semi-discrete approach depends on the number of time steps used for the forward model and the adjoint equation. It is shown for an extreme case, the semi-discrete approach can lead to wrong signed sensitivities because of inconsistencies in this approach. The fully discrete approach, on the other hand, always produces consistent sensitivities. The developed transient framework is then employed on a benchmark problem which deals with designing of an elastic partitioner in order to reduce the transmitted acoustic pressure. For time-harmonic topology optimization of vibroacoustic problems, the problem has been introduced in 24. By using a transient inlet sinusoidal acoustic plane wave and optimizing after the initial transient effects have passed, the previously reported "hour-glass" shaped structure is obtained. A transient application concerning the design of an acoustic pulse shaping device is considered to demonstrate the tailoring of an acoustic reading at a specified point. The structure is subjected to an incoming acoustic wave packet consisting of frequencies between 1000 Hz and 3000 Hz. The envelope of the transmitted acoustic pressure at the specified point is then calculated and fitted to a predefined shape. Compared to the initial configuration, the optimization realizes a 99.5% performance increase. The same problem setup is then modified to the tailoring of an envelope shape of the transmitted acoustic pressure averaged over a line. The optimized design shows a similar performance increase and has a final objective close to zero. More interestingly, the design obtained using the line objective also reveals significant topological changes. That is, the initial configuration has 45 holes whereas the optimized shape has 47. This is possible due to the versatility of the used level approach, which, to a large extend is based on ideas from density based topology optimization. Finally, the presented work will open the way for the optimization of complex transient signals containing broad frequency content as well as broadband filter applications for vibroacoustic problems.

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REFERENCES


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Transient shape optimization of vibroacoustic problems for broadband filter designs using cut elements
Abstract
The focus of this article is on generalized shape optimization of transient vibroacoustic problems. The goal is to demonstrate a transient problem formulation that allows to optimize for wide range of frequency content for complex signals which are often of interest in industry. The work employs time domain methods to realize wideband optimization in the frequency domain. To this end, the objective function is defined in frequency domain where the frequency response of the system is obtained through a fast Fourier transform (FFT) algorithm on the transient response of the system. The work utilizes a level set approach to implicitly define the geometry in which the zero level describes the interface between acoustic and structural domains. A cut element method is used in order to capture the geometry on a fixed background mesh by utilization of an special integration scheme to accurately resolve the interface. This allows for accurate solutions to strongly coupled vibroacoustic systems without having to re-mesh at each design update. Present work uses the so called explicit level set approach where the nodal level set values are used as design variables in order to use efficient gradient based optimizers. The discrete adjoint method is used to calculate the gradients of objective and constraint functions. A thorough explanation of the consistent sensitivity calculation is given involving the FFT operation which is needed to define the objective function in frequency domain. Moreover, the developed framework is applied to various vibroacoustic filter designs.

Keywords: Vibroacoustics, Cut finite elements, Immersed boundary methods, Transient optimization, Level set methods, Shape optimization

1. Introduction

Topology optimization [1] is a numerical method to determine optimal material distributions that minimizes a given performance criteria under a set of constraint. The method has gained increasing popularity across many areas in both research and industry since it allows for innovative designs through the free material distribution. Considerable number of studies on topology optimization paved the way for giga scale structural optimization for static problems [2]. The method has also been applied to the optimization of fluid systems [3, 4] as well as several multi-physics applications [5, 6, 7]. Considering dynamics, after the introduction of the adjoint method for transient problems [8, 9] examples of topology optimization under transient loadings can be found in the works of [10, 11, 12]. Moreover, optimizing for complex signals containing wide range of frequency content is usually of great interest in industry i.e optimizing a part of the hearing aid device that is usually subject to a good performance expectancy for a wide frequency window.

*Corresponding author
Email addresses: cedil@mek.dtu.dk (Cetin B. Dilgen), naage@mek.dtu.dk (Niels Aage)
Commonly, frequency domain modelling and optimization only deals with discrete frequencies which are usually selected from a limited window of the frequency band. Optimization can quickly become excessively expensive when many frequencies are considered in order to widen the zone of influence of optimization on the frequency response of the system. Examples of topology optimization in frequency domain can be found considering eigenvalue problems [13], optics [14], acoustics [15, 16, 17] and vibroacoustics [18]. Transient problem formulation is a promising alternative to address this issue since the optimization can be carried out using a complex and compact signal that contains broad range of frequencies. This idea can be seen in the works of [19, 20, 21] where a proper time-domain input pulse is selected to excite a broad frequency range in order to carry out transient topology optimization of antennas. However, this approach still does not provide the full control on the broad-band response in the frequency domain. This is because the objective function is defined in the time domain and the optimization only indirectly effects the frequency content of the signal that is being optimized.

Although density based topology optimization provides the most design freedom for optimization, there are issues exist for multi-physics problems that are strongly coupled through the interface. Main reasons for this can be listed as the lack of physical interpretation of the gray areas and the stair-case (pixelized) boundary description. Generally, strongly coupled problems, i.e vibroacoustics, require accurate modelling of the interface in order to correctly capture and model the interactions between the two physics. As an alternative to realize a generalized optimization framework suitable for coupled multi-physics problems, level set based methods [22] show great promise. The method implicitly defines the geometry, hence the interface by the zero level contour. However, when the method is used with an ersatz material approach [23], meaning the level set function is mapped onto a piece-wise constant density field and the interface is represented with an interpolated gray area, the level set method also suffers the same drawbacks as the topology optimization for coupled problems. The geometry defined by the zero level of the level set function can also be captured with body fitted meshes [24], i.e. classical level set approach, in which a very accurate modelling of the coupled physics can be realized depending on the quality of the elements along the re-meshed interface. This approach commonly uses the solution of a Hamilton-Jacobi type equation to update the design by moving the interface based on the calculated shape sensitivities. However, due to the re-meshing operation at each design iteration, the approach is not suitable for general parallel frameworks. Moreover, numerical noise may be introduced on the sensitivities due to the extrapolation from the fitted mesh onto the background mesh. Examples of classical level set approach for the optimization of vibroacoustic systems can be found in [25, 26, 27]. A detailed comparative review of density, level set and evolutionary based optimization methods for vibroacoustics can be found in the work of [28].

Cumbersome re-meshing operation can be avoided when the level set approach is coupled with immersed boundary methods [29] to capture the geometry. The present work utilizes an immersed boundary cut element method to model the exact boundary represented by the zero level of the level set function. Throughout the optimization, a fixed mesh is used and the method allows the elements to be cut by the interface boundary. Accurate modelling of the interface in the cut elements is realized through a special integration scheme used on the cut elements. The employed cut element method can be categorized as a special (simplified) case of CutFEM without stabilization [30], finite cell method [31] or X-FEM without enrichment [32]. For the optimization, the utilized cut element method is coupled with the so-called explicit level set approach [33, 34] in which the nodal level set values are directly tied to the mathematical design variables. This approach enables the utilization of nonlinear programming tools, such as the method of moving asymptotes (MMA) algorithm [45] that is used in the current work, and in turn allows for general optimization frameworks where multiple objective and constraint functions can easily be considered for the optimization.

The current work focuses on generalized shape optimization of transient vibroacoustic problems where a transient problem formulation that allows to realize wideband optimization in frequency domain is demonstrated. Throughout the work, the frequency response of the coupled vibroacoustic system is obtained through a fast Fourier transform (FFT) algorithm applied to the transient response of the system. This allows the objective function to be defined in frequency domain where the optimization can directly tailor the response of the coupled system. To the best of the authors' knowledge, utilization of time-domain methods to realize wideband optimization in frequency domain have not been demonstrated before for generalized shape optimization frameworks where multiple objective and constraint functions can easily be considered for the optimization.
optimization of strongly coupled vibroacoustic problems. Moreover, the work utilizes the discrete adjoint method for calculating the gradients of the objective function. A thorough explanation of the consistent sensitivity calculation through the discrete adjoint framework that involves the FFT operation, which is needed to define the objective function in frequency domain, is also among the contributions of the present work.

The current paper is organized as follows: The utilized governing equations for the coupled vibroacoustic system together with the spatial and temporal discretization aspects are introduced in section 2. Section 3 introduces the geometry description and the cut element method. The design parameterization used for the optimization is described in section 4. The optimization problem as well as the sensitivity analysis using the discrete adjoint method are introduced in section 5. Section 6 describes the numerical setup that is used for the considered examples throughout the work. The numerical examples are presented in section 7 where the developed framework is applied for the optimization of various vibroacoustic filter designs.

2. Governing equations

This section describes the governing equations that are used throughout the work. For the considered vibroacoustic systems, the structural response is defined with the elasticity equation and the solution of the acoustic pressure is obtained with the Helmholtz equation. In order to realize an efficient parallel modelling and optimization framework, the work utilizes a cut element method in which the solutions to both physics are obtained in the entire computational domain $\Omega$. Computational domain consists of both structural and acoustic domains as

$$\Omega = \Omega_s \cup \Omega_a$$

where $\Omega_a$ is the acoustic domain and $\Omega_s$ is the structure that is embedded in $\Omega$. In order to solve both physics in the total domain $\Omega$, a fictitious domain approach is employed. For the structure, a void phase is defined in the acoustic region $\Omega_a$ where its solution is obtained through modifying the material properties of the solid. For the solution of the acoustic pressure in its fictitious domain (structural domain $\Omega_s$), a rigid phase is defined with again modifying the material properties of the acoustic medium. Since the work deals with strongly coupled vibroacoustic systems, correct definition of the interface boundaries and the application of the coupling condition between the two physics are imperative to obtain accurate solutions. Coupling between the two physics is then realized along the interface $\Gamma_{sa}$. The cut element method allows the elements to be cut by the interface boundary $\Gamma_{sa}$. A special integration scheme is used in the cut elements to model the unfitted interface and the coupling condition between the two physics which will be introduced in the subsequent section 3.1.

The developed framework deals with a transient problem formulation that allows to optimize for wide range of frequencies. To this end, coupled vibroacoustic system will be modelled in time-domain where the system will be excited using a signal that contains broad range of frequencies. For optimization, the frequency response of the chosen performance criteria will be extracted using a FFT algorithm on its transient response. To this end, considering a transient motion, the linear elasticity equation governing the structure response is written as

$$\rho_s \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \mathbf{\sigma} + \rho_s \alpha_d \frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \left( \beta \frac{\partial \mathbf{\sigma}}{\partial t} \right) = 0 \quad \text{in} \quad \Omega$$

$$\mathbf{u} = 0 \quad \text{on} \quad \Gamma_{sd}$$

$$\mathbf{n}_s \cdot \mathbf{\sigma} = 0 \quad \text{on} \quad \Gamma_{sn}$$

$$\mathbf{n}_a \cdot \mathbf{\sigma} = p \mathbf{n}_a \quad \text{on} \quad \Gamma_{sa}$$

where $\mathbf{u}$ is the displacement vector, $p$ is the acoustic pressure, $\rho_s$ is the density of the solid, $\mathbf{n}_s$ is the normal vector pointing outwards from the acoustic region likewise $\mathbf{n}_a$ is the normal vector defined at the interface pointing outwards from the structural domain. In order to reflect the loss mechanism, the work also considers structural damping using the Rayleigh damping where $\alpha_d$ and $\beta_d$ are called Rayleigh damping parameters. Furthermore, Cauchy stress vector $\mathbf{\sigma}$ is defined as $\mathbf{\sigma} = \mathcal{C} (\mathbf{E}, \nu) \mathbf{\epsilon}$ in which the constitutive...
matrix $\mathbf{C}(E_s, \nu)$ is a function of the Young’s modulus $E_s$ and the Poisson’s ratio $\nu$ and the strain vector is defined as $\mathbf{e} = \begin{bmatrix} \frac{\partial u_1}{\partial x} & \frac{\partial u_1}{\partial y} & \frac{\partial u_2}{\partial x} & + & \frac{\partial u_2}{\partial y} \end{bmatrix}^T$. Moreover, equation 3 defines the fully clamped condition for the structure, equation 4 specifies the traction free boundary condition and the coupling to the acoustic medium is realized through the boundary condition given in equation 5. For calculating the transient response of the structure both in structural domain and in its void phase (acoustic domain), the material properties of the solid are altered as

$$E_s = \alpha \tilde{E}_s, \quad \rho_s = \alpha \tilde{\rho}_s,$$

(6)

where the tilde superscript specifies the original material properties and the parameter $\alpha$ is a dimensionless contrast parameter that is unity for the structural domain and taken as $10^{-8}$ for the void phase of the structure. The acoustic pressure on the other hand is governed by the transient Helmholtz equation which is written as

$$\frac{1}{K_a} \frac{\partial^2 p}{\partial t^2} - \frac{1}{\rho_a} \nabla^2 p = 0 \quad \text{in} \quad \Omega$$

(7)

$$\mathbf{n}_a \cdot \nabla p = 0 \quad \text{on} \quad \Gamma_{ad}$$

(8)

$$\mathbf{n}_a \cdot \nabla p = \rho_a \frac{\partial^2 (\mathbf{n}_a \cdot \mathbf{u})}{\partial t^2} \quad \text{on} \quad \Gamma_{as}$$

(9)

$$\mathbf{n}_a \cdot \nabla p + \frac{1}{c_a} \frac{\partial p}{\partial t} = \frac{2}{c_a} \frac{\partial p_{in}}{\partial t} \quad \text{on} \quad \Gamma_{ar}$$

(10)

where $\rho_a$ is the density of the acoustic medium, $c_a$ is the speed of sound in the acoustic medium. The bulk modulus $K_a$ for the acoustic domain is defined as $K_a = \rho_a c_a^2$. The boundary conditions that are used in the current work for the transient acoustic pressure solution are hard wall condition given in equation 8, coupling boundary condition for the acoustic domain written in equation 9 and the absorbing boundary condition given in equation 10. The absorbing boundary condition is written with a plane wave radiation where $p_{in}$ denotes the transient incoming acoustic wave. Similar to the structural equation, transient response of the acoustic pressure both in the acoustic domain and its rigid phase (structural domain) is calculated by changing the properties of the acoustic medium as

$$K_a = \frac{\tilde{K}_a}{\alpha}, \quad \rho_a = \frac{\tilde{\rho}_a}{\alpha}$$

(11)

Similarly, the dimensionless contrast parameter $\alpha$ takes the values of unity for the acoustic domain and $10^{-8}$ for the rigid phase of the acoustic solution. The illustration of the resulted coupled acoustic-structure system is given in figure 1 along with the representation of the boundary conditions used throughout the work.

Figure 1: Schematic illustration of the coupled acoustic-structural system. Physical domains, the coupled interface and the boundary conditions are showed.
2.1. Discretization

This section describes the general details of the spatial and temporal discretization for the coupled vibroacoustic system introduced in the previous section. Integration scheme to realize the interface boundary inside the cut elements will be described in section 3.1. Provided details are valid for the elements that are not cut by the interface boundary \( \Gamma \).

For general spatial discretization, standard continuous Galerkin method [36] is employed where the coupled system is multiplied with test functions and integrated over the domain \( \Omega \). Integration by parts is then applied to obtain the weak form. The computational domain is meshed with regular Q-4 elements and time independent linear shape functions are utilized to approximate the continuous variables through which the semi-discrete form of the coupled system is obtained as

\[
M \ddot{v}^n + C \dot{v}^n + K v^n = h^n
\]

where \( M \) is the mass matrix, \( C \) is the damping matrix and \( K \) is the stiffness matrix. The superscript \( n \) in equation 12 denotes the current time step. Solution vector \( v \) and the load vector \( h \) are given as

\[
v = \begin{bmatrix} u \\ p \end{bmatrix}, \quad h = \begin{bmatrix} 0 \\ g \end{bmatrix}
\]

where \( u \) and \( p \) are state vectors for structural displacement and acoustic pressure solutions, respectively. The vector \( g \) denotes the source vector for the acoustic equation which is active when the absorption boundary condition (Eq. 10) is utilized for radiating a plane wave. The weak form of the coupled system and the identification of the individual element matrices given in equation 12 are thoroughly described in [Cetin].

For the temporal discretization, the current work employs an implicit time stepping scheme, namely the Newmark algorithm [37]. The method expresses the first and the second time derivative of the solution vector \( v \) as

\[
\dot{v}^n = a_1 \dot{v}^{n-1} + a_2 \dot{v}^{n-1} + a_3 (v^n - v^{n-1})
\]

\[
\ddot{v}^n = -a_4 \ddot{v}^{n-1} - a_5 \ddot{v}^{n-1} + a_6 (v^n - v^{n-1})
\]

here the parameters \( a_1 \) to \( a_6 \) are called the Newmark parameters. In order to derive the linear system of equations which is solved for finding the solution vector \( v^n \) for the current time \( n \), the definitions given in equations 14 and 15 are substituted into the semi-discrete form of the coupled system (Eq. 12). The resulted equation reads

\[
\hat{K} v^n = \hat{h}^n
\]

where \( \hat{K} \) is the so-called effective stiffness matrix and \( \hat{h}^n \) is the effective load vector which are identified as

\[
\hat{K} = K + a_6 M + a_3 C
\]

\[
\hat{h}^n = h^n + M (a_4 v^{n-1} + a_5 v^{n-1} + a_6 v^{n-1}) + C (-a_1 v^{n-1} - a_2 v^{n-1} + a_3 v^{n-1})
\]

Furthermore, the Newmark parameters are identified as

\[
a_1 = 1 - \frac{\beta}{\bar{\beta}}, \quad a_2 = \left(1 - \frac{\gamma}{2\beta} \right) \Delta t, \quad a_3 = \frac{\gamma}{\bar{\beta} \Delta t}
\]

\[
a_4 = \frac{1}{\beta \Delta t}, \quad a_5 = \frac{1}{2\beta} - 1, \quad a_6 = \frac{1}{\beta \Delta t^2}
\]

where \( \Delta t \) is the time step size. The current work uses a specific family of the Newmark algorithm [38] in which the parameters \( \bar{\beta} \) and \( \bar{\gamma} \) are selected so that the employed time discretization becomes unconditionally stable. \( \beta \) and \( \gamma \) are given as

\[
\bar{\beta} = \frac{1}{4}, \quad \bar{\gamma} = \frac{1}{2}
\]

(21)
The work assumes the initial conditions $v^0$ and $\dot{v}^0$ as zero. The initial condition for the second time derivative of the solution vector $\ddot{v}^0$ is found by setting the $v^0$ and $\dot{v}^0$ to zero in equation 12 and solving the following equation

$$M\ddot{v}^0 = h^0$$  \hspace{1cm} (22)

The implementation for the framework that solves the coupled vibroacoustic system has been done using C++ in which PETSc library [39, 40, 41] is employed for making use of its parallel data management. Moreover, the parallel direct solver MUMPS [42, 43] is utilized for the solution of equation 16.

3. Geometry description

This section describes the utilized geometry description and the cut element method used to treat the elements that are cut by the interface boundary. Throughout the work, the geometry is represented by a scalar valued function $\bar{s}$ called the level set function. In order to identify the acoustic and structure domains embedded in the total computational domain $\Omega$, the following rule is used

- $\bar{s}(x) > 0$, $x \in \Omega_s$ (structural domain)
- $\bar{s}(x) = 0$, $x \in \Gamma_{sa}$ (interface)
- $\bar{s}(x) < 0$, $x \in \Omega_a$ (acoustic domain)

(23)

A robust way of defining or capturing complex geometries is realized using the rule given in equation 23 in which the positive values represent the structural domain and the negative values identify the acoustic domain where the total of structural and acoustic domains forms the whole domain $\Omega$. Here, the zero iso-level of the function $\bar{s}$ captures a clear definition of the interface $\Gamma_{sa}$ between the structural and acoustic domains. This way, the geometry is implicitly represented by the level set function $\bar{s}$ using a fixed background mesh. In general, obtaining an accurate description of the interface $\Gamma_{sa}$ is critical for the accurate modelling when a multi-physics system that is coupled from the interface is considered. Discretely, the level set function $\bar{s}$ is defined directly on the nodes of the computational mesh and represented by linear shape functions. The resulted interface $\Gamma_{sa}$ from the zero iso-level of the level set field is then represented by linear straight curves inside cut elements. An example level set function $\bar{s}$ is given in the figure 2a. The figure identifies the embedded structural and acoustic domains and the resulted interface using the rule given in equation 23.

(a) $\bar{s}(x) > 0$  \hspace{1cm} (b) $\bar{s}(x) = 0$

Figure 2: An example level set function showing the embedded physical domains. (a) shows the rule that is used for specifying different physical domains embedded with the level set function. (b) finite element mesh where white color shows the uncut elements in the acoustic domain, gray color shows the uncut elements in the solid region and the blue color shows the cut elements.
Nodal level set values also provide an appropriate way of identifying the cut elements. To this end, an element based indicator function is introduced to mark each element as cut or uncut element based on their nodal level set values. As an example, if an element’s nodal level set values contain both negative and positive values then this element is marked as a cut element. This situation is visually illustrated in figure 2b where cut elements are identified using the nodal level set values of elements. Furthermore, if an element’s nodal level set values only contain positive values (\( s > 0 \)) then it is marked as uncut solid domain element in \( \Omega_s \). Likewise if all of the nodal level set values are \( s < 0 \), then that particular element is marked as uncut acoustic domain element in \( \Omega_a \). For uncut elements, no special further treatment is done for the discretization of the coupled governing equations (section 2.1) where the integration is carried out using the standard Gaussian quadrature rule considering bilinear quadrilateral (Q-4) elements. As described in section 2, fictitious domain solutions for uncut elements are realized through changing their material properties appropriately.

3.1. Cut element method

This section describes the cut element method which is used for modelling of non-conforming boundaries. The main motivation behind using an immersed boundary method like the cut element method is that it eliminates the expensive operation of re-meshing the interface with conforming elements. Using the method, the exact boundary representation is obtained only by integration in the elements that are cut by the interface. Meaning that the cut element method does not enrich the shape functions and the degrees of freedom of the discrete system remains unchanged. Since the integration that is done in the cut elements is only a local operation, the method can easily be included in an efficient parallel framework.

![Figure 3: Illustration of a sub-cell integration in a cut element. Physical domains are identified in the cut elements where the gray color is the structural domain, white color is the acoustic domain and the blue line is the interface. The figure shows the process of placing the Gauss points on iso-parametric triangle and line elements then mapping the integration points to the reference domain of the parent element for integration.](image)

Cut elements use the Gaussian quadrature rule for weighted integration in order to realize the effect of the partial interface inside the cut elements. Hence, correctly placing the integration points carries importance. After the cut element is identified, a triangulation algorithm is utilized in order to divide the parent element into sub-triangle elements. Here the triangulation is only used to ensure the correct placements of the integration points inside the parent cut element using the sub-triangle elements and the interface line element. The current work uses the marching squares algorithm [44] to carry out the
triangulation which determines the location of the partial interface inside the cut element using the nodal
level set values.

An example cut element can be seen in the figure 3 in which the sub-elements are obtained with tri-
angulation. Nodal level set values are further utilized to mark the sub-elements in order to distinguish
whether they belong to Ωs or Ωa. This information is utilized to correctly set the material properties of
the structural and acoustic domain solutions for both physics inside the cut elements. The illustration of the sub-cell integration process is also given in the figure 3. After the triangulation, firstly the Gauss points are inserted to the sub-triangle element in its reference domain. Gauss points of the iso-parametric triangle sub-element are then mapped to the reference domain of the parent element for integration. As it can be seen from the figure, the final integration only contributes to the degrees of freedom of the parent Quad element through which the original layout of the sparse system matrix is attained throughout the optimization. The final integration uses the Gaussian quadrature rule with the Gauss points that are mapped from the reference domain of the sub-triangle to the reference domain of the parent element. The associated weights for the sub-triangle’s Gauss points are scaled with the factor of $4\frac{\Delta V_T}{\Delta V_Q}$ where $\Delta V_T$ and $\Delta V_Q$ are the volumes of the sub-triangle and the parent quad element, respectively. The factor 4 comes from the area scaling between a triangle and a quad element considering a local coordinate system. Figure 3 also shows the process of integrating along the partial interface in the cut element. The line integration is utilized to implement the coupling boundary conditions given in equations 5 and 9. After the interface boundary line is identified, Gauss points are inserted in the reference domain of an iso-parametric linear line element. Integration points are then mapped to the reference domain of the parent quad element where the integration is carried out. For the illustrated line integration inside the cut element, associated weights for the sub-line element’s Gauss points are directly used in the final integration. For further information on the cut element method and its implementation details, the reader is referred to the works of [45][Cetin, Sumer].

4. Design parameterization

In this section the design variable used for the optimization and the employed design parameterization
for the current work are introduced. Throughout the work the mathematical design variable is denoted
as $s$ and the previously introduced level set function $\bar{s}$ is referred as the physical design variable since the
current design configuration is contained in $\bar{s}$ and the finite element analysis is performed based on that.
The employed design parameterization describes the link between the design variable $s$ and the physical
design variable $\bar{s}$. Similar to $\bar{s}$, the design variable $s$ is also defined on the nodal points of the computational
mesh in which the utilization of the gradient based optimizers can be facilitated for the solution of the
optimization problem. Moreover, the design variable $s$ has the following upper and lower bounds

$$0 \geq s \geq 1 \tag{24}$$

Utilizing the above limits for the design variable $s$ allow the usage of the gradient based optimizers in a
similar way that is employed for the density based topology optimization methods. In order to realize an
implicit limit on the speed at which the zero iso-level can change in one design update, the design variable $s$
is further mapped to the variable $\bar{s}$ which has the upper and lower bounds of the half of the element size as

$$-0.5h_e \geq \bar{s} \geq 0.5h_e \tag{25}$$

In order increase the zone of influence of the design variables for optimization a filtering operation is applied
on $\bar{s}$. The utilization of a filter also stabilizes the optimization with providing a smoother interface boundary
description. The current work employs a filter based on a Helmholtz type differential equation from the
work of [46]. Here it is noted that the filter equation is implemented using the finite volume method in which
the variables are represented as piece-wise constants and stored in cell centers. Due to the finite volume
discretization, solutions obtained from the filter equation are always stable independent of the chosen filter
size. In order to facilitate the filtering operation, the variable ˜s is first interpolated to cell centers. The filter equation is given as

\[ -r^2 \nabla^2 \tilde{s}_c + \tilde{s}_c = \tilde{s}_n \]  

Here \( r \) is filtering radius and the subscript \( c \) specifies the variables that are stored in cell centers. After the filter operation, the solution \( \tilde{s}_c \) is interpolated back to the nodes of the mesh through which the physical design variable \( \tilde{s} \) is obtained. Physical design variable \( \tilde{s} \) holds the current design configuration on which the cut element method is utilized to carry out the finite element analysis in order to obtain the response of the coupled vibroacoustic system. Here it is noted that, since the filter equation is solved in the element centers, the two interpolation operations provide extra filtering effect which is always present even in the case the filter radius \( r \) is set to zero. Unlike the density based topology optimization methods, the utilization of the filter equation does not provide a minimum feature size for the considered framework. Since, the zero iso-

5. Optimization problem

This section describes the general optimization problem which is solved for the optimization of wideband vibroacoustic problems. The coupled system is solved in time domain in order to obtain the transient response of the system. Objective function, which is sought to be minimized, is defined in frequency domain to be able to tailor the specific frequencies present inside the transient response of the system. Objective function uses the state variables defined in frequency domain which are obtained through a FFT operation after the time domain solution is done.

The vectors of state variables and residuals are denoted as \( U^n \) and \( R^n \), respectively. As stated previously, \( n \) specifies the current time step. The vector \( U^n \) contains the solution vector and its first and second time derivatives due to the utilization of the Newmark algorithm for temporal discretization. The vector \( R^n \) holds the corresponding residuals which are written here as

\[
R^n = \begin{bmatrix} r^n_1 \\ r^n_2 \\ r^n_3 \end{bmatrix}, \quad U^n = \begin{bmatrix} \psi^n \\ \dot{\psi}^n \\ \ddot{\psi}^n \end{bmatrix}
\]  

Here the individual residual vectors \( r^n_1, r^n_2 \) and \( r^n_3 \) are identified from the discretized coupled system given in the equations 14 to 18

\[
\begin{align*}
r^n_1 &= [K + a_0M + a_3C] \psi^n - \left([a_0M + a_3C] \psi^{n-1} - [a_2M - a_1C] \psi^{n-1} + [a_2C - a_3M] \psi^{n-1} - h^n \right) \\
r^n_2 &= \ddot{\psi}^n - a_1 \dot{\psi}^{n-1} - a_2 \psi^{n-1} - a_3 \left[ \psi^n - \psi^{n-1} \right] \\
r^n_3 &= \dddot{\psi}^n + a_4 \ddot{\psi}^{n-1} + a_5 \dot{\psi}^{n-1} - a_6 \left[ \psi^n - \psi^{n-1} \right]
\end{align*}
\]

Moreover, the generic optimization problem that is considered for the current work has the following form

\[
\min \Phi = \sum_{m=0}^{M} \psi^{m}(U^m(\tilde{s}))
\]  

s.t. \( R^n(\tilde{s}, U^n(\tilde{s})) = 0 \), for \( n = 0, 1, \ldots, N \)  

\[
s_{\min} \leq \tilde{s} \leq s_{\max}
\]  

\[
\psi_i \leq 0
\]  

where \( \Phi \) is the objective function defined in frequency domain, \( N \) is the total number of time steps, \( M \) is the total number of discrete frequencies that is considered in objective function. \( U^m_\psi \) is the vector of state
variables in frequency domain that is obtained via FFT applied on the solution $U^n$. Here it is noted that due to the FFT operation, the state vector in frequency domain $U^m_f$ consists of complex numbers. Discretely, length of the vectors $U$ and $U_f$ are equal to each other. Formally, the discrete Fourier transform is defined as

$$U^m_f = \sum_{n=0}^{N-1} U^n e^{-\frac{i 2 \pi n m}{N}}$$

(35)

where $i$ is the imaginary unit defined as $i = \sqrt{-1}$. Moreover, $\psi_i$ denotes additional constraint functions considered for the optimization. The vector of design variables is denoted as $s$ where $s_{min}$ and $s_{max}$ are its lower and upper bounds (Eq. 24) which are set as 0 and 1, respectively. The vector of physical design variables $\bar{s}$ is utilized for calculating the response of the coupled system as seen from the equation 32 and it contains the current topology for the optimization. The link between $s$ and $\bar{s}$ is explained in section 4 and the resulted chain rule that is used to obtain the gradient of the objective function $\Phi$ with respect to design variables $s$ will be explained in the following section 5.1.

The optimization problem stated in equations 31 to 34 is solved employing the method of moving asymptotes (MMA) algorithm [35]. Specifically, the present work includes the method’s parallel PETSc implementation from [47] into the developed framework.

5.1. Sensitivity analysis

This section describes the sensitivity analysis considering the objective function given in equation 28. The objective function is defined in frequency domain. Since the modelling is done in time domain, the sensitivity analysis also considers the transformation from time domain to frequency domain via the utilized FFT operation. The current work uses the FFTW library [48] for computing the discrete Fourier transform of the transient response of the coupled system.

A common trend in time dependent sensitivity analysis is to use the so called semi-discrete adjoint approach in which the problem is considered discrete in space but continuous in time. However, the semi-discrete approach is not suitable for cases where the objective function is defined in frequency domain. This is because the semi-discrete approach derives the adjoint equation assuming the objective function is defined in time domain. This means that using a discrete FFT cannot be incorporated within the semi-discrete approach. Recently in the work of [Cetin], it has also been shown that even for pure transient optimization problems, the semi-discrete method may not produce consistent sensitivities which can result in gradients having wrong signs. Hence, for calculating consistent and exact sensitivities, the work utilizes a fully discrete sensitivity analysis for calculating the gradient of the objective function with respect to the design variable.

In order to carry out the discrete sensitivity analysis, firstly the objective function is augmented with using a vector of Lagrangian multipliers $\Lambda$. Lagrangian function $\mathcal{L}$ reads as

$$\mathcal{L} = \Phi (U_f(U(\bar{s}))) + \sum_{n=0}^{N} \Lambda^n R^n(\bar{s}, U^n(\bar{s}))$$

(36)

The objective function is written as a function of the state variables in frequency domain $U_f$ which is an explicit function of the transient state variables $U$. State variables are in turn an implicit function of the physical design variables $\bar{s}$. Here the Lagrangian function $\mathcal{L}$ equals to the original objective function $\Phi$ since for each time step the residual of the coupled system is satisfied $R^n = 0$. Due to the Newmark algorithm, similar to the state variables, the vector of Lagrangian multipliers also consists of three fields as

$$\Lambda^n = \begin{bmatrix} \Lambda^n \\ \dot{\Lambda} \\ \ddot{\Lambda} \end{bmatrix}$$

(37)
The derivative of the Lagrangian function with respect to the physical design variable $\bar{s}$ is written as

$$\frac{dL}{ds} = \sum_{n=0}^{N} \left( \frac{\partial \Phi}{\partial U_f} \frac{\partial U^n}{\partial s} \right)^n \frac{\partial U^n}{\partial s} + \Lambda^n \left[ \frac{\partial R^n}{\partial s} + \frac{\partial R^n}{\partial U^n} \frac{\partial U^n}{\partial s} \right]$$

(38)

The term $\left( \frac{\partial \Phi}{\partial U_f} \frac{\partial U^n}{\partial s} \right)^n$ on the right hand side of the equation 38 constitutes the partial derivative of the objective function with respect to the transient state variable $\frac{\partial \Phi}{\partial U^n}$ which also contains the chain rule describing the connection between frequency and time domain. In order to calculate $\frac{\partial \Phi}{\partial U^n}$, firstly the term $\frac{\partial \Phi}{\partial U_f}$ is calculated. Since $U_f$ consists of complex numbers defined in frequency domain, the partial derivative $\frac{\partial \Phi}{\partial U_f}$ also consists of complex numbers which is realized as

$$\frac{\partial \Phi}{\partial U_f} = \frac{\partial \Phi}{\partial U_f^r} + i \frac{\partial \Phi}{\partial U_f^i}$$

(39)

where the subscripts $r$ and $i$ denote the real and imaginary parts of a complex number. The term $\frac{\partial U_f}{\partial U}$ links the frequency domain to time domain. Since the applied discrete Fourier transform operation can be seen as a linear transformation, the partial derivative $\frac{\partial U_f}{\partial U}$ describes the discrete Fourier transform operation itself. Hence, the partial derivative of the objective function with respect to the transient state variable $\frac{\partial \Phi}{\partial U^n}$ is rewritten as

$$\frac{\partial \Phi^n}{\partial U} = \left( \frac{\partial U_j^T}{\partial U^n} \frac{\partial \Phi}{\partial U_f} \right)^n$$

(40)

where $\frac{\partial U_j^T}{\partial U^n}$ is the inverse discrete Fourier transform operation. Order of operations in equation 40 are written as: Firstly the calculation of the partial derivative $\frac{\partial \Phi}{\partial U_f}$ is done, then the inverse discrete Fourier transform operation is applied on it to calculate $\frac{\partial \Phi}{\partial U^n}$ which is defined in time domain.

Having introduced the chain rule describing the link between frequency and time domains, in order to continue the sensitivity analysis, the derivative of the Lagrangian function with respect to the physical design variable (Eq. 38) is rewritten as

$$\frac{dL}{ds} = \sum_{n=0}^{N} \Lambda^n \left[ \frac{\partial R^n}{\partial s} + \frac{\partial R^n}{\partial U^n} \frac{\partial U^n}{\partial s} \right]$$

(41)

Using the fact that the Lagrangian vector can be freely chosen, the underlined part in the above equation is set to zero to prevent the calculation of the partial derivative $\frac{\partial \Phi}{\partial U^n}$. This gives rise to the adjoint equation

$$\frac{\partial R^T}{\partial U} \Lambda = -\frac{\partial \phi}{\partial U}$$

(42)

where the superscript $n$ notation is dropped in order to illustrate that the adjoint equation written in equation 42 contains the all time steps considered in the given problem. The partial derivative of the residual vector with respect to the state variables $\frac{\partial R}{\partial U}$ has the following general form

$$\frac{\partial R}{\partial U} = \begin{bmatrix}
A_0^n \\
B_0^n \\
A_1^n \\
B_1^n \\
\vdots \\
A_{N-1}^{N-2} \\
B_{N-1}^{N-2} \\
A_N^{N-1} \\
B_N^{N-1} \\
A_N^n
\end{bmatrix}$$

(43)
Here, the subscripts show the current time step and the superscripts denote the corresponding state variables. Sub-matrices in \( \frac{\partial}{\partial U} \) written in general form considering a time integration scheme that depends on the current time step and one previous time step in which the residual function for a time step \( n \) can be written as

\[
R^n = A^n U^n + B U^{n-1}
\] (44)

Generally, as it can be seen from the above equation, the sub-matrices \( A \) and \( B \) remain constant for each time step and can be identified from the residual equations given in equations 28 to 30. Explicit definitions of the sub-matrices \( A \) and \( B \) considering the Newmark algorithm can be found in \([\text{Cetin}]\). Moreover, the sub-matrix \( A_0 \) is easily identified from the initial conditions.

Due to the transpose operation applied on \( \frac{\partial}{\partial U} \) for the adjoint equation given in equation 42, the solution of the adjoint equation is realized from reverse pseudo time steps which are written as

\[
(A)^T \Lambda^N = -\frac{\partial \phi}{\partial U}^N
\] (45)

\[
(A)^T \Lambda^{N-1} = -\frac{\partial \phi}{\partial U}^{N-1} - (B)^T \Lambda^N
\] (46)

\[
\vdots
\]

\[
(A_0)^T \Lambda^0 = -\frac{\partial \phi^0}{\partial U} - (B)^T \Lambda^1
\] (47)

After the adjoint equation is solved for the Lagrangian variables \( \Lambda^n \), the final sensitivity of the objective function is calculated as

\[
\frac{d\Phi}{ds} = \Lambda_0^T \left[ \frac{\partial A_0}{\partial s} U^0 \right] + \sum_{n=1}^{N} \Lambda^n \left[ \frac{\partial A}{\partial s} U^n + \frac{\partial B}{\partial s} U^{n-1} \right]
\] (49)

Considering a Newmark time stepping scheme, the explicit definitions of the partial derivatives \( \frac{\partial A_0}{\partial s} \), \( \frac{\partial A}{\partial s} \) and \( \frac{\partial B}{\partial s} \) are given in \([\text{Cetin}]\). As it can be seen from the gradient calculation in equation 49, state variables from the solution of the transient coupled vibroacoustic system needs to be stored in order to carry out discrete adjoint method for transient optimization problems. It is noted that the gradient calculation given in equation 49 is only done for the cut elements since the partial derivatives \( \frac{\partial A_0}{\partial s} \), \( \frac{\partial A}{\partial s} \) and \( \frac{\partial B}{\partial s} \) are zero elsewhere.

Sensitivity analysis provides the gradient of the objective function with respect to the physical design variable \( s \), the gradient with respect to the mathematical design variable \( \tilde{s} \) is obtained with applying the following chain rule

\[
\frac{d\Phi}{ds} = \frac{d\Phi}{d\tilde{s}} \frac{d\tilde{s}}{d\tilde{s}} \frac{d\tilde{s}}{ds} \frac{d\tilde{s}}{d\tilde{s}}
\]

As it can be seen from the above chain rule, the partial derivatives describe the link between the physical design variable \( s \) and mathematical design variable \( \tilde{s} \). The partial derivatives in the chain rule are applied in reverse order in order to calculate the gradient of the objective function with respect to the design variable \( \frac{d\Phi}{d\tilde{s}} \). Here, the partial derivative \( \frac{d\tilde{s}}{d\tilde{s}} \) describes changing the bounds on the mathematical design variable, \( \frac{d\tilde{s}}{ds} \) describes interpolating \( \tilde{s} \) from nodes to the element centers, \( \frac{d\tilde{s}}{d\tilde{s}} \) is the chain rule regarding the employed PDE filter in which its implementation details are thoroughly given in \([46]\) and \( \frac{d\tilde{s}}{d\tilde{s}} \) describes the interpolation operation from element centers to the nodes of the mesh.

Here it is noted that, for each optimization case that is considered for the current work, the calculated sensitivities are checked against a first order finite difference calculation. In the worst case, the difference between the calculated sensitivity and the finite difference computation was well below 0.1% since the utilized discrete adjoint method always yields exact and consistent sensitivities.
6. Numerical setup

This section presents the numerical setup that is used for the optimization of transient vibroacoustic filter designs. The section also introduces the objective function along with the computational domain and material properties that are used throughout the work. In order to define the objective function which is used for the optimization of acoustic filter designs for a wide frequency range, a measure of transmission is needed to be defined. To achieve this, after the transient response of the state variables are obtained from the solution of the transient coupled vibroacoustic system, the transmitted acoustic pressure signal is integrated at the outlet of the considered acoustic duct as

\[ \hat{p}(t) = \int_{r_{\text{out}}} p(t) \, d\Gamma \]  

(51)

the frequency response of the transmitted acoustic pressure is found by the discrete Fourier transform

\[ \hat{p}(f) = \text{FFT}(\hat{p}(t)) \]  

(52)

and the transmission \( S(f) \) is then defined as

\[ S(f) = \frac{\hat{p}(f)}{\hat{p}_0(f)} \]  

(53)

where the subscript 0 denotes the transmitted acoustic pressure when there is no structure in the acoustic duct which is calculated the same way as \( \hat{p}_0(f) \). As it can be seen from the above equation 53, when the value of \( S(f) \) is unity for a particular frequency a full transmission is achieved. Meaning that the recorded amplitude of the transmitted acoustic pressure for an empty acoustic duct at a certain frequency is equal to that of an acoustic duct with a vibrating structure present in it. Moreover when the value of \( S(f) \) is zero for a certain frequency, there is no transmission realized compared to the transmission of the empty duct. In other words, the vibrating structure does not transmit acoustic pressure towards to outlet of the duct.

In order to reflect the so called pass-band and stop-band regions in the considered frequency span, two objective functions are considered which are written as

\[ \Phi_1 = \sum_{f=n_1}^{n_2} \frac{(S(f) - a)^2}{a^2}, \quad a = 1 \]  

(54)

\[ \Phi_2 = \sum_{f=n_3}^{n_4} \frac{(S(f) - b)^2}{b^2} \]  

(55)

where the minimization of the function \( \Phi_1 \) fits the frequency response of the transmitted acoustic pressure to that of an empty acoustic duct hence realizes a full transmission in a frequency window defined between \( n_1 \) and \( n_2 \). The minimization of \( \Phi_2 \) on the other hand lowers the amplitude of the frequency response of the transmitted acoustic pressure compared to the response of an empty acoustic duct in a frequency range defined between \( n_3 \) and \( n_4 \). The order of magnitude difference between the transmitted acoustic pressure in the stop-band region and the empty acoustic duct is defined by the parameter \( b \) in equation 55. The study on the selection of \( b \) in order to realize an effective zero-transmission and its effect on the overall optimization performance are given in section 7.1.

In order to realize an optimization problem where multiple objective functions are equally minimized, the problem can be formally written in a so-called min-max formulation. However, since the min-max formulation is not differentiable an additional variable is introduced and the optimization problem is cast...
as a bound formulation as

\[
\min_{\mathbf{s}, \beta} \beta \\
\text{s.t.} \quad R^n(\mathbf{s}, \mathbf{U}^n(\mathbf{s})) = 0, \quad \text{for} \quad n = 0, 1, \ldots, N \\
\Phi_1 < \beta \\
\Phi_2 < \beta \\
0 \leq \mathbf{s} \leq 1
\]

(56) (57) (58) (59) (60)

where the additional variable \( \beta \) is the upper bound for the optimization. The formulation realizes the minimization of the upper bound \( \beta \) where the objective functions \( \Phi_1 \) and \( \Phi_2 \) are defined as constraints in the optimization problem, hence effectively minimizing both \( \Phi_1 \) and \( \Phi_2 \).

Figure 4: Schematic illustration of the optimization case for the design of acoustic filters showing the boundary conditions of the optimization problem. Gray color shows the design domain. Incoming acoustic white noise and an example desired filter shape at the outlet are also shown.

A schematic illustration of the numerical setup for the optimization of acoustic filter designs is given in figure 4. As it can be seen from the figure, both top and bottom boundaries of the acoustic duct are set as hard-wall condition for the acoustic pressure while the structure is considered to be clamped. For the acoustic domain, both right and left most boundaries are treated as absorbing conditions. The incoming acoustic plane wave from the left most boundary is also shown in the figure. In order to excite broad frequency range in the coupled system, the incoming plane wave is realized as a white noise with random acoustic pressure values between \(-1 \text{ Pa} \) and \(1 \text{ Pa}\). Moreover, the figure also illustrates an example filter shape at the right most boundary (at the acoustic duct outlet) where the acoustic transmission of the design \( S(f) \) is calculated in frequency domain and a certain filter shape is applied to it. Here it is noted that the presented filter shape in the schematic illustration is given as an example. The work considers various different filters for the optimization which are presented in the following sections.

The overall calculation time for the considered cases throughout the work is chosen as \(0.02\text{s} \) as it can also be seen from the incoming transient acoustic plane wave plot given in figure 4. In order to adequately resolve the coupled vibroacoustic problem in time, the time step size is set to \(\Delta t = 2 \times 10^{-5}\text{s} \). The frequency content of the white noise applied at the inlet of the acoustic duct to excite broad frequency range in the system is given in figure 5. As it can be seen from the figure, the incoming acoustic wave has an approximately constant energy content across all the frequencies present in the signal.
For the optimization, the acoustic domain is taken as air while the structure is considered to be a rubber-like material. The material properties used for the structure and acoustic domains are listed in the tables 1 and 2, respectively.

<table>
<thead>
<tr>
<th>$E$ [Pa]</th>
<th>$\nu$</th>
<th>$\rho_s$ [kg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$50 \times 10^6$</td>
<td>0.4</td>
<td>1000</td>
</tr>
</tbody>
</table>

Table 1: Material properties considered for the structure.

<table>
<thead>
<tr>
<th>$c_a$ [m/s]</th>
<th>$\rho_a$ [kg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.21</td>
<td>343</td>
</tr>
</tbody>
</table>

Table 2: Material properties considered for the acoustic domain.

As described in section 2, the work also considers Rayleigh damping for structural damping. Damping for structure is utilized both for the added stabilization of modeling and the subsequent optimization and to reflect the loss mechanism of the real world. The Rayleigh parameters $\alpha_d$ and $\beta_d$ are calculated according to [49] as

$$\alpha_d = 2\zeta \frac{\omega_1 \omega_2}{\omega_1 + \omega_2}$$

$$\beta_d = 2\zeta \frac{1}{\omega_1 + \omega_2}$$

(61) (62)

here $\zeta$ is called the damping ratio and is taken to be $\zeta = 0.1$. Moreover, the work assumes that the two natural frequencies $\omega_1$ and $\omega_2$ are $\omega_1 = 1600 \times 2\pi$ rad/s and $\omega_2 = 2200 \times 2\pi$ rad/s. Throughout the work, the computational domain given in figure 4 is meshed with structured quad elements in which the each element has an edge length of $2 \times 10^{-3}$m. For optimization, the filter radius $r$ is set to $8 \times 10^{-3}$m.

Throughout the work, the utilized MMA algorithm for solving the optimization problem presented in equations 56 to 60 uses the asymptote parameters of 0.5, 0.7 and 1.2 which are used for controlling the initial adaptation, decrease and increase of the asymptotes, respectively. The penalty parameter which is used for constraints in MMA algorithm is chosen as 1000. For all of the optimization cases that are considered, the work does not consider a specific stopping criteria. Presented results are run for a set number of iterations. Optimization iterations are terminated once a design having a good performance is obtained. Moreover, the considered optimization problem does not include a volume constraint on the structure. Since, having only a slab of solid material in the design domain does not form a trivial answer to the optimization problem.
7. Numerical examples

7.1. Objective function study

This section presents the study that is done for the considered objective functions given in the equations 54 and 55. As it is introduced in the previous section 6, the pass-band and stop-band regions for the objective functions are controlled with the parameters \( a \) and \( b \), respectively. Minimizing the objective function \( \Phi_1 \) with having the \( a \) parameter as unity fits the calculated transmission value \( S(f) \) of the structure inside an acoustic duct to 1, effectively realizing full transmission in the considered frequency range. Ideally, the parameter \( b \) on the other hand needs to be set as 0 in order to realize zero transmission \( S(f) = 0 \) in the frequency range defining the stop-band region of the filter that is considered for the optimization. However, as it can be seen from the equations 54 and 55, an inverse weighting is utilized in the objective functions. Through the carried out numerical experiments it has been found that, the utilized inverse weighting provided designs with superior performances compared to the designs obtained using objective functions without any weighting. Hence, a small positive number is used for the \( b \) parameter in order to avoid division by zero in the objective function \( \Phi_2 \). This section investigates the effect of the \( b \) parameter on the optimization and the final performance of the optimized design.

Moreover, the section considers a low-pass acoustic filter design for the study. The objective function \( \Phi_1 \) defining the pass-band region operates on the frequencies between \( 1000 \text{ Hz} \leq f \leq 2500 \text{ Hz} \). For the stop-band, the objective function \( \Phi_2 \) on the other hand is chosen to be active on the frequencies between \( 2500 \text{ Hz} < f \leq 4000 \text{ Hz} \). Three different \( b \) parameters are selected to carry out the study which are \( 1 \times 10^{-2} \), \( 1 \times 10^{-3} \) and \( 1 \times 10^{-4} \).

Figure 6a shows the initial configuration that is used for the optimization. The physical design variables \( \bar{s} \) that specifies the initial design is obtained first by calculating the following expression

\[
s_v = \cos \left( \frac{r_1 \pi X}{l_x} \right) \cos \left( \frac{r_2 \pi Y}{l_y} \right) + 0.1 \quad (63)
\]
where $x$ and $y$ are the nodal coordinates of the mesh in the design domain, $l_x$ and $l_y$ is taken to be 0.1 and $r_1$ and $r_2$ is chosen as 7. After calculating $s_v$, the mathematical design variables $s$ are obtained with the
following rule as

\[ s_i = \begin{cases} 
0, & \text{if } s_{v,i} \geq 0.01 \\
1, & \text{if } s_{v,i} < 0.01
\end{cases} \]  

(64)

With applying the design parameterization described in section 4, the physical design variables \( \vec{\mathbf{s}} \) containing the initial design is obtained. Physically, the initial design given in figure 6a can be considered as an infinitely long acoustic duct in the out of plane direction where the two dimensional approximation realizes its cross section view from the mid-section of the channel.

Figure 6b shows the desired acoustic low-pass filters with the three different levels of stop-band in which the transmission \( S(f) \) is to be fitted to the values of \( 1 \times 10^{-2}, 1 \times 10^{-3} \) and \( 1 \times 10^{-4} \). As it can be seen from the figure, the initial configuration nearly has a full transmission across the considered frequency range of 1000Hz to 4000Hz. Table 3 lists the calculated objective values for the initial configuration for each optimization case. As expected, since the same initial design is utilized and the parameter \( a \) is set to \( a = 1 \) for each case, the values of \( \Phi_1 \) are the same. However, the values of \( \Phi_2 \) increase two orders of magnitude for each order of magnitude decrease in the \( b \) parameter. Since, the objective values \( \Phi_1 \) and \( \Phi_2 \) are inversely weighted with the square of \( a \) and \( b \), respectively.

The result of the comparative study is given the figure 7. As it can be seen from the figures 7a to 7c, although the optimized designs have highly complex topologies, a similar trend can be seen in how the structures clustered inside the design domain for each case. Also, due to the lack of feature size control in the optimization, minimum feature size is bound by the element size used in the computational mesh which can be seen in the thin connections and small island structures present in the optimized designs.

The frequency responses of the optimized designs can be seen in the figure 7d where the calculated transmission \( S(f) \) at the outlet is plotted for all optimized designs. It can be seen from the figure that the calculated transmission \( S(f) \) for each case respects the desired low-pass filter shape for the considered frequency range. However, as the parameter \( b \) is decreased for having a lower transmitted acoustic pressure

Figure 8: Optimization for an acoustic low-pass filter design. (a) optimized design for \( b \times 10^{-5} \). (b) transmission of the optimized design in the considered frequency range. Black line is the desired low-pass filter, blue line is the response of the optimized design.
response at the stop-band region, the resulted optimized designs’ performances for the transition between
the pass-band and stop-band regions also decrease. This effect can also be seen in the presented objective
function values \( \Phi_1 \) and \( \Phi_2 \) for each optimized design in figures 7a to 7c where the objective values increased
as the transmission value is decreased in the stop-band of the acoustic filter. As it can also be seen from
the presented objective values, optimized designs’ \( \Phi_1 \) values actually end up at higher values compared to
the initial configuration which is due to the transition between the pass-band and stop-band regions for the
considered low-pass filter.

Overall, compared to the initial transmission given in figure 6b, it can be seen from the figure 7d
that the developed optimization framework can successfully tailor the frequency content obtained from
the transient response of the coupled vibroacoustic system, effectively designing acoustic filters. Moreover,
figure 7e compares the averaged sound pressure level (SPL) values at the outlet of the acoustic duct for the
considered frequency range. Compared to the SPL response of the empty acoustic duct, the considered low-
pass filter shape can also be seen from the SPL values of each optimized design. Here, the optimized designs
have nearly the same averaged SPL response with the empty acoustic duct from 1000 Hz to approximately
2250 Hz and after a sharp transition into the stop-band region, transmission \( S(f) \) values of \( 1 \times 10^{-2}, 1 \times 10^{-3} \)
and \( 1 \times 10^{-4} \) roughly corresponds to the averaged SPL values of 20 dB, 0 dB and -20 dB for the stop-band
region of the low-pass acoustic filter, respectively.

As a further study, the same optimization setup is again considered with a low-pass filter design where
the \( b \) parameter is lowered to \( b = 1 \times 10^{-3} \). Figure 8a shows the optimized design where a similar trend is
seen compared to the design presented in figure 7c. However, as it can be seen from the performance of the
acoustic filter given in figure 8b, optimization resulted in a low quality local-minimum. Meaning that the
optimized design fails to lower the transmission to \( S(f) = 1 \times 10^{-3} \) for the stop-band region of the considered
low-pass filter. Considering the SPL values given in figure 7e and the corresponding performances for each \( b \)
parameter that is used for the objective function \( \Phi_2 \), \( b = 1 \times 10^{-3} \) is deemed the most effective for optimizing
acoustic filters within the developed framework which will be used for the remaining of the work.

7.2. Initial guess study

This section carries out an initial guess study for the optimization of acoustic filters. Instead of the
low-pass filter design that is presented in the previous section 7.1, the section considers the optimization
of high-pass acoustic filters. For the optimization, the objective function \( \Phi_1 \) defining the pass-band of the
high-pass filter operates on the frequencies between \( 2500 \text{ Hz} \leq f \leq 4000 \text{ Hz} \). Whereas, \( \Phi_2 \) for the stop-band
region of the high-pass filter is active between \( 1000 \text{ Hz} \leq f < 2500 \text{ Hz} \). The desired high-pass filter is
given in figure 9d in which the calculated transmission \( S(f) \) of the designs are to be lowered to a value
\( S(f) = 1 \times 10^{-3} \) in the stop-band region of the filter.

For the current study, three different initial configurations will be considered. The first initial design is
the same that was used in the previous section. The other two initial guesses are obtained with decreasing
the \( r_1 \) and \( r_2 \) parameters given in equation 63 from 7 to \( r_1, r_2 = 6 \) and \( r_1, r_2 = 5 \), respectively. Decreasing
the parameters \( r_1 \) and \( r_2 \) reduce the total number of circle structures in the initial configuration while
making their size bigger.

Figures 9a to 9c presents the initial configurations that are used for the optimization of acoustic high-
pass filters. As it is seen from the figures, initial structures have sparsely clustered features in order to
allow a high transmission across the frequencies that are considered in the high-pass filter given in figure 9d.
Initial structures’ features become larger from figure 9a to 9c. The figures also presents the objective values
\( \Phi_1 \) and \( \Phi_2 \) calculated with the initial designs where similar results are obtained. This points out similar
transmission responses between 1000Hz and 4000Hz for the initial configurations.

Figure 9e presents the transmission \( S(f) \) responses calculated at the outlet of the acoustic duct over the
considered frequency range. Here, the initial configurations given in figures 9a and 9b resulted in transmission
responses that closely follow each other between 1000Hz and 4000Hz where the calculated transmission \( S(f) \)
values are clustered around unity. Meaning that the initial configuration for the first two cases allows for
nearly full transmission in the frequency range that is considered for the optimization. Likewise, the initial
design given in figure 9c also allows for frequencies between 1000Hz and 2800Hz to pass. However, after
approximately around 2800Hz, the last initial design has a lowered transmission response as it can also be seen from the figure 9e which corresponds to the pass-band region of the considered high-pass acoustic filter.

The results of the optimization for the initial guess study are presented in figure 10. Moreover, the optimized designs can be seen in figures 10a to 10c which are the optimized results of the initial designs given in figures 9a to 9c, respectively. Here, the designs given in figures 10a and 10b have a similar structure layout where the optimized structures in the design domain separated the domain roughly into three acoustic partitions. Optimized design given in figure 10c resulted in the largest features compared to the first two cases. Also, from the investigation of the objective values Φ₁ and Φ₂ given in figures 10a to 10c, it is seen that the first two optimized designs successfully captured the high-pass filter response whereas the last optimization failed in the pass-band region of the considered high-pass filter shape. This is also visually shown in figure 10d where the calculated transmission $S(f)$ for each optimized design is plotted over the
Figure 10: Optimization for an acoustic high-pass filter design. (a) optimized design for the initial guess shown in Fig. 9a. (b) optimized design for the initial guess shown in Fig. 9b. (c) optimized design for the initial guess shown in Fig. 9c. (d) transmission of the optimized designs in the considered frequency range. Black line is the desired high-pass filter, blue line is the response of the design in shown Fig. 10a, orange line is the response of the design shown in Fig. 10b, green line is the response of the design shown in Fig. 10c. (e) averaged SPL response of the designs calculated at the output, gray line is the empty acoustic duct, blue line is the response of the design shown in Fig. 10a, orange line is the response of the design shown in Fig. 10b, green line is the response of the design shown in Fig. 10c.

considered frequency range. It can be seen in the figure that the optimized designs given in figures 10a and 10b perform successfully as acoustic high-pass filters with lowering the transmission to $S(f) = 1 \times 10^{-4}$ in the stop-band and, after a sharp transition around 2500Hz, realizing nearly full transmission in the pass-band region of the high-pass filter.

Furthermore, the figure 10d also shows the response of the design given in figure 10c in which the design successfully realizes the stop-band of the high-pass filter. However, after the transition into the pass-band, the design’s performance deteriorates as the calculated transmission $S(f)$ lowers in the pass-band. Figure 10e compares the designs’ averaged SPL values at the outlet of the acoustic duct for the considered frequency range against the response of an empty acoustic channel. Here for the optimized designs in figures 10a and
10b, the SPL values in the stop-band are clustered around 0dB and goes up to around 60dB in the pass-band with closely following the response of an empty acoustic channel. The failure of the design given in figure 10c can also be seen from the figure where the SPL values diverge from the response of an empty acoustic channel in the pass-band of the high-pass filter.

Overall, the developed transient optimization framework for coupled vibroacoustic problems is successfully applied for the design of acoustic high-pass filters. Initial configuration given in figure 9c resulted in a failed design due to the starting guess having larger structure members which limits the design complexity. It is seen that the initial configurations that allow nearly full transmission (Figs. 9a and 9b) across the frequencies that are considered by the optimization resulted in efficient acoustic high-pass filters.

7.3. Band-pass and band-stop acoustic filter designs

This section presents the optimization results for the design of acoustic band-pass and band-stop filters. The section firstly carries out the optimization for the band-pass filter where the objective function $\Phi_1$, defining the pass-band region of the band-pass filter, operates on the frequencies between $2500 \, \text{Hz} \leq f \leq 4000 \, \text{Hz}$. Stop-band regions defined by the objective function $\Phi_2$ are considered in the frequency window of $1000 \, \text{Hz} \leq f < 2500 \, \text{Hz}$ and $4000 \, \text{Hz} < f \leq 5500 \, \text{Hz}$. Initial structure considered for the optimization is the same as in the figure 9a where the initial objective values are listed here as $\Phi_1 = 0.0154458, \Phi_2 = 1.15859 \times 10^8$.

Figure 11a shows the optimized design while the transmissions $S(f)$ of the optimized design and the initial configuration are given in figure 11b. As it can be seen from the figure 11b, the initial configuration has a nearly full transmission across the frequencies 1000 Hz to 5500 Hz. The optimized design on the other hand closely follows the desired band-pass filter shape. Interestingly, the optimized design (Fig. 11a) has a similar structure arrangement compared to the design in 9a in which both designs have similar transmission responses from 1000 Hz to 4000 Hz for a high-pass filter shape. The current design further tailors the frequency response of the coupled system to realize an additional stop-band from 4000 Hz to 5500 Hz. Also, from the optimized design’s objective values given in figure 11a and the visual inspection of the transmission response in figure 11b, it can be said that the performance of the pass-band region is slightly lowered compared to the designs presented in previous sections. This is mainly due to the added complexity of the optimization where an additional stop-band is considered to realize a band-pass filter.

Figure 11c shows the calculated averaged SPL response of at the outlet of the acoustic channel, comparing the optimized design and the empty acoustic channel. It can be seen from the figure that the optimized design’s calculated SPL response at the outlet is clustered around 0dB for the stop-band regions of the band-pass filter. At the pass-band, the design’s SPL response closely follow the SPL response of an empty acoustic channel. Overall, the developed transient optimization framework is shown to successfully tailor the frequency response of the coupled vibroacoustic system with designing an efficient acoustic band-pass filter.

The framework is lastly applied for the design of a band-stop filter. The objective function $\Phi_1$ for the pass-band regions of the considered band-stop filter operates on the frequency window of $1000 \, \text{Hz} \leq f < 2500 \, \text{Hz}$ and $4000 \, \text{Hz} < f \leq 5500 \, \text{Hz}$. For the stop-band region, the objective function $\Phi_2$ is active between the frequencies of $2500 \, \text{Hz} \leq f \leq 4000 \, \text{Hz}$. Again, the same initial configuration as the previous band-pass filter optimization is utilized which resulted in initial objective values of $\Phi_1 = 0.0552177, \Phi_2 = 5.8754 \times 10^7$.

The optimized design is shown in figure 12a. Moreover, the desired band-stop filter shape along with the transmissions $S(f)$ of the optimized and initial designs are given in figure 12b. When the optimized design is compared to the low-pass filter design given in figure 7b, it can be said that the both designs have a similar performance between the frequencies from 1000 Hz to 4000 Hz with acting as an acoustic low-pass filter. Overall, it can be seen in figure 12b that the initial transmission $S(f)$ is successfully tailored during the optimization in which the optimized design’s response closely follow the desired band-stop filter between the frequencies of 1000 Hz to 5500 Hz. The performance of the optimized acoustic band-stop filter is also seen from the averaged SPL values calculated at the outlet of the acoustic channel which is given in figure 12c. The figure shows that pass-band regions attains the overall 60dB SPL response while the stop-band region of the filter lowers the SPL response to approximately around 0dB.
Figure 11: Optimization for an acoustic band-pass filter design. (a) optimized design. (b) transmission of the optimized design in the considered frequency range. Black line is the desired band-pass filter, blue line is the response of the optimized design, gray dashed line is the response of the initial guess design. (c) averaged SPL response of the optimized design calculated at the output, gray line is the empty acoustic duct, blue line is the response of the optimized design.

8. Conclusions

The article presents the utilization of time-domain methods to realize wideband optimization in frequency domain. The developed framework carries out generalized shape optimization of transient vibroacoustic problems in which the optimization considers acoustic filter designs. In order to achieve this, the objective function is defined in frequency domain where the FFT operation is utilized to obtain the frequency response from the transient response of the coupled system. Throughout the work, the level set approach is utilized for the geometry description where its zero iso-level specifies the interface between acoustic and structural domains. An immersed boundary method called the cut element method is employed for capturing the geometry which operates on a fixed background mesh. The method uses a special integration scheme to accurately resolve the interface between the two physics without the addition of extra degrees of freedom to the system. Hence, the employed cut element method is suitable to include into the existing parallel FEM frameworks with ease. Moreover, the work utilizes the discrete adjoint method for carrying out the sensitivity analysis in order to calculate the gradients of the objective functions. The derivation of the sensitivity analysis is kept general to allow for the inclusion of different time integration schemes in which the handling of the FFT operation is explained to be able to define the objective function in frequency domain. Furthermore, a study for the utilized objective function is carried out to assess the effect of the inverse weighting that is used in the objective function where a design of acoustic low-pass filter is considered.
It has been found that having $b = 1 \times 10^{-3}$ for the objective function $\Phi_2$ to realize the stop-band region of the considered filter resulted in a relatively sharp transition between the pass-band and the stop-band, realizing an effective filter performance. The selected $b$ parameter also reduces the averaged SPL values at the outlet of the acoustic channel to approximately around 0dB in the stop-band. An initial guess study is then carried out to determine the effect of different initial configurations to the end design considering the optimization of an acoustic high-pass filters. It has been illustrated that with using initial configurations that allow for nearly full transmission in the frequency range that is considered for the optimization, efficient acoustic high-pass designs are obtained. The outcomes from both the objective function and the initial guess studies are then utilized in optimization for more complex acoustic band-pass and band-stop filters. Overall, the developed transient optimization framework is shown to successfully tailor the frequency response of the coupled vibroacoustic system for the design of acoustic band-pass and band-stop filters. The presented work will pave the way for the optimization of acoustic devices to realize efficient wideband operation. Also, different objective functions may be studied to increase the stability of the optimization framework with decreasing the effect of the initial configuration to the optimized design.

References


