Topology optimization for multiphysics problems:

Thermoelectric energy conversion and fluid-structure-interaction

Christian Lundgaard
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Preface

This thesis is submitted in partial fulfilment of the requirements for obtaining the degree of PhD. in mechanical engineering at the Technical University of Denmark (DTU). The PhD. project has been funded by the Danish Council for Independent Research through the TopTen project. The work has been carried out at the Department of Mechanical Engineering, Section of Solid Mechanics, at DTU during the period from the 1th of April 2015 and the 1th of June 2018. The main supervisor has been Professor Dr.techn. Ole Sigmund and the co-supervisor has been Associate Professor PhD. Kurt Engelbrecht and Senior Researcher PhD Boyan Stefanov Lazarov.

To complete this PhD project would have been impossible without the help from a lot of individuals. Especially, I wish to thanks Ole Sigmund for being an inspiring, educational and motivating supervisor. I also wish to thanks Kurt Engelbrecht and Rasmus Bjørk for many good discussions about thermoelectricity. I would also like to thanks a number of present or former colleagues who have provided academic guidance or simply good company at various stages of the project: Joe Alexandersen, Casper Schoesboe Andreasen, Rasmus Christensen and Sebastian Nærgaard, Jeroen Groen, Said Zeidan, Anders Clausen, Erik Andreassen, Christopher Nelleman and Niels Frandsen, Niels Aage, Mingdong Zhou, Randi Møller, Viggo Tvergaard, Gerda Helene Fogt, Hansotto Kristensen, Marie Brauns, Sümer Bartug Dilgen, Cetin Bartug Dilgen, Kristian Jørgensen Juul and Rasmus Grau Andersen. On a personal level I wish to thanks my friends and family for providing good company.
Abstract

The aim of this thesis is to develop topology optimization methodologies for two different multiphysical problems: Thermoelectric energy conversion and fluid-structure-interaction. The thesis is divided into four chapters: The motivation of the study, the relevant literature and a general introduction to the concept of topology optimization are layout in Chapter 1. To develop a topology optimization framework is an iterative process where a considerable amount of challenges are faced. With a point of departure in my own PhD project, recommendations to overcome these challenges are discussed in Chapter 2. The chapter can be skipped without loosing the meaning of the remaining part of the thesis. Chapter 3 and 4 are build up equivalently, can be read independently and are concerned with topology optimization for thermoelectric energy conversion and fluid-structure-interaction problems, respectively. The chapters begin with an introduction to the multiphysics concepts where important model parameters are identified, relevant literature is reviewed and the governing partial differential equations are stated. The chapters are concluded with suggestions to future research and a bread overview of the most important findings of the journal papers which have been submitted as part of the thesis.
List of publications

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

**Thermoelectric energy conversion**


**Fluid-structure-interaction**

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1 Introduction

This thesis expounds a density-based topology optimization methodology for two different types of multiphysical problems: thermoelectric energy conversion and fluid-structure-interaction. Thermoelectric energy conversion is concerned with the interaction between electric and thermal energy in semi-conducting materials [48, 79] and fluid-structure-interaction is concerned with the interaction between moving fluids and elastic structures [70, 77]. Thermoelectric energy conversion and fluid-structure-interaction belong to two different classes of multiphysical problems for which reason two topology optimization methodologies has been developed. Despite the offsets in very different classes of physical problems, the methodologies turn out to share a considerable amount of concepts. The development and usage of these two topology optimization methodologies are accounted for in the present thesis.

1.1 Motivation

Thermoelectric energy conversion are predicted to be an entrant in the changeover from fossil to sustainable energy resources, as devices powered by thermoelectric energy conversion can be used in applications such as waste heat recovery and refrigeration [28]. Even though a considerably amount of scientific attention has addressed the effectiveness of thermoelectric devices [41], the main efforts have so far been limited to a broad search and development of advanced thermoelectric materials [93]. To compete economically with conventional technologies, it is necessary to increase the effectiveness of thermoelectric devices [106]. In the present thesis it is studied if topology optimization is a suitable methodology for achieving this goal.

Many topology optimization methodologies are developed with the purpose of solving industrially relevant design problems. Fluid-structure-interaction problems have been studied intensively in the literature [55, 78, 118], however the branch of research still requires a considerable amount of maturation before it can be applied to industrially relevant design problems. The maturing of a topology optimization methodology is an iterative process and in the pursuit of achieving a design methodology which is capable of solving industrially relevant design problems, we aim at pushing the limits for what is possible with topology optimization in fluid-structure-interaction problems.

1.2 Topology optimization

To fully understand the theory and methods of topology optimization, readers are required to acquire some degree of knowledge in numerical methods [112], linear algebra [95], finite element analysis [32] and partial differential equations [96]. A thorough introduction to topology optimization is provided in the books [17, 59] and a comparative review of the available classes of topology optimization methodologies is provided by Deaton and Grandhi [33], Sigmund and Maute [91]. If the reader has
ambitions about developing a topology optimization framework, I suggest him/her to consult journal papers such as Andreasen [7], Sigmund [87] as a point of departure.

With reference to Fig. 1.1, structural optimization can be sorted into three different classes: size optimization, shape optimization, and topology optimization. The concept of the structural optimization classes can be explained with basis in a solid structure with a circular shape. The basic form of the circle is preserved in sizing optimization and only the radius of the circle is changeable. The external boundary of the circle can be changed in shape optimization, however the design process allows no freedom to create internal or external features. Topology optimization allow full design freedom which means that both internal and external features can be created. Topology optimization is therefore the most versatile form of structural optimization.

![Figure 1.1: An overview of the three main classes of structural optimization approaches.](image)

**The design problem**

The optimization problems solved in this thesis can all be cast from this general design problem formulation:

\[
\begin{align*}
\min_{\rho} \quad & \max_k \left(f^k\right) \\
\text{s.t.} \quad & \bar{R}^k(\tilde{\rho}^k, S^k) = 0 \\
& g(\tilde{\rho}^k) = N^e \sum_{i} \tilde{\rho}^k v_i/V \leq V_f \quad \forall \rho_i \in \Omega_D \\
& 0 \leq \rho_i \leq 1 \quad \forall \rho_i \in \Omega_D
\end{align*}
\]

The optimization problems are formulated in a min-max form [89, 108] for \( k = \{1, 2, ..., N^k\} \) projected realizations of the design variable field \( \tilde{\rho}^k \), where \( f^k \) is the objective function of the \( k \)'th realization of the design field (the superscripted \( k \) denotes the design realizations); \( \bar{R}^k \) is the residual equations; \( \tilde{\rho}^k \) is the filtered and projected design field realization; \( S^k \) is the state field vectors; \( g \) is the volume inequality constraint; \( N^e \) is the number of elements in the design domain, \( \Omega_D \); \( v_i \)
is the volume of element $i$, $V$ is the total volume of the $\Omega_D$ and $V_f$ is the volume fraction.

The robust formulation has been applied with successful outcomes to linear elasticity problems, heat problems [108], optical problems [107], acoustics problems [30], time dependent fluid problems [74], elasticity problems with spatially varying manufacturing errors [82], among many more.

**Design procedure**

The operations of the topology optimization routine is easiest explained with a point of departure in the following flowchart of the design procedure:

- Initialize the problem.
  - Set up design problem: Discretize partial differential equations, choose boundary conditions; objective function, $f$; constraint function(s), $g$, and other important model parameters.
  - Initialize mathematical design field, $\vec{\rho}_n$; number of design realizations, $k$; density-filtered design variable field, $\vec{\bar{\rho}}_n$; projected design variable field, $\vec{\tilde{\rho}}_n$, where $n$ is the design iteration number.
- Start optimization loop, for $n = 1$ to $n_{\text{max}}$
  - Apply filter operation, $F(\cdot)$, on $\vec{\bar{\rho}}$ to get $\vec{\tilde{\rho}}$: $F(\vec{\bar{\rho}}_n) \rightarrow \vec{\tilde{\rho}}_n$.
  - Apply projection filter operation, $P^k(\cdot)$, with $k$ different thresholds to get the projected design realizations: $P^k(\vec{\tilde{\rho}}_n) \rightarrow \vec{\tilde{\rho}}^k_n$.
  - Solve the state field problem with finite element analysis, $\mathcal{F}\mathcal{E}\mathcal{A}$, to get the state field, $\vec{S}_k$: $\mathcal{F}\mathcal{E}\mathcal{A}(\vec{\tilde{\rho}}^k_n) \rightarrow \vec{S}_k$.
  - Use adjoint sensitivity analysis, $\mathcal{A}\mathcal{S}\mathcal{A}(\cdot)$, to get the gradients of the objective function and the constraint functions with respect to $\vec{\tilde{\rho}}$: $\mathcal{A}\mathcal{S}\mathcal{A}(\vec{\tilde{\rho}}, \vec{S}_k) \rightarrow df/\partial \vec{\tilde{\rho}}^k$ and $\mathcal{A}\mathcal{S}\mathcal{A}(\vec{\tilde{\rho}}, \vec{S}_k) \rightarrow dg/\partial \vec{\tilde{\rho}}^k$.
  - Use the chain rule, $\mathcal{C}\mathcal{R}\mathcal{R}(\cdot)$, to compute sensitivities based on mathematical design variables: $\mathcal{C}\mathcal{R}\mathcal{R}(\mathcal{C}\mathcal{R}\mathcal{R}(df/\partial \vec{\tilde{\rho}}^k_n)) \rightarrow df/\partial \vec{\tilde{\rho}}^k_n$ and $\mathcal{C}\mathcal{R}\mathcal{R}(\mathcal{C}\mathcal{R}\mathcal{R}(dg/\partial \vec{\tilde{\rho}}^k_n)) \rightarrow dg/\partial \vec{\tilde{\rho}}^k_n$.
  - Solve the optimization problem with the method of moving asymptotes, $\mathcal{M}\mathcal{M}\mathcal{A}(\cdot)$, to get the next design field update: $\mathcal{M}\mathcal{M}\mathcal{A}(\vec{\rho}_n, df/\partial \vec{\tilde{\rho}}^k_n, dg/\partial \vec{\tilde{\rho}}^k_n) \rightarrow \vec{\rho}_{n+1}$.
- Break optimization loop if a stopping criteria is fulfilled.

**Post processing**

With reference to the flowchart, the three critical operations in the topology optimization frameworks are: (A) the filter operations, (B) the finite element analysis and (C) the adjoint sensitivity analysis. These operations have been layout in the following sections:
Filters and projection strategies

The physical design variables used in the finite element analysis, $\tilde{\rho}_i^k$, are obtained by imposing the projection filter Eq. (1.2) [88, 109]:

$$\tilde{\rho}_i^k = \frac{\tanh(\beta \eta^k) + \tanh(\beta (\tilde{\rho}_i - \eta^k))}{\tanh(\beta \eta^k) + \tanh(\beta (1 - \eta^k))}$$

(1.2)

where $\beta$ is the Heaviside projection parameter, $\eta^k$ is the projection filter threshold value, $k$ is the design realization, and $\tilde{\rho}_i$ is the density filtered design variables. The density filtered design variables $\tilde{\rho}_i$ are obtained from the mathematical design variables by the following filter operation [24, 26]:

$$\tilde{\rho}_i = \frac{\sum_{j \in N_i} w(\vec{x}_j) v_j \rho_j}{\sum_{j \in N_i} w(\vec{x}_j) v_j}$$

(1.3)

where $v_j$ is the area of the $j$th element, $N_i$ is the index set of the design variables which is within the radius $R$ of design variable $i$, $w(\vec{x})$ is the filter weighting function, $\rho_j$ is the mathematical design variables and $\vec{x}_j$ is the spatial location of the element $j$. The filter weighting function is given by:

$$w(\vec{x}_j) = \begin{cases} R - |\vec{x}_j| & \forall |\vec{x}_j| \leq R \land \vec{x}_j \in \Omega_D \\ 0 & \text{otherwise} \end{cases}$$

(1.4)

where $R$ is the filter radius, $|\vec{x}_j| = |x_j - x_i|$ and $w(\vec{x}_j)$ is a weighting function.

The field sensitivities are obtained by utilizing the chain rule twice:

$$\frac{\partial f}{\partial \rho_i} = \sum_{j \in \Omega_D} \frac{\partial f}{\partial \tilde{\rho}_j^k} \frac{\partial \tilde{\rho}_j^k}{\partial \rho_i^k}$$

(1.5)

Finite element formulation

In this work, the finite element equations are solved using rectangular elements and linear basis functions. Each finite element consists of one design variable and four nodes with five degrees of freedom in fluid-structure-interaction problems and two degrees of freedom in thermoelectric energy conversion problems. The residual equation is written as: $\vec{R}(\tilde{S}, \tilde{\rho}) = \vec{M}(\tilde{S}, \tilde{\rho}) \tilde{S} - \vec{F} = \vec{0}$, where $\vec{R}$ is the residual vector, $\vec{F}$ is the force vector, $\vec{M}$ is the system matrix and $\tilde{S}$ is the state field vector. For fluid-structure-interaction problems, the state field vector is $\tilde{S} = \{\vec{U}, \vec{P}, \vec{D}\}$ where $\vec{U}$ is the fluid velocity vector, $\vec{P}$ is the fluid pressure vector, $\vec{D}$ is the structural displacements vector. For thermoelectric energy conversion problems, the state field vector is $\tilde{S} = \{\vec{T}, \vec{V}\}$ where $\vec{T}$ is the temperature and $\vec{V}$ is the electric potential difference. The residual equations are solved by a combination of the undamped Newton’s method (see e.g. Deuflhard [36]) and Picard iterations. Newton iterations provide fast convergence for initial guesses close to the solution, where Picard iterations provide fast convergence for initial guesses far away from the solution.
Adjoint sensitivity analysis

Gradients of the objective function with respect to the design variable field, in this study denoted *sensitivities*, are required in order to solve the optimization problem in Eq. (1.1). The sensitivities of the *k*’th design realization, \( \frac{dL^k}{d\bar{\rho}} \), where *L* is the general Lagrangian functional, are computed by the discrete adjoint approach, see Bendsøe and Sigmund [17], Michaleris et al. [68], which reads:

\[
\begin{pmatrix}
\frac{\partial \tilde{R}^k}{\partial \bar{S}^k} \\
\frac{\partial \bar{S}^k}{\partial \bar{\rho}}
\end{pmatrix}^T \bar{\lambda}^k = \begin{pmatrix}
\frac{\partial f^k}{\partial \bar{\rho}} \\
\frac{\partial \bar{S}^k}{\partial \bar{\rho}}
\end{pmatrix}^T
\]  \hspace{1cm} (1.6)

where \( \bar{\lambda}^k \) is the vector of adjoint variables and \( \Box^T \) denotes the transpose. The sensitivities can now be computed by the following expression:

\[
\frac{dL^k}{d\bar{\rho}} = \frac{\partial f^k}{\partial \bar{\rho}} - \left[ \bar{\lambda}^k \right]^T \frac{\partial \tilde{R}^k}{\partial \bar{\rho}}
\]  \hspace{1cm} (1.7)

where \( \frac{\Box}{\Box} \) denotes the total derivative and \( \frac{\partial \Box}{\partial \Box} \) denotes the partial derivative. A thorough derivation of the adjoint sensitivity analysis is provided in Andreasen [8].
To develop a topology optimization methodology is an iterative process where a considerable amount of challenges are faced. With basis in my own research experience, I present some general recommendations to overcome these challenges. The present chapter is addressing students and researchers on master or PhD level (i.e. a past version of myself), who have ambitions about developing their own topology optimization methodology. By following the recommendations laid out in this chapter, the methodologies may potentially reach a higher level of quality in a smaller amount of time. To include this chapter in my PhD thesis may be considered unorthodox, however I believe that the chapter may be useful and beneficial for young and/or unexperienced researchers. All statements are completely my own and the chapter can be skipped without losing the meaning of the remaining part of the thesis.

2.1 Identify an important problem

With a point of departure in an engineering application, identify a challenge which can be solved by using a material distribution method such as topology optimization. Consider the engineering application and answer questions such as: What is the governing physics? Is it a multiphysical problem [65]? Is the problem strongly [4] or weakly coupled [64]? To adequately capture the features of the physics, consider if it is necessary to solve the physical problem time-dependently [74]; with non-linearly material parameters [66] or in one, two or three dimensions [10, 11]. A literature review of multiphysics design methodologies is provided in [33].

Numerical optimization approaches are often, compared to e.g. analytical approaches or engineering intuition [63], suitable for coupled, non-linear and high dimensional physical problems. Natural convection [5] and wave-propagation[30] problems are examples on physical problems where topology optimization is a very suited design approach.

Assess whether topology optimization is a suited methodology for solving the design problem at hand. Identify important model parameters such as objective functions, boundary conditions, material parameters and assess how the underlying physical model and model assumptions are related to the design problem. Consider and imagine how the important and dominant features of the governing physics are related to the design problem and the design solutions.

When these matters have been considered, it is now time to derive the governing partial differential equations. Topology optimization approaches are always constrained by partial differential equations, and it is therefore critical to state the exact equations such that the design methodology can be communicated with coworkers.
2.2 Search for relevant literature

A critical part of developing a topology optimization methodology is to carry out a thorough literature study to meet at least three important concerns: (A) to ensure the originality of the research, (B) to identify adequate benchmark examples and (C) to classify the present and related optimization approaches.

The originality of scientific research is critical and precious time can easily be wasted on developing methodologies which have already been invented and reported in the literature, compare e.g. [15, 57]. Advanced numerical methodologies are often easier to present to skeptical co-workers, if their performances are benchmarked against other accepted and used optimization approaches in the literature [6, 66]. An important part of developing design methodologies is to objectively assess how they perform in relation to other and already accepted methodologies.

To consult coworkers, advisors and other researchers may be an effective strategy in the search for relevant literature, as people often are happy to share their knowledge. The image search feature of many search engines can be useful to identify related design problems in the literature\(^1\). If a relevant paper is identified, investigate if the paper has been cited in other works. A relevant paper for a specific study are most often cited by other related studies. Many scientific search engines offer functionalities which can identify these mechanisms.

To formulate “a good story” is a critical part of presenting scientific work. With an offset in an academic or an industrial problem, it is most often easier to explain advanced design methodologies [9] and to confine the amount of presented information. Information about literature searches and research study planning are provided in e.g. Hoogenboom and Manske [51] and Whitesides [111], respectively.

2.3 Discretization of the model

The discretized finite element equations are obtained by multiplying the strong forms of the partial differential equations with suitable test functions and integrating over the domain [53]; introducing a design variable field [18]; performing integration by parts of higher dimensions on relevant terms [81] and introducing the design field dependent interpolation functions [17, 123]. In the process of developing a topology optimization framework, it is critical to develop a scientific notation and use it consistently in the reporting and programming, see e.g. Andreassen et al. [12], Sigmund [87]. A meaningful, simple and consistent scientific notation provides a platform for discussion. The time used to develop this is experimentally well-spent as it makes debugging and discussions concerning the methodology much more efficient.

The number of material phases (total number of solids and void) and type of material phases (solid-solid, solid-solid, etc) have a large influence on the design problems and design solutions. To set up a suitable number and type of phases are therefore critical in the development of a topology optimization methodology, compare e.g. [64, 99] and consider the three phase formulation in [92].

\(^1\)Try e.g. to make an image search for constructal heat trees or negative Poisson’s ratio in your favorite search engine.
As the fundamental concepts of the design framework have been decided, it is time to lay out a programming strategy. Take the appropriate time to plan a consistent programming strategy and do not compromise with the quality of the code. Sometimes it may be tempting to take an offset in educational codes such as Aage et al. [2], Andreassen et al. [12], Sigmund [87], however for advanced topology optimization frameworks these educational codes may not be the best suited point of departure.

2.4 Validate the finite element model

As the finite element routine seems to be correctly derived and implemented, it is time to perform the first validation study. With point of departure in the simplest possible problem, assess whether the finite element solutions are consistent with physical intuition. Continuously increase the complexity of the finite element problems while ensuring that the finite element routine is working properly. Continue this process until the most advanced example is validated and save the results for future reference.

The next step is to validate the finite element routine with predictions derived from analytical approaches and commercial finite element codes. Compare state fields for different boundary conditions, discretizations and model parameters such as time steps, load increments, material properties, etc. To build confidence in the finite element framework, it is critical to make a broad search for corner-cases and ensure that the finite element formulation, the commercial codes and the analytical predictions (do probably not exist for more advanced examples) are similar for all problems. The rate of convergence of the Newton solver can be used to assess whether the coding or derivations are prone to errors. The slightest deviation in the expected rate of convergence are most often an indication of an error in the tangential system matrix. As the validation study is completed, the next step is to build intuition about the physics and the framework. Identify important model parameters and study their interaction such that the important features of the underlying physics a detected. Save the results for future reference.

2.5 Develop the optimization framework

Formulate the design problem mathematically by defining an objective function and constraint functions. Obtain the gradients of these functions with adjoint sensitivity analysis [17, 69], automatic differentiation [75] or other applicable methods for sensitivity analysis. For the same reasons as already discussed in Sec. 2.3, it is important to report mathematical derivations consistently and in this relation to distinguish between the weak form, the finite element form and the implementation form [64].

2.6 Validate the optimization framework

To validate the derived sensitivities is a critical part of the implementation and development of a topology optimization methodology. The validation study is
performed by implementing a routine which is capable of comparing the analytical adjoint sensitivities with an approximation to the sensitivities [90]. Errors in the sensitivity analysis may not necessarily be expressed in all problems, and an important part of the sensitivity validation study is therefore to search for corner cases. Corner cases can be identified by conducting validation studies for different boundary conditions, initial design fields, discretizations, time-step length, material parameters and so forth. Conduct the validation studies with different perturbations in the design field and for all elements in the design field (sometimes called full finite difference checks colloquially). To thoroughly validate the adjoint sensitivities build confidence in the framework as implementation and derivation errors can be identified and corrected. To find such errors in an early stage of the development of the methodology, may save a considerable amount of time, as design solutions solved with incorrect adjoint sensitivities are useless.

2.7 Solve design problems

As the adjoint sensitivities are validated, it is time to solve some design problems. With basis in the model parameters identified in Sec. 2.4, solve different design problems and investigate how the design solutions and model parameters are related. Take basis in questions such as: Can general tendencies be derived from the interplay between the design solutions and the model parameters? How are the design solutions and the governing physics related? Explain why the features of the design solutions are “optimal” for the specific design problems [3]. Large parameter studies can often be used to identify important regimes of model parameters and gain insight in the governing physics. Use such studies to search for interesting features of the design problems.

Multiphysic topology optimization frameworks may provide intermediate or poor performing design solutions and remedies to such issues may be to impose double filtering [30], robust formulations [108], projection filtering [49], solve other physical fields to impose specific features in the design solutions [55], formulate the design problem with multiple and weighted objective functions [65], scale sensitivities, continuation strategies, different optimizers [97, 98], parameters tuning (the parameters in the method of moving asymptotes, various filter radii, interpolation function parameters, projection filter thresholds parameters, etc) or investigate the monotonicity of the adjoint sensitivity gradients. The smoothness, the well-posedness and convexity of the design problems are related to the monotonicity of the adjoint sensitivities. Studying the interplay between these may increase smoothness, well-posedness and convexity of the design problems [65].

2.8 Validate the design solutions

To prove that the design solutions are physical and not obtained by artificial features of the underlying mathematical model, it is necessary to conduction design solution validation studies. Such studies are conducted in four steps:
2.8.1 State fields

With basis in a well-performing design solution and the corresponding state field plots, identify the governing features of the design solution and how they are related to the model parameters. Search for non-physical design and modeling features. Non-physical design features are most often caused by intermediate design variables, discretization issues [64], poor or no continuation strategies [22] or poorly resolved physics [73]. Unless intermediate design variables are physical meaningful [115], design solutions shall always be validated without intermediate design variables.

2.8.2 Cross-check studies

With basis in a sequence of well-performing design solutions obtained for different model parameters, it is time to conduct a cross-check study. A cross-check study can be used to determine how much significance one may attribute to the features of the design solutions, see e.g. [4, 66]. The reliability of the topology optimization framework is increased with the number of design solutions passing the cross-check. To explain the concept of a cross-check study let us consider two design solutions and two sets of model parameters: Design solution A solved for model parameter A and design solution B solved for model parameters B. The following must be fulfilled for these designs to pass a cross-check: Design solution A must outperform design solution B when both design solutions are evaluated for model parameters A. Design solution B must outperform design solutions A when both design solutions are evaluated for model parameters B. To further increase the reliability of the proposed design methodology, design solution obtained by engineering intuition, from the literature or related optimization approaches can be included in the cross-check studies. To discuss design features of design solutions are meaningless unless the design solutions have passed a cross-check.

2.8.3 The modeling approaches

The design solutions may take advantages of non-physical features of the underlying mathematical formulation which may not have been captured in the initial validation studies in Sec. 2.4. By evaluating the design solution with a boundary fitted mesh [1, 45] and a segregated solver in a commercial finite element application, pitfalls such as discretization issues [64] and inadequately modeling [74] may be identified. With basis in the state field plots ensure that the unified and segregated modeling approaches provide the same results. To further increase the reliability of the design solutions, conduct various finite element validations such as mesh-refinement studies [32].

2.8.4 The physical modeling

Assess whether a simpler mathematical model can generate the same or almost the same design solutions. This can be done by solving design problems with simpler versions of the mathematical model. Topology optimization frameworks can sometimes resolve different types of physics or non-linear effects which only have a
small influence on the design solutions [55, 100]. Approaches such as those already
discussed in Secs. 2.8.1 and 2.8.3 can be used as a point of departure for conducting
this study.

2.8.5 Experimental validations

Conduct experimental validations of the design solutions. Quantify how the numerical
predictions compare with experimental results and use this very strong insight in
assessing the applicability of the proposed design framework [6, 31].
The scientific and commercial interest in thermoelectric energy conversion has increased considerably in recent decades due to the increasing demand for non-polluting and renewable energy sources. Many researchers predict that the need for renewable energy resources will be partly covered by thermoelectric energy conversion [28] and this prediction has made the field of research subject to a considerable amount of scientific attention [48, 67, 79]. To make the thermoelectric energy conversion technology economically profitable and competitive with conventional technologies, it is required to improve the effectiveness of thermoelectric devices and materials [106]. As a contribution for achieving this goal, we have developed and reported a numerical topology optimization approach which is capable of designing thermoelectric devices for specified performance measures.

The build-up of the chapter is the following: An introduction to thermoelectricity and the topology optimization methodology is provided in Sec. 3.1. An overview of the design problems investigated in [P1-P4] is given in Sec. 3.2. Studies which did not yield obvious applicable results, but may provide guidance for future research, are presented in Sec. 3.3. The most important findings and suggestions for future research within topology optimization of thermoelectric energy conversion problems are discussed in Sec. 3.4.

3.1 Introduction

Thermoelectricity is a multi-physic problem which concerns the interaction and coupling between electric and thermal energy in semi conducting materials. Thermoelectric energy conversion can be described by two separately identified effects: The Seebeck effect and the Peltier effect. The Seebeck effect concerns the conversion of thermal energy into electric energy and the Peltier effect concerns the conversion of electric energy into thermal energy [48, 79]. With reference to the sketch in Fig. 3.1, thermoelectric devices consist of three main components: (A) legs, (B) electric conductors and (C) interface substrates. Conversion of electric or thermal energy occur in the legs due to the physical properties of the thermoelectric materials. The electric conductors connect the legs electrically and ensure that a sufficiently large electric potential or thermal cooling powers are established for thermoelectric generators or thermoelectric coolers, respectively. The substrates constitute the interface between the thermal hot reservoir (heat source), the thermal cold reservoir (heat sink) and the thermoelectric device. Two thermoelectric legs (shown with different colors in Fig. 3.1) and an electric conductor are in combination denoted a module. Modules consists of two dissimilar types of semiconductors: P and N types, which are charged (electrically) positively or negatively.

The effectiveness of a thermoelectric material depends on the properties of the P and N type semi-conducting materials and is often characterized by the thermoelectric
Chapter 3: Thermoelectric energy conversion

Figure 3.1: A schematic of a thermoelectric device.

The fundamental concept of the density-based topology optimization approach [17, 18, 91] proposed in the present study is to distribute two different materials in a one, two or three dimensional design space in order to optimize a specified performance measure. With reference to the design problem sketches in Fig. 3.2, we have studied three different classes of optimization problems in [P1-P4]: (A) diagonal problems sketched in Fig. 3.2a and inspired by [116, 117], (B) off-diagonal problems sketched in Fig. 3.2b and inspired by [80] and (C) PN problems sketched in Fig. 3.2c and inspired by [13].

With reference to Fig. 3.2, the three design problems are classified by the primary directions of the electric current and the thermal heat flux. The primary directions are either horizontal or vertical. Devices in diagonal configurations convert a vertical electric current into a vertical thermal flux or vice versa. Devices in off-diagonal configurations convert a horizontal electric current into a vertical thermal flux or vice versa. Devices in PN configurations have complex interplays between the vertical thermal flux and the electric current.

To assess the best suited configuration class for a specific type of application is a compromise between several parameters: Thermoelectric devices in diagonal configurations provide a relatively large electric power output and conversion efficiency, however the thermo-mechanical stresses and wear in the electrodes are relatively large, because they are connected directly to the hot and cold reservoirs. The thermo-mechanical stresses and wear of the electrodes are relatively smaller for devices in off-diagonal and PN configurations, however the electric power output and conversion

\[ ZT = \frac{\alpha^2 \sigma}{\kappa T} \]  

where \( T \) is the temperature [K], \( \alpha \) is the Seebeck effect, \( \sigma \) is the electric conductivity and \( \kappa \) is the thermal conductivity [79, 103, 114, 116]. All physical quantities and measures are in the present thesis and in [P1-P5] given in SI base units.

3.1.1 Classes of design problems

The fundamental concept of the density-based topology optimization approach [17, 18, 91] proposed in the present study is to distribute two different materials in a one, two or three dimensional design space in order to optimize a specified performance measure. With reference to the design problem sketches in Fig. 3.2, we have studied three different classes of optimization problems in [P1-P4]: (A) diagonal problems sketched in Fig. 3.2a and inspired by [116, 117], (B) off-diagonal problems sketched in Fig. 3.2b and inspired by [80] and (C) PN problems sketched in Fig. 3.2c and inspired by [13].

With reference to Fig. 3.2, the three design problems are classified by the primary directions of the electric current and the thermal heat flux. The primary directions are either horizontal or vertical. Devices in diagonal configurations convert a vertical electric current into a vertical thermal flux or vice versa. Devices in off-diagonal configurations convert a horizontal electric current into a vertical thermal flux or vice versa. Devices in PN configurations have complex interplays between the vertical thermal flux and the electric current.

To assess the best suited configuration class for a specific type of application is a compromise between several parameters: Thermoelectric devices in diagonal configurations provide a relatively large electric power output and conversion efficiency, however the thermo-mechanical stresses and wear in the electrodes are relatively large, because they are connected directly to the hot and cold reservoirs. The thermo-mechanical stresses and wear of the electrodes are relatively smaller for devices in off-diagonal and PN configurations, however the electric power output and conversion

\[ ZT = \frac{\alpha^2 \sigma}{\kappa T} \]  

where \( T \) is the temperature [K], \( \alpha \) is the Seebeck effect, \( \sigma \) is the electric conductivity and \( \kappa \) is the thermal conductivity [79, 103, 114, 116]. All physical quantities and measures are in the present thesis and in [P1-P5] given in SI base units.
Figure 3.2: Sketches of the three classes of design problems studied in [P1-P4]. Material A and B are not necessarily the same for each design problem.

efficiency are relatively smaller compared to devices in the diagonal settings. Please notice that the notation stated on Fig. 3.2 is slightly different from [P1], but conforms with the notation used in [P2-P4].

3.1.2 The brief introduction to the concept of thermoelectricity

The concept of thermoelectric energy conversion is expounded with basis in the trivial solution\(^1\) of a diagonal thermoelectric generator in Fig. 3.2a. To resolve the thermoelectric energy conversion problem, it is required to resolve four different state fields: (A) The temperature, (B) the electric potential, (C) the heat flux and (D) the electric current density.

The temperature and electric potential fields solved for \(T^C = 0\) (temperature of the thermal cold reservoir) and \(T^H = 1000\) (temperature of the thermal hot reservoir), the material parameters of Material B in [P4] and various convection coefficients, \(h^{HC}\), have been plotted in Figs. 3.3 and 3.4.

\(^1\)all design variables are fixed to one material phase
The importance of the convection coefficients can be recognized by pairwise comparing the state field plots solved for the same model parameters in Figs. 3.3 and 3.4. Due to the Seebeck effect and Newton’s law of cooling [32, 64], the temperature and electric potential differences between $\Gamma^H$ and $\Gamma^C$ are increased as the convection coefficients are increased. A large temperature difference between $\Gamma^H$ and $\Gamma^C$ is therefore critical to maintain the effectiveness of a thermoelectric generator.

The importance of the impedance in the external electric load, $z^{imp}$, is shown in the state field plots for the electric potential in Fig. 3.4 and the electric current density in Figs. 3.5a and 3.5b. The figures demonstrate two important features: (A) thermoelectric generators in open circuit configuration, $z^{imp} = 0$, are subject to zero electric currents which means that no electric power is produced for such configurations. (B) thermoelectric generators in closed circuit configurations, $z^{imp} \neq 0$, are subject to finite electric currents which means that electric power is produced for such configurations. The electric power output of a thermoelectric generator is maximized if the internal and external electric resistances are matched in magnitude, compare this with what you already know about batteries.

The heat flux for $z^{imp} = 10^3$ and various convection coefficients have been plotted in Fig. 3.5c, 3.5d and 3.5e. The heat flux is dependent on $z^{imp}$ as the Joule heating is dependent on the electric current density and the convection coefficients. This interplay constitutes the primary non-linear coupling in thermoelectric problems.

3.1.3 Ohm’s and Fourier’s equations

With basis in Figs. 3.3, 3.4 and 3.5, the readers of this text have hopefully accepted that a temperature difference may generate an electric current in thermoelectric active materials. It is now time to consider the governing partial differential equations. Thermoelectricity is governed by the Fourier’s and Ohm’s generalized equations and
Section 3.1: Introduction

(a) electric potential field for $h^{HC} = 5$ and $z^{imp} = 10^3$
(b) electric potential field for $h^{HC} = 10^2$ and $z^{imp} = 10^3$
(c) electric potential field for $h^{HC} = 10^3$ and $z^{imp} = 10^3$
(d) electric potential field for $h^{HC} = 5$ and $z^{imp} = 0$
(e) electric potential field for $h^{HC} = 10^2$ and $z^{imp} = 0$
(f) electric potential field for $h^{HC} = 10^3$ and $z^{imp} = 0$

Figure 3.4: Electric potential fields for various convection coefficients, $h^{HC}$, and impedances in the external resistive load, $z^{imp}$. As the convection coefficients are increased the temperature difference and electric potential between $\Gamma^H$ and $\Gamma^C$ are increased. The electric potential difference is therefore both dependent on $z^{imp}$ and $h^{HC}$.

are in steady state given by [14, 79]:

\[
\frac{\partial Q_i}{\partial x_i} = \dot{q} \quad \text{in} \quad \Omega_D \quad (3.2a)
\]

\[
\frac{\partial J_i}{\partial x_i} = 0 \quad \text{in} \quad \Omega_D \quad (3.2b)
\]

\[
Q_i = T \alpha_{ij} J_j - \kappa_{ij} \frac{\partial T}{\partial x_j} \quad (3.2c)
\]

\[
J_i = \sigma_{ij} \left( E_j - \alpha_{ik} \frac{\partial T}{\partial x_k} \right) \quad (3.2d)
\]

where $Q_i$ is the heat flow density; $x_i$ is the spatial coordinates; $\dot{q} = J_i E_i$ is the Joule heating term; $T$ is the temperature; $\alpha_{ij}$ is the Seebeck coefficient; $J_i$ is the electric current density; $\kappa_{ij}$ is the thermal conductivity of the medium; $\sigma_{ij}$ is the electric conductivity of the medium; and $E_j = -\partial V/\partial x_j$ is the electric field. The tensor indices, $i$ and $j$, have two entries, $x$ and $y$, which are corresponding to the spatial directions in a Cartesian coordinate system.

These equations can the discretized with the finite element method [32, 123] by multiplying the strong forms of the equations with a suitable test functions and
integrating over the domain $\Omega$; performing integration by parts of higher dimensions on relevant terms [81]; and introducing the design field dependent interpolation functions, $\alpha_{ij} = \alpha_{ij}(\rho), \sigma_{ij} = \sigma_{ij}(\rho), \kappa_{ij} = \kappa_{ij}(\rho)$ [17, 64]. This yields the following discrete variational problem: Find $T^h \in P^h$ and $V^h \in Q^h$ such that $\forall p^h \in P^h_0$ and $\forall q^h \in Q^h_0$.

\[
\begin{align*}
\int_\Omega \frac{\partial p^h}{\partial x_i} \kappa_{ij}(\rho) \frac{\partial T^h}{\partial x_j} \, \mathrm{d}V - \int_\Gamma \frac{\partial p^h}{\partial x_i} T \alpha_{ij}(\rho) J_j \, \mathrm{d}V - \int_\Gamma p^h E_i J_i \, \mathrm{d}V &= 0 \quad (3.3a) \\
\int_\Omega \frac{\partial q^h}{\partial x_i} \sigma_{ij}(\rho) \frac{\partial V^h}{\partial x_j} \, \mathrm{d}V + \int_\Omega \frac{\partial q^h}{\partial x_i} \sigma_{ij}(\rho) \alpha_{jk}(\rho) \frac{\partial T^h}{\partial x_k} \, \mathrm{d}V + \int_\Omega z_{imp} q^h V^h \, \mathrm{d}S &= 0 \quad (3.3b)
\end{align*}
\]

Details on the derivation and implementation of Eqs. (3.2)-(3.3) can be found in [P1].
3.1.4 State of the art

Mathematical optimization approaches concerned with thermoelectric energy conversion can be sorted into three different classes: (A) functionally graded materials studies, (B) segmentation and compatibility approaches and (C) geometrical optimization approaches (size and shape). The topology optimization approach proposed in present thesis is a sub-class of (B).

Functionally graded materials studies are aiming at identifying spatial profiles of relevant material parameters which optimize a prescribed performance measure. The design solutions of functionally graded material studies are characterized by macroscopic gradients in the material parameters, which may be linked to the composition (including doping) or micro structures of the functional properties of the material, see e.g. the works of [19–21, 46, 47, 71, 83, 83]. Segmentation and compatibility approaches were originally suggested for thermoelectric generators in the work of Ursell and Snyder [104] and have later been developed in a series of studies in e.g. Seifert et al. [84, 85], Snyder et al. [94]. Segmentation approaches with two material phases for diagonal and off-diagonal problem were studied in Sakai et al. [80], Yang et al. [116, 117]. A topology optimization approach was proposed in Takezawa and Kitamura [99] and geometrical optimization (size) was studied in Hegmanns and Beitzelschmidt [50]. These design approaches and the corresponding design solutions are very different compared to the design solutions presented in the present thesis. A detailed literature review of optimization approaches for thermoelectric energy conversion can be found in [P4].

3.2 An overview of the findings

The journal papers concerned with thermoelectricity and submitted as part of the present thesis can generally be sorted in three different classes: (A) reporting on the proposed methodology, (B) design studies of thermoelectric generators and (C) design studies of thermoelectric coolers. An introduction to the proposed topology optimization methodology is laid out in [P1]. The paper contains details on the derivation and implementation of the framework. [P2,P3] are concerned with diagonal and off-diagonal thermoelectric generator design problems, respectively. The papers are primarily addressing design problems relevant for scientists in the thermoelectric society. [P4] is concerned with topology optimization problems of diagonal thermoelectric coolers. The paper has the same scope as [P2,P3]. To provide the reader with an easy accessible overview of [P1-P4], I have summarized the different branches of the studies in the following list:

1. Classes of design problems
   a) Diagonal [P1,P2,P4]
   b) Off-diagonal [P3]
   c) PN [P1]

2. Type of devices
a) Thermoelectric generators [P1,P2,P3]

b) Thermoelectric coolers [P1,P4]

3. Important model parameters

a) Objectives functions:
   i. Relevant for thermoelectric generators
      A. Electric power output [P1,P2,P3]
      B. Conversion efficiency [P1,P2,P3]
   ii. Relevant for thermoelectric coolers
      A. Cooling power [P1,P4]
      B. Coefficient of performance [P1,P4]
   i. Heat transfer rates (convection coefficients) [P1,P2,P4]
   ii. Temperatures of the thermal reservoirs [P4]
   iii. Impedance in the external resistive load [P1,P3] (relevant for thermoelectric generators)
   iv. Applied electric potential [P1,P4] (relevant for thermoelectric coolers)

b) Device geometry (height and length of the design domain) [P2,P3]

c) Material parameters [P1,P2]

The various branches of the study are further layout in the following sections.

3.2.1 Classes of design problems

The three classes of devices have already been accounted for in Sec. 3.1.1 and Fig. 3.2.

3.2.2 Type of devices

Design solutions solved in diagonal configurations and presented throughout [P1,P3,P4] have a considerable amount of similarities even through they are solved for different model parameters. As a demonstration of this statement, I have plotted two design solutions solved for different objective functions and material parameters in Figs. 3.6a and 3.6b. The design solution in Fig. 3.6a is solved for electric power output, $h^{HC} = 595$ and temperature dependent material parameters (see [P3] for more information). The design solution in Fig. 3.6b is solved for cooling power, $h^{HC} = 344$, and temperature independent materials, (see [P4] for more information). The design solutions are both governed by spike-shaped design features, even though the design solutions are obtained by solving very different design problems. The spike-shaped design features are seen in design solutions of diagonal problems for both thermoelectric generators and coolers. The design solutions solved for off-diagonal and PN design problems have been plotted in Figs. 3.6c and 3.6d, respectively [P1,P2]. These design solutions are very different, and it has not been possible to derive any general characteristics of the design features across the problem configurations.
Section 3.2: An overview of the findings

(a) diagonal  (b) diagonal  (c) off-diagonal  (d) PN

Figure 3.6: Design solutions for different classes of optimization problems and different model parameters. The design solution in (a) and (b) are solved for electric power output or cooling power in diagonal configurations, respectively [P3,P4]. The design solutions in (c) and (d) are solved for electric power output in off-diagonal or PN configurations, respectively [P1,P2].

3.2.3 Important model parameters

Throughout our studies with the topology optimization framework, we have identified several important model parameters which are relevant for both thermoelectric generators and coolers. These model parameters have already been listed in the beginning of Sec. 3.2 and I refer to the respective papers for detailed information. To demonstrate the importance of one of the model parameters, I have plotted the design solutions solved for maximum cooling and various convection coefficients in Fig. 3.7 [P4]. By comparing the design solutions in [P3,P4], it is possible to derive some general tendencies for diagonal thermoelectric generator and thermoelectric cooler problems: (A) the design solutions are governed by spike-shape design features in the transitions between the material phases for some specific magnitudes of the convection coefficients. (B) as the convection coefficients are increased, the extend of the spike-shaped design features are decreased and the transition between the material phases go toward a simple one dimensional line interface.

(a) $h^{HC} = 175$  (b) $h^{HC} = 276$  (c) $h^{HC} = 344$  (d) $h^{HC} = 412$  (e) $h^{HC} = 530$  (f) $h^{HC} = 10^3$

Figure 3.7: Design solution solved for maximum cooling power and different convection coefficients. The relationship between the convection coefficients and the topology of the design solutions is characteristic for design problems of diagonal thermoelectric generators and coolers.
3.3 Unpublished results

A design problem which did not yield obvious applicable results, but may provide guidance for future research, is expounded in this section. The study is inspired by the work of Yang et al. [116] and takes basis in the thermoelectric figure-of-merit. Yang et al. [116] show that a device consisting of two different thermoelectric materials can exceed the performance of the constitutive materials if the electric potential difference is sufficiently large when the electric conductivity is evaluated. With a point of departure in the problem sketch in Fig. 3.2a, the objective of the design problems is to increase the thermoelectric figure-of-merit by using the topology optimization approach laid out in [P1]. The material parameters used for the study are similar to those used in Yang et al. [116] aside from the thermal conductivity of the material with the lowest figure-of-merit. This parameter has been decreased such that the figure-of-merit of the two materials are equal in magnitude.

The thermoelectric figure-of-merit is computed by solving three different load-cases for each of the material parameters in Eq. (3.1). The load cases are computed with basis in two different sets of boundary conditions: (A) the Yang et al. [116] boundary conditions and (B) the perturbation boundary conditions, see [P3] for more information. By using the perturbation boundary conditions, the figure-of-merit is computed with small differences in the state fields such that the governing equations stays in the linear regime where the Joule heating is negligible. This approach is consistent with the analytic and experimental approaches seen in e.g. Rowe [79], Sakai et al. [80]. Aside from an inconsistently large electric potential difference used to evaluate the electric conductivity, the Yang et al. [116] boundary conditions are equivalent to the perturbation boundary conditions. The highly conductive surface electrodes on $\Gamma^H$ and $\Gamma^C$ in Fig. 3.2a have considerably influence on the design problems and to demonstrate this, I have decided to present design solutions solved with and without the electrodes. Two and three dimensional design solutions solved for the thermoelectric figure-of-merit, with and without surface electrodes and with the two sets of boundary conditions have been plotted in Figs. 3.8 and 3.9. By comparing the two and three dimensional design solutions across the different boundary conditions, I point out that the features of the design solutions seem quite similar.

The relationship between the figure-of-merit and the volume ratio between the two material phases, $\nu(x)$, for vertically layered unit cells, horizontally layered unit cells and the design solutions in Figs. 3.8 and 3.9 have been plotted in Fig. 3.10. With reference to the figures, I notice that it is not possible to exceed the performance of the constitutive materials if consistent boundary conditions (perturbation boundary conditions and highly conductive surface electrodes) are used in the evaluation of the objective function. Design solutions solved for the figure-of-merit do not necessarily provide good thermoelectric energy conversion properties and this optimization problem may therefore after-all have less relevance and importance, please consult the discussions in [P3] for more information.
Section 3.4: Conclusion

The general conclusions across [P1-P4] have been summarized in the following list:

1. The interplay between the objective functions, heat transfer rates, applied electric potentials (thermoelectric coolers), impedance in the external resistive load (thermoelectric generators), device dimensions and the material parameters are important for design problems of thermoelectric generators and thermoelectric coolers in diagonal, off-diagonal and PN generator configurations.

2. Design solutions solved for electric power output and thermal cooling power are in diagonal configurations governed by spike-shape design features. The
3. Modeling the thermal heat transfer between the thermal hot reservoir, the thermal cold reservoir and the thermoelectric device with convective boundary conditions (Newton’s law of cooling) seems to be an adequate modeling approach for the design problems studied in the present thesis.

4. By spatially distributing two thermoelectric materials in a two dimensional design space with the topology optimization methodology laid out in [P1], it is not possible to exceed the figure-of-merit of the constitutive materials if consistent boundary conditions is used to evaluate the material parameters.

5. The density-based topology optimization approach is best suited for complex design problems such as thermoelectric generators and coolers in PN and off-diagonal configurations.

6. The interplay between the spike-shaped design features, the convection coefficients and the design performances may provide an offset to the development of an analytical optimization approach.

7. Thermal and electric losses between the material phases are neglected in the underlying finite element routine. To include these losses are considered an important study for future research.

8. To manufacture and experimental test the design solutions and quantify the difference between the predicted and measured performance is an interesting and important study for future work.
9. To include multiple material phases in the topology optimization framework may deepen the design space, such that more complex design features are taken into consideration. This may provide larger performance improvements than those already presented.
4 Fluid-Structure-Interaction

Fluid-structure-interaction problems have been studied extensively over the recent decades [16, 27, 70], however only a limited amount of studies have been concerned with topology optimization [54, 55, 61, 78, 105, 118–120]. This chapter expounds an introduction to the main findings in [P5] and is written with the scope of providing a soft introduction for readers who are less familiar with the topic.

To achieve full profit of reading this chapter, the reader is advised to be versed in fluid mechanics [110], structural mechanics [72], computational methods for structural mechanics [32], computational methods for fluid mechanics [124] and topology optimization [17]. The structure of the chapter is the following: An introduction to fluid-structure-interaction is given in 4.1, a design problem is discussed in Sec. 4.2, and a summary of the most important conclusions is provided in Sec. 4.3.

4.1 Introduction

Fluid-structure-interaction is a strongly coupled phenomenon and concerns the interaction between a stationary or moving fluid and an elastic structure. Many engineering applications and natural phenomena are subject to fluid-structure-interaction and to take such effects into consideration is therefore critical in the design of many engineering applications [37, 40, 42, 43, 60, 86, 102, 113].

4.1.1 Classes of design problems

The fundamental concept of the density-based topology optimization approach [17, 18, 91] proposed in the present study is to distribute solid or fluid in a two-dimensional design space in order to optimize a specified performance measure. With reference to the design problem sketches in Fig. 4.1, three different design problems have been studied: (A) the wall flow problem in Fig. 4.1a, (B) the flow obstacle problem in Fig. 4.1b and (C) the fluid gripper in Fig. 4.1c.

To develop a framework which is suited for solving all three design problems is challenging, as each of the design problems put requirements on different parts of the underlying finite element formulation [P5].

4.1.2 A brief introduction to the concept of fluid-structure-interaction

The concept of fluid-structure-interaction problems is expounded with basis in the trivial\(^1\) solution of the wall flow problem in Fig. 4.1a [P5]. To resolve the fluid-structure-interaction problems studied in this thesis, it is required to resolve three different state fields: (A) the fluid velocity, (B) the fluid pressure and (C) the structural displacement. The velocity and pressure fields are related as in classical

\(^1\) all design variables fixed to the fluid phase
fluid mechanics: gradients in the fluid field result in gradients in the pressure field and vice versa. The fluid (pressure and velocity) fields and the displacement field is related though the pressure field.

The fluid velocity and the pressure fields for different Reynolds numbers, \( Re = \{1, 10, 50\} \) have been plotted in Figs. 4.2b-4.2g. The fluid and the structure is coupled via the pressure field and the direction and the magnitude of the reaction forces of the structure against the fluid pressure is plotted with the blue arrows in Fig. 4.2h. The dependency between the Reynolds number and the fluid fields is a key feature in fluid-structure-interaction problems and the design problems investigated in the present thesis. As the pressure field depend on the Reynolds number, the design problems solved for structural objective functions are also dependent on the Reynolds number. The state fields are computed in all elements (the unified formulation), however the pressure-coupling forces are only imposed on the surface of the structure. The coupling between the fluid and the structure results in structural displacements which have been plotted in Fig. 4.2i. As the unified formulation makes it rather difficult to identify the important information in the displacement field, the undeformed and deformed configurations of the design solution have been plotted in Fig. 4.2j. This figure can be used to investigate the features of the design solutions, but recall that the structural deformations aren’t influencing to the fluid field.

### 4.1.3 Navier-Cauchy and Navier-Stokes equations

It is now time to discuss the governing partial differential equations which are solved with the finite element method to obtain the state field plots in Fig. 4.2. The
Section 4.1: Introduction

Figure 4.2: State fields for the trivial solutions of the wall flow problem in Fig. 4.1a

The fluid velocity, the fluid pressure and the structural displacement are dependent on the Reynolds number, the structure and the fluid is coupled via the pressure field, and the state fields are solved in a unified formulation.

underlying physical model of the fluid-structure-interaction framework is modeled with the Navier-Cauchy and Navier-Stokes equations [32, 39, 110]. The mathematical modeling is limited to steady state, constant material properties and negligible shear stresses on the interface between the fluid and the structure. The equations are given by:
\[ \frac{\partial \sigma^s_{ij}}{\partial x_j} + f_i = 0 \quad \text{in} \quad \Omega_S \]  

\[ \sigma^s_{ij} = C_{ijkl} \varepsilon^k_{li} \]  

\[ \varepsilon^s_{kl} = \frac{1}{2} \left( \frac{\partial d_k}{\partial x_l} + \frac{\partial d_l}{\partial x_k} \right) \]  

\[ \sigma^f_{ij} = 2 \frac{\rho f}{Re} \dot{\varepsilon}^f_{ij} - \delta_{ij} p \]  

\[ \dot{\varepsilon}^f_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

\[ \frac{\partial u_i}{\partial x_j} = 0 \quad \text{in} \quad \Omega_F \]  

\[ \sigma^f_{ij} n_j = \sigma^s_{ij} n_j \quad \text{on} \quad \Gamma_{SF} \]  

where \( \sigma^s \) is the Cauchy stress tensor, \( x_j \) is the spatial variables, \( f_i \) is the external applied loads, \( C_{ijkl} \) is the structural stiffness tensor, \( \varepsilon^s_{kl} \) is the structural strains, \( d_k \) is the structural displacements, \( u_i \) is the fluid velocity, \( \sigma^f_{ij} \) is the fluid stress tensor, \( b_i \) is the fluid body forces, \( Re \) is the Reynolds number, \( \dot{\varepsilon}^f \) is the fluid strain rate, \( \delta_{ij} \) is Kronecker’s delta, \( p \) is the fluid pressure and \( n_j \) is the normal vector to the surface \( \Gamma \). The tensor indices \( i, j, k, l \) have two entries, \( x \) and \( y \), which refer to the spatial directions \( x \) and \( y \). The Reynolds number is defined as \( Re = \frac{U_{max} \rho}{\mu} \), where \( U_{max} \) is a maximum fluid velocity in the inlet, \( \rho^f \) is the fluid density, \( \mu \) is the fluid viscosity and \( L \) is the width in the inlet.

The finite element discretized equations of the Navier-Cauchy and Navier-Stokes equations are obtained by multiplying Eqs. (4.1) with suitable test functions and integrating over the domain [53]; assuming that the forces on the structure and the fluid are in equilibrium, i.e. \( \sigma^f_{ij} n_j = \sigma^s_{ij} n_j \) [39]; introducing a design variable field, \( 0 \leq \rho \leq 1 \) [18]; performing integration by parts of higher dimensions operation on the boundary load terms [81]; introducing the design dependent pressure-coupling filter function, \( \Psi = \Psi(\rho) \), on the pressure coupling terms [118]; adding a Brinkman penalization term, \( b_i = -\alpha(\rho) u_i \), to the Navier-Stokes equations [23]; introducing design-dependent material parameters for the structural stiffness \( E = E(\rho) \) and the Brinkman penalization parameter, \( \alpha = \alpha(\rho) \); and introducing Pressure-Stabilising Petrov-Galerkin (PSPG) and the Streamline-Upwind Petrov-Galerkin (SUPG) terms to suppress oscillations in the pressure and velocity fields [25, 52, 101]. The weak form of the governing equation in Eq. (4.1), can hereafter be written as the following discrete variational problem after defining the following suitable finite dimensional spaces, \( \mathcal{D}^h, \mathcal{Q}^h \) and \( \mathcal{U}^h \): Find \( d^h \in \mathcal{D}^h, p^h \in \mathcal{Q}^h \) and \( u^h \in \mathcal{U}^h \) such that \( \forall v^h \in \mathcal{D}^h \), \( \forall p^h \in \mathcal{P}^h \) and \( \forall \varphi^h \in \mathcal{U}^h \). With basis in works of [4, 54, 54, 118], the weak form of the equations is given by:
where $\Box^h$ denotes that the term has been discretized and $v^h$ denotes the basis functions and $\tau^{SU}$ and is the SUPG and PSPG stabilization parameters, respectively [4].

### 4.1.4 State-of-the-art

The topology optimization approach reported in [P5] is inspired by structural optimization approaches in Andreassen et al. [12], Sigmund [87, 89], Wang et al. [109] and fluid dynamical optimization approaches in Borrvall and Petersson [23], Gersborg-Hansen et al. [44], Yoon [118]. The approach is further related to other fluid mechanical optimization approaches such as fluid-structure-interaction problems in poroelasticity [10], transport problems [11], reactive flows problems [76], transient flows problems [34, 62], flow driven by constant body force [35] and natural convection problems [3].

Topology optimization of fluid structure interaction problems can sorted in three classes. (A) density-based methodologies, (B) bi-directional evolutionary methodologies and (C) immersed boundary methodologies. The concept of density-based topology optimization for fluid-structure-interaction problems was proposed by Yoon [118] and later applied an additional design problem in [119]. A bi-directional evolutionary topology optimization method was used to optimize structural compliance problems under design-dependent pressure loads in [78, 105]. Jenkins and Maute [54, 55] used an immersed method with explicit boundary representation, an ex-
tended finite element method and an explicit level set method to solve different fluid-structure-interaction design problems. The three different approaches have different modeling assumptions and solve different design problems, which are discussed thorough in [P5]. The proposed methodology in this study can be sorted under class (A).

4.2 An overview of the findings

Design problems concerned with fluid structure-interaction are challenging due to the deepness of the design space, the non-linearity of the underlying physics and the computational burden of the underlying finite element method. The wall flow problem in Fig. 4.1a has been studied in all three classes of optimization approaches for fluid-structure-interaction problems [54, 78, 118] and due to the large scientific interest in the problem, it is used as a point of departure to summarize the main findings of [P5].

The design solutions solved for structural compliance and \( Re = \{1, 5, 10, 40\} \) and the corresponding state fields have been plotted in Figs. 4.3, 4.4, 4.5, 4.6, respectively. The pressure field is dependent on the Reynolds number (recall the difference between Figs. 4.2e, 4.2f and 4.2g) and the design solutions are therefore adjusted to maximizing stiffness and minimizing the pressure load even though the pressure load isn’t explicitly stated in the objective function of the design problem. With reference to the pronounced relationship between the design solutions, the Reynolds number and the passed crosscheck in Tab. 4.1, I confidently conclude that the weak coupling between the fluid and the structure is adequately resolved in the design solutions. To develop a well-performing and robust methodology which provides design solutions that pass cross-checks and validation studies turned out to be much more challenging than initially assessed. To provide guidance for future research, I have discussed the most focal contributions in the following sections.

![State fields and design solutions solved for \( Re = 1 \).](image)

**Figure 4.3:** State fields and design solutions solved for \( Re = 1 \).

4.2.1 The robust formulation

To ensure length scale control and manufacturable tolerant design solutions, the design problems in [P5] are solved with the so-called robust formulation [89, 109]. Beside the original objective of the formulation, it has been proved useful in many design problems which suffered from design solutions with a considerable amount of
Section 4.2: An overview of the findings

(a) Pressure-coupling  
(b) Pressure field  
(c) Velocity field

Figure 4.4: State fields and design solutions solved for $Re = 5$.

(a) Pressure-coupling  
(b) Pressure field  
(c) Velocity field

Figure 4.5: State fields and the design solutions solved for $Re = 10$.

(a) Pressure-coupling  
(b) Pressure field  
(c) Velocity field

Figure 4.6: State fields and design solutions solved for $Re = 40$.

intermediate design variables, see e.g. [30, 74]. Design solutions with intermediate
design variables are most often providing excellent performance, however this is most
often caused by the intermediate design variables and the corresponding nonphysical
interpolation between the material phases. Design problems formulated in the robust
form are experientially less sensitive to the choice of interpolation function parameters,

Table 4.1: A cross-check study between the structural compliance and the Reynolds
number for the designs solutions in Figs. 4.3, 4.4, 4.5 and 4.6.

<table>
<thead>
<tr>
<th>Design evaluated for</th>
<th>$Re = 1$</th>
<th>$Re = 5$</th>
<th>$Re = 10$</th>
<th>$Re = 40$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Re = 1$</td>
<td>$2.8359\cdot10^{-7}$</td>
<td>$1.1579\cdot10^{-8}$</td>
<td>$3.1559\cdot10^{-9}$</td>
<td>$5.1549\cdot10^{-10}$</td>
</tr>
<tr>
<td>$Re = 5$</td>
<td>$2.8373\cdot10^{-7}$</td>
<td>$1.1411\cdot10^{-8}$</td>
<td>$3.0552\cdot10^{-9}$</td>
<td>$4.7432\cdot10^{-10}$</td>
</tr>
<tr>
<td>$Re = 10$</td>
<td>$2.9226\cdot10^{-7}$</td>
<td>$1.1478\cdot10^{-8}$</td>
<td>$2.9915\cdot10^{-9}$</td>
<td>$4.3669\cdot10^{-10}$</td>
</tr>
<tr>
<td>$Re = 40$</td>
<td>$3.8645\cdot10^{-7}$</td>
<td>$1.4423\cdot10^{-8}$</td>
<td>$3.5304\cdot10^{-9}$</td>
<td>$4.2497\cdot10^{-10}$</td>
</tr>
</tbody>
</table>
model parameters, and penalization and continuation strategies.

### 4.2.2 Interpolation functions

Topology optimization for fluid-structure-interaction problems are highly non-linear, ill-posed and non-convex and a considerable amount of parameter tuning is required to achieve well-performing design solutions. In the appendix of [P5] we presented a methodology which was used to formulate well-posed design problems. By using interpolation functions which cause strictly monotonic relationship between the objective function and some specified design variables, it was shown that the smoothness and convexity of the design problems were increased considerably. A similar approach with an equivalent outcome was used for the thermoelectric design problems in [P1-P4]. The approach can probably be generalized to all multi-physical design problems and may therefore be the most important finding in [P5].

### 4.2.3 Validations

To build confidence in the design solutions, we have in [P5] conducted various validations such as cross-check studies and body-fitted meshes studies. The cross-checks studies are used to determine how much significance we can attribute to the features of the design solutions. To compare the features of the design solutions solved for different model parameters is meaningless unless the corresponding cross-check study is conducted and passed. The design solutions presented in [P5] have all passed cross-checks for which reason we confidently concluded that the coupling between the fluid flow, the elastic structure and the optimization problem was resolved. By fitting a body-fitted mesh to the design solutions and solving the finite element problem with a segregated solver in a commercial finite element software, we realized that the Brinkman penalization parameter of the solid domains is required to be in the order of $10^9$ or larger to adequate resolve the pressure field. Too low Brinkman penalization parameters result in non-physical low pressure drops which is indeed a very fatal flaw in fluid-structure-interaction problems as the coupling between the fluid and the structure is transferred via the pressure field.

### 4.2.4 Free floating elements

By formulating the design problems with multiple weighted objective functions, we demonstrated that free-floating islands of solid elements could be removed from the design solutions. This approach is concerned with a considerable amount of parameters tuning and the level of complexity in the interpretation of the design features are increased drastically, as it is almost impossible to assess how each of the objective functions exactly influence the features of the design solutions. For future research, my advice is therefore to search for other methods which resolve the issue with free-floating island of solid elements.
4.2.5 Derivation details

The derivation of the unified finite element formulation of the fluid-structure-interaction problem is elaborated in [P5]. The discretized weak form of the governing equations in [P5] differ from the counterpart equations in Yoon [118]. The equations reported in Yoon [119] are equivalent to the equations in [P5], however it has not been possible to assess which set of equations that were actually used to solve the design problems in Yoon [118, 119].

4.3 Conclusion

The most important conclusions in [P5] have been summarized in the following list:

1. A density-based topology optimization approach is used to solve design problems for low and moderate Reynolds numbers. The framework takes basis in the finite element discretization of the Navier-Cauchy and Navier-Stokes equations. The physical modeling is limited to two dimensions, steady state, constant material properties and the coupling between the structural deformations and the fluid flow is neglected.

2. The coupling between the fluid flow, the elastic structure and the optimization problem is clearly captured and demonstrated for several design problems with different objective functions and model parameters. All design solutions are thoroughly validated with cross-checks and segregated finite element solvers with body-fitted meshes.

3. The derivation of the unified finite element formulation for fluid-structure-interaction problems is elaborated.

4. The robust formulation ensures length-scale-control of the design solutions and make the design problems less sensitive to the choice of interpolation functions, model parameters and continuation strategies.

5. The importance of solving the design problems with a “sufficiently” large Brinkman penalization parameter is reported.

6. The smoothness of the design problems can be considerable increased, by ensuring a strictly monolithic relationship between the objective function of the design problem and some specified design variables.

7. Free-floating islands of solid elements can be removed from the design solutions by solving the design problems with a multi-objective formulation.

8. The study procures new insight in the field of topology optimization for fluid-structure-interaction problems and may provide guidance for future research.
Bibliography


Publications
Publication [P1]:

A density-based topology optimization methodology for thermoelectric energy conversion problems

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Abstract
A density-based topology optimization approach for thermoelectric (TE) energy conversion problems is proposed. The approach concerns the optimization of thermoelectric generators (TEGs) and thermoelectric coolers (TECs). The framework supports convective heat transfer boundary conditions, temperature dependent material parameters and relevant objective functions. Comprehensive implementation details of the methodology are provided, and seven different design problems are solved and discussed to demonstrate that the approach is well-suited for optimizing TEGs and TECs. The study reveals new insight in TE energy conversion, and the study provides guidance for future research, which pursuits the development of high performing and industrially profitable TEGs and TECs.

Keywords
Topology optimization · Thermoelectric energy conversion · Electric power output · Conversion efficiency · Thermoelectricity · Renewable energy · Thermoelectric cooling · Thermoelectric coolers

1 Introduction
This paper presents a density-based topology optimization approach for thermoelectric (TE) energy conversion problems. The approach concerns the optimization of thermoelectric generators (TEGs) and thermoelectric coolers (TECs). The framework supports convective heat transfer boundary conditions, temperature dependent material parameters and relevant objective functions. Comprehensive implementation details of the methodology are provided, and seven different design problems are solved and discussed to demonstrate that the approach is well-suited for optimizing TEGs and TECs. The study reveals new insight in TE energy conversion, and the study provides guidance for future research, which pursuits the development of high performing and industrially profitable TEGs and TECs.

Thermoelectric energy conversion is described by two separately identified effects: the Seebeck effect and the Peltier effect. The Seebeck effect concerns the conversion of thermal energy into electric energy and the Peltier effect concerns the conversion of electric energy into thermal energy (Rowe 2005; Goldsmid 2009). TE energy conversion is an interesting and important engineering field due to the globally increasing demand on non-polluting and renewable energy resources. The increasing demand is predicted by many researchers to be partly covered by TE energy conversion in e.g. large scale commercial waste heat recovery and cooling applications (Champier 2017). Improvements in efficiencies of thermoelectric generators (TEGs) and thermoelectric coolers (TECs) are required to make TE energy conversion economically profitable and competitive with conventional waste heat recovery and cooling technologies (Vining 2009). As TE energy conversion is predicted to have large-scale application perspectives, a topology optimization approach as presented in this study, may be used to reach important performance improvements. The topology optimization approach provides a road to systematically optimize an arbitrary TE energy conversion problem with respect to realistic boundary conditions, arbitrary dimensions and length-scales, realistic non-linear material parameters and relevant objective functions.

Thermoelectric energy conversion is described by two separately identified effects: the Seebeck effect and the Peltier effect. The Seebeck effect concerns the conversion of thermal energy into electric energy and the Peltier effect concerns the conversion of electric energy into thermal energy (Rowe 2005; Goldsmid 2009).

A TE device (thermoelectric generator (TEG) or thermoelectric cooler (TEC) is sketched in Fig. 1a, and a TE module is sketched in Fig. 1b. With reference to Fig. 1a, a TE device consists of three major parts: legs consisting of TE active materials which drive the TE energy conversion (components colored with blue and yellow); electric conductors which connect the TE legs electrically (components colored with gray) and substrates which constitute the interface between the heat source and cooling sink (components colored with dark gray). With reference to Fig. 1b, a TE module consists of two dissimilar types of semiconductors: n-types legs which are charged negatively and p-types legs

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Fig. 1 A schematic of a TE device and TE module

which are charged positively. If \( p \) and \( n \)-type legs are subject to a temperature gradient in the same direction, the legs will generate electric potential gradients in opposite directions. If a \( p \) and \( n \)-type legs are subjected to an electric potential difference in different directions, the legs will be subject to heat fluxes in the same direction. The TE device in Fig. 1 is electrically in series and thermally in parallel. This configuration is utilized to build up a working electric potential over the device for TEGs and direct the thermal energy transfer from one surface to the other for TECs.

The efficiency of TE devices depends on the type of TE active materials utilized. The efficiency of a TE material is positively correlated with the Seebeck coefficient, \( \alpha \), positively correlated with the electric conductivity, \( \sigma \), and negatively correlated with the thermal conductivity, \( \kappa \). A high \( \alpha \) facilitates a large amount of Seebeck and Peltier work for a given temperature gradient or electric potential gradient. A high \( \sigma \) facilitates a low electric energy loss due to Joule heating. A low \( \kappa \) facilitates a large temperature gradient between the heat source and the cooling sink. The TE figure-of-merit, \( ZT = \alpha^2\sigma/\kappa T \), where \( T \) is the temperature [K], is prone to much scientific attention in the thermoelectric society (Yang et al. 2012; Yamashita et al. 2003; Tritt and Ma 2006), as the magnitude of \( ZT \) of a TE material is positively correlated with the ability and efficiency of the material to carry out thermoelectric energy conversion. However, we believe that the end goal device application is a better performance measure than \( ZT \), for which reason we in this study focus on objectives such as electric power output, \( f_P \), electric conversion efficiency, \( f_\eta \), temperature, \( f_T \), thermal heat flux, \( f_Q \) and coefficient of performance \( f_\mu \).

The topology optimization approach presented in this study takes basis in the idea of distributing two different TE active materials in a two dimensional design space in order to optimize for a performance measure such as \( f_P \), \( f_\eta \), \( f_T \), \( f_Q \) or \( f_\mu \).

Topology optimization for TE energy conversion problems are related to the topology optimization of piezoelectric actuators with respect to the governing physics and the boundary conditions. Piezoelectric actuators have been investigated in the e.g. Sigmund (1998).

A topology optimization approach for TEGs has been proposed previously in the work by Takezawa and Kitamura (2012). Takezawa and Kitamura proposed a single material COMSOL-based topology optimization framework which supported \( f_P \) and \( f_\eta \) objectives and temperature dependent materials. The design solutions were primarily governed by an active volume constraint, a solid-void material phase formulation, an L-shaped design domain and fixed temperature boundary conditions between the boundaries of heat source and cooling sink. The methodology proposed in this study facilitates a completely different design problem, as two TE material phases are distributed in the design space. The configuration with two design phases and no void in the design domain complies with realistic configurations of TEGs and TECs.

Heghmanns and Beitelschmidt (2015) presented a genetic approach to optimize the electric power output and the thermo-mechanical-stress for TEGs. Heghmanns and Beitelschmidt parameterized the height of the insulators; and the number, the width and the height of the TE legs. Such approaches are not applicable to topology optimization as discussed in Sigmund (2011).

Analytically founded approaches for TEGs have been presented in the works of Yang et al. (2012, 2013), Sakai et al. (2014) and Ursell and Snyder (2002). The approaches took basis in two materials phase optimization for the non-dimensional figure-of-merit, the electric power output and the conversion efficiency for segmented and off-diagonal
problems. All these approaches were limited to fixed temperature boundary conditions, simple topological design solutions and constant material parameters.

The topology optimization approach presented in this study supports TEGs and TECs relevant application objectives, physically realistic convective heat transfer boundary conditions, temperature dependent material parameters, and full control of length-scales and device dimensions. The numerical framework provides a road to systematic optimization of TEGs and TECs in industrially relevant settings. The study demonstrates that optimal geometric designs of TEGs and TECs depend on many factors, such as material parameters, boundary conditions, length-scales, model dimensions and objective functions. Furthermore, it is possible to achieve design performance of two materials which exceed the performance of the individual materials. The primary aim of the study is to communicate the methodology and test the approach on academic problems, however, the approach can straightforwardly be applied to other and/or industrially relevant designs problems.

The paper is organized as follows. The physical model is introduced in Section 2, the finite element formulation is introduced in Section 3, the topology optimization framework is introduced in Section 4, the implementation details are covered in Section 5, numerical examples are presented in Section 6, and finally, Section 7 contains discussions and conclusions.

2 Physical model

The continuity of thermal energy and electric charge is in an arbitrary domain, \( \Omega \), given by:

\[
\nabla_x \cdot \mathbf{Q} = \dot{\mathbf{q}} \quad \text{in} \quad \Omega \tag{1}
\]

\[
\nabla_x \cdot \mathbf{J} = 0 \quad \text{in} \quad \Omega \tag{2}
\]

where \( \mathbf{Q} \) is the heat flow density [W/m\(^2\)]; \( \nabla_x \) denotes the spatial derivative with respect to Cartesian directions \( x \) and \( y \); \( \dot{\mathbf{q}} = \mathbf{J} \cdot \mathbf{E} \) is the Joule heating term [W/m\(^3\)]; \( \mathbf{E} = -\nabla V \) is the electric field [V/m] and \( \mathbf{J} \) is the electric current density [A/m\(^2\)]. In thermoelectric analysis, the thermal and electric energies are coupled by the constitutive equations (Rowe 2005):

\[
\mathbf{Q} = T \mathbf{\alpha} \cdot \mathbf{J} - \kappa \cdot \nabla_x T \tag{3}
\]

\[
\mathbf{J} = \sigma \cdot (\mathbf{E} - \mathbf{\alpha} \cdot \nabla_x T) \tag{4}
\]

where \( T \) is the temperature [K]; \( V \) is the electric potential; \( \mathbf{\alpha} \) is the Seebeck coefficient [V/K]; \( \kappa \) is the thermal conductivity [W/m-K] and \( \sigma \) is the electrical conductivity [S/m]. The material parameters are temperature dependent for which reason \( \alpha = \alpha(T), \sigma = \sigma(T), \kappa = \kappa(T) \). The boundary conditions for (1)-(4) are:

Fixed electric potential: \[ V = c_1 \] (5a)

Fixed temperature: \[ T = c_2 \] (5b)

Thermal insulation: \[ \mathbf{n} \cdot \mathbf{Q} = 0 \] (5c)

Electric insulation: \[ \mathbf{n} \cdot \mathbf{J} = 0 \] (5d)

Electric current in outer load: \[ \mathbf{n} \cdot \mathbf{J} = c_3 \] (5e)

Electrodes on boundary: \[ \mathbf{r} \cdot \mathbf{J} = c_4 \] (5f)

Convective heat transfer: \[ \mathbf{n} \cdot \mathbf{Q} = c_5 \] (5g)

where \( \mathbf{n} \) is a vector normal to the boundary, where the boundary condition is imposed; \( \mathbf{r} \) is a vector perpendicular to the boundary where the boundary condition is imposed; and \( c_1, c_2, c_3, c_4 \) and \( c_5 \) are numbers larger than 0. The electric current in the external resistive load is given by:

\[
\mathbf{n} \cdot \mathbf{J} = z_{imp} (V - V_{fl}) \tag{6}
\]

where \( z_{imp} \) is the impedance of the resistive load [m/S] and \( V_{fl} \) is a reference electric potential [V]. The electric current in surfaces electrodes is given by:

\[
\mathbf{r} \cdot \mathbf{J} = \sigma_{per} V \tag{7}
\]

where \( \sigma_{per} \) is the conductivity of the surface electrode [S/m]. The heat transfer due to convection is given by:

\[
\mathbf{n} \cdot \mathbf{Q} = h_{conv}(T - T_{fl}) \tag{8}
\]

where \( h_{conv} \) is the convective heat transfer coefficient [W/m\(^2\)] and \( T_{fl} \) is the temperature of the ambient [K].

3 Finite element formulation

The topology optimization approach takes basis in the idea of spatially distributing two different material phases, \( \Omega_A \) and \( \Omega_B \) in a design space \( \Omega_{D} \), in order to optimize for some performance measure. With basis in (1)-(4), \( \Omega_A \) and \( \Omega_B \) are initially clearly separated by a well-defined boundary \( \Gamma \). The material phases represent two different TE active materials, Material A and Material B. The equations are rewritten in a unified domain formulation, where no well-defined boundary between the material phases is required, by introducing a design variable field, \( 0 \leq \rho \leq 1 \), so that (1)-(4) become a functional of the design field, i.e. \( \alpha(T) = \alpha(T, \rho), \sigma(T) = \sigma(T, \rho) \) and \( \kappa(T) = \kappa(T, \rho) \). A schematic of the concept of the unified domain, the design variable field and the corresponding boundary conditions in (5a-5g) have been sketched in Fig. 2. Elements with \( \rho = 0 \) behave physically like Material A; elements with \( \rho = 1 \) behave physically like Material B; and elements with \( 0 < \rho < 1 \) are in an intermediate state between Material A and Material B. The thermal and electrical contact resistances in the transition between the materials are neglected.
The discretized finite element equations are obtained by multiplying the strong forms of the equations in (1)–(4) with a suitable test function; integrating over the domain; performing integration by parts of higher dimensions on relevant terms; and introducing the design field dependent interpolation functions (Yushanov et al. 2011; Antonova and Looman 2000; Cook et al. 2007).

The unified version of (1)–(4) are discretised using bilinear quadrilateral finite elements with linear shape functions. The discrete variational problem is based on the Galerkin method where suitable finite dimensional solution spaces are introduced. Without further details, the discretized finite element equations are obtained by (Antonova and Looman 2000; Cook et al. 2007):  

$$\begin{bmatrix} K^{TT}(\rho, T) + H^{TT} & 0 \\ K^{VT}(\rho, T) & K^{VV}(\rho, T) + H^{VV} + H^{VT} \end{bmatrix} \begin{bmatrix} T \\ V \end{bmatrix} = \begin{bmatrix} Q^T(T, V) + Q^E(T, V) \\ 0 \end{bmatrix} \quad (9)$$

where $K^{TT}$ is the thermal stiffness matrix; $H^{TT}$ is the heat transfer due to convection stiffness matrix; $K^{VT}$ is the electric stiffness matrix; $K^{VV}$ is the Seebeck stiffness matrix; $H^{VV}$ is the electric resistance in outer load stiffness matrix; $H^{VT}$ is the electric conductivity of the surface electrode stiffness matrix; $Q^T$ is the Peltier heat load vector; and $Q^E$ is the Joule heating load vector. Lower case letters denote generally element stiffness matrices and vectors, and capital letters denotes generally global stiffness matrices and vectors. The global system matrices and load vectors in (11a) are assembled from the local stiffness matrices with a standard finite element assembly procedure:

$$K^{TT} = \sum_{e=1}^{N} k^{TT}_e, \quad H^{TT} = \sum_{e=1}^{N} k^{VT}_e, \quad ... \quad (10)$$

The element system matrices are given by:

$$k^{TT} = \int_{\Omega} B^T \kappa B \, dV \quad (11a)$$
$$h^{TT} = \int_{\Gamma} h_{conv} N^T N \, dS \quad (11b)$$
$$k^{VV} = \int_{\Omega} B^T \sigma B \, dV \quad (11c)$$
$$k^{VT} = \int_{\Omega} B^T \alpha B \, dV \quad (11d)$$
$$h_1^{VV} = \int_{\Gamma} \zeta_{imp} N^T N \, dS \quad (11e)$$
$$h_2^{VV} = \int_{\Gamma} \sigma_{per} N^T N \, dS \quad (11f)$$
$$q^P = \int_{\Omega} B^T \tau \alpha J \, dV \quad (11g)$$
$$q^E = \int_{\Omega} N^T B^T V^T J \, dV \quad (11h)$$

where $\alpha$ is the Seebeck coefficient; $\sigma$ is the electric conductivity matrix; $\kappa$ is the thermal conductivity matrix; $N$ is the matrix of element shape functions; $B$ is the derivative of $N$, i.e. $B = \nabla N$, $T_e$ and $V_e$ are the element temperature and element electric potentials, respectively, and are given by:

$$V_e = N^T v \quad (12)$$
$$T_e = N^T t \quad (13)$$

where $t$ and $v$ are the nodal element temperatures and electric potentials. The element electric current density and the element heat flux can now be computed as:

$$J(T, V) = -\sigma B^T V_e - \sigma \alpha B^T T_e \quad (14)$$
$$Q(T, V) = T_e \alpha J - \kappa B \quad (15)$$

where the element material parameter matrices are given by:

$$\alpha(\rho, T) = \begin{bmatrix} \alpha_{xx}(\rho, T) & \alpha_{xy}(\rho, T) \\ \alpha_{xy}(\rho, T) & \alpha_{yy}(\rho, T) \end{bmatrix} \quad (16a)$$
$$\sigma(\rho, T) = \begin{bmatrix} \sigma_{xx}(\rho, T) & \sigma_{xy}(\rho, T) \\ \sigma_{xy}(\rho, T) & \sigma_{yy}(\rho, T) \end{bmatrix} \quad (16b)$$
$$\kappa(\rho, T) = \begin{bmatrix} \kappa_{xx}(\rho, T) & \kappa_{xy}(\rho, T) \\ \kappa_{xy}(\rho, T) & \kappa_{yy}(\rho, T) \end{bmatrix} \quad (16c)$$

The material parameters are in this study assumed isotropic, so $\alpha_{xy} = \sigma_{xy} = \kappa_{xy} = 0$. However, the framework can easily support anisotropic materials, simply by imposing non-zero values of the material parameters in the off-diagonal in (16a–16c). The Seebeck coefficient, the electric conductivity and the thermal conductivity are
interpolated between Material A and B by the following interpolation functions:

\[ \sigma_{ij}(\rho) = \frac{\kappa_{ij}^A(1 - \rho)\sigma_{ij}^A + \kappa_{ij}^B \rho \sigma_{ij}^B}{\kappa_{ij}^A(1 - \rho) + \kappa_{ij}^B \rho} \]  
(17a)

\[ \sigma_j(\rho) = \frac{\sigma^A_j(1 - \rho) + \sigma^B_j \rho}{\kappa_j^A(1 - \rho) + \kappa_j^B \rho} \]  
(17b)

\[ \kappa_{ij}(\rho) = \frac{\kappa_{ij}^A(1 - \rho) + \kappa_{ij}^B \rho}{\kappa_{ij}^A(1 - \rho) + \kappa_{ij}^B \rho} \]  
(17c)

where the indices \( i \) and \( j \) can take the values \( x \) and \( y \), and \( \kappa_{ij}^A, \kappa_{ij}^B, \sigma_{ij}^A, \sigma_{ij}^B, \sigma_j^A, \sigma_j^B \) are the interpolation functions in \((16a – 16c)\). The interpolation functions in \((17a – 17c)\) describe the relationship between two materials interpolated between Material A and B by the following interpolation functions:

4.1 Problem definition

The optimization problem is formulated in a min/max form for \( k \in \{1, 2, \ldots, N^k\} \) projected realizations of the design variable field to ensure length-scale control and robustness toward manufacturing variations (Sigmund 2009; Wang et al. 2011). The so-called robust formulation is given by:

\[
\min_{\rho} \max_k \left( f^k \right) \quad \text{s.t.} \quad R_k^T \rho = 0, \quad 0 \leq \rho \leq 1, \quad \forall \rho \in \Omega_D
\]  
(19)

The optimization problem in (19) is solved for three realizations \( N^* = 3 \), denoted the eroded, the nominal and the dilated designs, respectively. The nominal design variable field is plotted throughout in this paper.

4.2 Adjoint sensitivities

The gradients of the objective function with respect to the design variable field are required in order to solve the optimization problem in (19). The sensitivities of the \( k \)’th design realization, \( dL^k / d\rho \), where \( L \) is the general Lagrangian functional, are computed by the discrete adjoint approach (see Bendsoe and Sigmund 2003 and the references therein). The discrete adjoint approach requires the solution of the nonlinear forward problem in (18) and an additional linear adjoint problem:

\[
- \left( \nabla_{\rho^T} R \right)^T \lambda^k = \left( \nabla_{\rho^T} f^k \right)^T
\]  
(20)

where \( \lambda^k \) is the vector of adjoint variables and \( \nabla^T \) denotes the matrix or vector transpose operation. The term is (20) is written as:

\[
\frac{dL^k}{d\rho} = d f^k = \nabla_{\rho^T} f^k - (\lambda^k)^T \nabla_{\rho^T} R^k
\]  
(21)

where \( \rho \) denotes the design variable vector, \( \nabla \) denotes the total derivative and \( \nabla^T \) denotes the partial derivative. Dropping the design realization notation, the tangent residual matrix, \( \nabla_\rho R \), in (20) is given by:

\[
\nabla_\rho R = \nabla_\rho M \cdot S - \nabla_\rho F
\]  
(22)

where

\[
\nabla_\rho M \cdot S = \left[ \begin{array}{cc}
\nabla_{\rho^T} K_{TT} \cdot T & 0 \\
\nabla_{\rho^T} K_{TV} \cdot T + \nabla_{\rho^T} K_{VV} \cdot V & 0
\end{array} \right]
\]  
(23)

and

\[
\nabla_\rho F = \left[ \begin{array}{cc}
\nabla_{\rho^T} Q^F + \nabla_{\rho} Q^E & \nabla_{\rho} Q^E + \nabla_{\rho^T} Q^F \\
0 & 0
\end{array} \right]
\]  
(24)

Here, \( \nabla_{\rho^T} \nabla \) and \( \nabla_{\rho^T} \nabla \) denote the derivative of \( \nabla \) with respect to \( T \) and \( V \), respectively. The dot product notation \( [\cdot] \) between a matrix and a vector corresponds to sum over the nearest indices in tensor notation: If \( A \) is a matrix and \( b \) is a vector, then \( A \cdot b \) is equivalent to \( A_i b_i \) in tensor notation. Notice that (22) is zero if the material parameters are assumed temperature independent. The tangent residual matrix with respect to the design variable field is given by:

\[
\nabla_{\rho^T} R = \left[ \begin{array}{cc}
\nabla_{\rho^T} K_{TT} \cdot T - \nabla_{\rho^T} Q^F + \nabla_{\rho^T} Q^E \\
\nabla_{\rho^T} K_{TV} \cdot T + \nabla_{\rho^T} K_{VV} \cdot V
\end{array} \right]
\]  
(25)

The adjoint load \( \nabla_{\rho^T} f \) and the load in (21), \( \nabla_{\rho^T} f \), depend on the objective function and these terms will be accounted for in relevant sections.
4.3 Filters and Projection Strategy

The physical design variables, $\tilde{\rho}_i$, are used in the FE analysis and are obtained by the projection:

$$\tilde{\rho}_i^k = \frac{\tanh(\beta(\tilde{\rho}_i^k)) + \tanh(\beta(\tilde{\rho}_i^k - \eta^k))}{\tanh(\beta(\tilde{\rho}_i^k)) + \tanh(\beta(1 - \eta^k))}$$  \hspace{1cm} (26)

where $\eta^k$ is the projection filter threshold. The filtered design variables $\tilde{\rho}_i$ are obtained from the mathematical design variables, $\rho_i$, by the filter operation:

$$\tilde{\rho}_i = \sum_{j \in N_i} w(x_j) v_j \rho_j$$ \hspace{1cm} (27)

where $v_j$ is the area of the $j$th element, $N_i$ is the index set of the design variables which are within the radius $R$ of design variable $i$, $w(x)$ is the filter weighting function and $x_i$ and $x_j$ are the spatial location of elements $i$ and $j$. The filter weighting function is given by:

$$w(x_j) = \begin{cases} R - |x_j|, & \forall x_j \leq R \wedge x_j \in \Omega_D \\ 0, & \text{otherwise} \end{cases}$$ \hspace{1cm} (28)

where $R$ is the filter radius, $|x_j| = x_i - x_j$.

Finally, gradients with respect to design variables, $\rho_i$, require a transformation of the sensitivities by the chain rule:

$$\frac{\partial L}{\partial \rho_i} = \sum_{j \in \Omega_D} \frac{\partial f^j}{\partial \rho_i} \frac{\partial \tilde{\rho}_j^k}{\partial \rho_j}$$ \hspace{1cm} (29)

5 Implementation

The finite element equations and sensitivities are derived in Maple and implemented in Matlab. The electric current density $J$ and the thermal heat flux $Q$ are evaluated in the centers of the elements. The finite element implementation has been verified with the commercial finite element software COMSOL and analytic derivations from Yang et al. (2012) and Rowe (2005).

The optimization problems are solved using the method of moving asymptotes (Svanberg 1987) with the standard settings and a move limit of 0.25. The Heaviside projection parameter is updated every 50th design iteration after the scheme: $\beta = \{4, 8, 16, 32, 64, 128\}$. The design process is stopped when $\beta = 128$ and the design process is converged, i.e. when the max difference between the design variables in iteration $k$ and $k - 1$ is less than 0.1%.

The projection filter threshold values for the eroded, nominal and dilated designs are $\eta^k = \{0.3, 0.5, 0.7\}$, respectively. The density filter radius $R$ is chosen to provide a physical minimum length scale, relative to the design domain height, $L_y$, of 0.05 (see Wang et al. 2011 for more informations).

The robust topology optimization formulation ensures length-scale control and manufacturable designs, and the choice of interpolation functions provide, to our experience, well-posed and fast converging optimization problems.

6 Numerical examples

To demonstrate the capability and versatility of the density-based topology optimization approach presented in Section 4, we have solved and discussed seven different optimization problems for various boundary conditions, objective functions and material parameters. The numerical examples take basis in the schematic in Fig. 3 which illustrates an isolated leg of a TE module in Fig. 1b. The design domain, $\Omega_D$, is rectangular with length $L_x$ and height $L_y$. The northern, southern, eastern and western surfaces of the design domain are denoted $\Gamma_N$, $\Gamma_S$, $\Gamma_E$ and $\Gamma_W$, respectively. The thermal energy entering $\Omega_D$ through $\Gamma_N$, $\Gamma_S$, $\Gamma_E$ and $\Gamma_W$ is modeled by convective heat transfer with convection coefficients $h_{conv}^N, h_{conv}^S, h_{conv}^E$ and $h_{conv}^W$ and reference temperatures $T_{ref}^N, T_{ref}^S, T_{ref}^E$ and $T_{ref}^W$, respectively. If convection coefficients $h_{conv}^N, h_{conv}^S, h_{conv}^E$ and $h_{conv}^W$ are equal they may be denoted $h_{conv}^N$, to simplify the notation. An outer resistive load (for TEG problems) or an electric potential difference (for TEC problems) is applied between $\Gamma_W$ and $\Gamma_E$. The optimization problems are solved for $L_x = L_y = 0.01$ and $\Omega_D$ is discretized into $100 \times 100$ finite elements.

The approach presented in Sections 3–4 supports arbitrary combinations of temperature dependent and independent material parameters, model dimensions and boundary conditions provided that the material parameters
are in a range where the Newton solver is numerically stable. Three different sets of material parameters with different characteristics have been listed in Table 1. The constant material parameters are named after the authors of the papers in which the material parameters have been found. The color map used to present design solutions is chosen such that blue corresponds to Material A and yellow corresponds to Material B.

The relationships between $\alpha$, $\sigma$, $\kappa$ and $T$ for the temperature dependent material parameters have been plotted in Fig. 4. The temperature dependent materials are self-invented and do not refer to any physical materials. The blue curves are Material A and the yellow and black curves are Material B. Please notice the similarity between the colors of the curves and the colors of the materials phases in Table 1 and the design solutions. The relationships between $\alpha$, $\sigma$, $\kappa$ and $T$ are chosen such that complex interactions between the material parameters occur in the temperature range between 0 and 1000 K. The temperature dependent material parameter set is purely academic and is primarily serving as a demonstration of the framework. However, physical realistic materials can easily be implemented if the polynomial relationships between the temperature and the material parameters are known.

The convection coefficients for various flow types and flow conditions have been listed in Table 2. These values are basis for the convection boundary conditions of the design problems discussed in the following sections.

In the following sections we will consider seven different optimization problems: In Section 6.1.1–6.1.2 we optimize TEGs for electric power output and conversion efficiency. We optimize TECs for temperature in Section 6.2.1, for heat flux in Section 6.2.2 and for coefficient of performance in Section 6.2.3. In Section 6.3 we optimize TEGs for electric power output and conversion efficiency for asymmetric boundary conditions. Finally, in Section 6.4 we investigates an electric power output design problem for so-called $p$-$n$ generators.

6.1 Thermoelectric generators

We aim at optimizing for two different objective functions for TEGs: The electric power output, $f_P$, and the electric conversion efficiency, $f_\eta$. The boundary conditions for the $f_P$ problem are summarized in Table 3. The problem setup is inspired by waste heat recovery applications in e.g. power plants, where designers aim at maximizing electric power production by utilizing the thermal energy exchange between hot exhaust gas and the cold ambient. $h_{E,\text{conv}}$ and $h_{W,\text{conv}}$ control the magnitude of the thermal input available in the hot and the cold reservoirs. If $h_{E,\text{conv}} = 0$ there is no thermal energy available. If $h_{E,\text{conv}} = \infty$ (equivalent to fixed boundary conditions) there is an infinite amount of
energy available. The convection coefficients depend on the flow types on \( \Gamma^E \) and \( \Gamma^W \), however physical convection coefficients are somewhere in between these (nonphysical) extremes, compare with Table 2. A comprehensive review of heat transfer mechanics in TE materials and devices is discussed in Tian et al. (2014).

### 6.1.1 Electric power output

The first numerical example aims at optimizing the electric power output, \( f_P \), by converting the thermal heat inputs on \( \Gamma^E \) and \( \Gamma^W \) into electric energy. TEGs are similar to batteries in electric circuits: To maximize the electric power output, it is necessary to match the internal and external resistance of the TEG. The electric power output objective is in weak form given by:

\[
f_P = \frac{1}{L_y} \int_{\Gamma^E} V \, dS \int_{\Gamma^E} J_x \, dS
\]

which can be rewritten in what we call finite element form as:

\[
f_P = \left( \sum_{i \in N_E} \frac{1}{L_{N_i}} V_{N_i} \right) \sum_{j \in M_E} J_j
\]

where \( N_E \) is the index sets of the nodes on \( \Gamma^E \) and \( M_E \) is the \( x \)-directional index sets of the \( x \) and \( y \) directions of the centers of the elements on \( \Gamma^E \). By introduction of the vectors \( L_{N_i}^T \) and \( L_{M_i}^T \), (31) can be written in the following form:

\[
f_P = \left( L_{N_i}^T V \right) \left( L_{M_i}^T J \right)
\]

Computing the gradients of the objective function with respect to the state field, \( \nabla_S f_P \), provides at this instance all terms in (31). \( \nabla_S f_P \) is given by:

\[
\nabla_S f_P = \left\{ \left( L_{N_i}^T V \right) \left( L_{M_i}^T V_J \right) + L_{N_i}^T \circ \left( L_{M_i}^T J \right) \right\}
\]
where $\odot$ denotes the Hadamard product (element wise multiplication).

The $f_P$ optimized designs for various $h_{EW}$ have been plotted in Fig. 5. The design solutions are based on the temperature dependent material parameters in Table 1 and Fig. 4. The design solutions are indeed dependent on $h_{EW}$. Low magnitudes of $h_{EW}$ result in "spike-shaped" transitions between the two material phases. Large magnitudes of $h_{EW}$ result in abrupt transitions between the two material phases. The spike-shaped design features enable the designs to perform in an intermediate state between the two design phases. Design problems solved for large $h_{EW}$ prefer a relatively larger amount of Material B compared to design problems solved for low $h_{EW}$. The design optimized for $h_{EW} = 10000$ has two transitions between the two material phases. This design feature is caused by Material B’s large magnitude of $\alpha$ for large $T$, confer Fig. 4. To provide additional insight, Fig. 6 plots the relationships between the temperature along the spatial direction, $x$, for the design solutions in Fig. 5. The figure shows the relationships between $T_{EW}$ and the temperature fields. The temperature difference between $T^E$ and $T^W$ is controlled by the magnitude of $h_{EW}$, where a large $h_{EW}$ yield a large temperature difference and vice versa. Increasing $h_{EW}$ causes the temperatures on $T^E$ and $T^W$ to approach $T_{EW}^f$ and $T_{EW}^s$, respectively.

$$f_P = \frac{(L_\eta^T \mathbf{T})(L_\eta^T \mathbf{J})}{L_\eta^T \mathbf{Q}}$$ (35)

6.1.2 Conversion efficiency

In the second numerical example we aim at optimizing the TE conversion efficiency, $f_\eta$. The boundary conditions and material parameters for this problem are similar to the boundary conditions and material parameters for the $f_P$ problem in Section 6.1.1. The electric conversion efficiency is in implementation form given by:

$$f_\eta = \frac{(L_\eta^T \mathbf{T})(L_\eta^T \mathbf{J})}{L_\eta^T \mathbf{Q}}$$
Fraction symbols are in implementation notation interpreted as elementwise vector division. With reference to (20) and (21), $\nabla \rho f_\eta$ and $\nabla S f_\eta$ can now be computed as:

$$\nabla \rho f_\eta = \left( L_N^T V \right) \left( L_M^T J \right) L_M^T Q - \left( L_N^T V \right) \left( L_M^T J \right) \nabla \rho Q L_M^T \left( Q \circ Q \right)$$

(36a)

$$\nabla S f_\eta = \left\{ \begin{array}{l} \left( L_N^T V \right) \left( L_M^T J \right) \nabla T \left( Q \circ Q \right) \\ \left( L_N^T V \right) \left( L_M^T J \right) \nabla \left( Q \circ Q \right) \end{array} \right\}$$

(36b)

The design solution for the $f_\eta$ design problem have been plotted in Fig. 7. Two design features are similar to the $f_P$ design problem in Section 6.1.1: The spike-shaped transitions between the material phases for low $h_{EW}$ and the design solution dependency of $h_{EW}$ for high $T$. The two transitions between the two material phases for $h_{EW} = 10000$ are not observed for this optimization problem, which may be explained by the high magnitude of $\kappa_B$ for high magnitudes of $T$, confer Fig. 4. The high $\kappa_B$ for high $T$ decreases the effective thermal conductivity of the design which allow passage of more thermal heat from $\Gamma_W$ to $\Gamma_E$. The available energy in the hot and cold reservoirs is controlled by the magnitude of $h_{EW}^{con}$ and $h_{EW}^{con}$. With reference to Fig. 3, $h_{EW}^{con} = 0$ is equivalent as cooling into a completely insulated boundary. $h_{EW}^{con} = \infty$ is equivalent as cooling into an infinitely large heat reservoir. A convection coefficient model parameters, well-chosen interpolation functions and the diffusion-type nature of the governing physics. By comparing the convergence plot and the design evolution in Figs. 8–9, we notice that the difference in objection functions between the spike-shaped designs the abrupt transitions design is small for this particular example.

### 6.2 Thermoelectric coolers

In TEC problems, we consider three different objective functions: the temperature average, $f_T$, the heat flux, $f_Q$, and the coefficient of performance (COP), $f_\mu$. The problem setup is inspired by a household refrigerator and takes basis in the design problem sketched in Fig. 3. The boundary conditions are listed in Table 4. A TEC is utilized to transfer energy from the thermal cold reservoir on $\Gamma_E$ to the thermal hot reservoir on $\Gamma_W$ by converting the electric energy imposed via an electric potential difference between $\Gamma_E$ and $\Gamma_W$ into cooling energy on $\Gamma_E$. The available energy in the hot and cold reservoirs is controlled by the magnitude of $h_{EW}^{con}$ and $h_{EW}^{con}$. With reference to Fig. 3, $h_{EW}^{con} = 0$ is equivalent as cooling into a completely insulated boundary. $h_{EW}^{con} = \infty$ is equivalent as cooling into an infinitely large heat reservoir. A convection coefficient
in both of these extremes are nonphysical. Some physically realistic convection coefficients have been listed in Table 2 for comparison.

6.2.1 Temperature

The third optimization problem aims at optimizing \( f_T \) objective which in implementation form is given by:

\[
f_T = L N T \tag{37}
\]

With reference to (20) and (21), \( \nabla \rho f_T \) and \( \nabla S f_T \) can now be computed as:

\[
\nabla \rho f_T = 0 \tag{38a}
\]

\[
\nabla S f_T = \left\{ L N T \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right\} \tag{38b}
\]

Table 4 Boundary conditions for the \( f_T, f_Q, f_\mu \) optimization problems

<table>
<thead>
<tr>
<th>Boundary</th>
<th>( f^N )</th>
<th>( f^S )</th>
<th>( f^E )</th>
<th>( f^W )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_{fl} )</td>
<td>-</td>
<td>-</td>
<td>300</td>
<td>270</td>
</tr>
<tr>
<td>( h_{conv} )</td>
<td>-</td>
<td>-</td>
<td>( h_{conv}^{E} )</td>
<td>( h_{conv}^{W} )</td>
</tr>
<tr>
<td>( V )</td>
<td>-</td>
<td>-</td>
<td>( V )</td>
<td>0</td>
</tr>
<tr>
<td>( \sigma_{per} )</td>
<td>-</td>
<td>-</td>
<td>( 10^{10} )</td>
<td>-</td>
</tr>
<tr>
<td>( z_{imp} )</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

The design solutions for the \( f_T \) optimization problem optimized for the Yang et al. (2012) material parameters and various magnitudes of \( h_{conv}^{E, W} \) have been plotted in Fig. 10. The design features are generally similar to what we observed in Sections 6.1.1 and 6.1.2. However, there are two details which differ slightly from the governing design features of the \( f_P \) and \( f_\eta \) design solutions: The spike-shaped transitions between the material phases are extended over a larger part of the design domain, and the transitions between the material phases occur for different \( h_{conv} \).

To obtain the “optimal” \( f_T \) for a given design problem, the electric energy input needs to be matched such that a compromise between the Peltier effect and the Joule heating is found. A cost ineffective high amount of internal Joule heating is generated for too high electric power inputs. A cost ineffective low amount of Peltier work is generated for too low electric power inputs. To demonstrate this compromise, the relationship between \( V \) and \( f_T \) for the design optimized for \( h_{conv}^{E, W} = 400 \) has been plotted in Fig. 11.

To determine how much significance we can attribute to the design solutions, we have crosschecked the relationship between \( f_T \) and \( h_{conv} \) in Fig. 12 for the design solutions in Fig. 10. All entries in the figure are evaluated for the optimal choice of electric potential difference between \( f^E \) and \( f^W \). The figure shows that a design optimized for one \( h_{conv}^{E, W} \) indeed has superior performance compared to designs optimized for an other \( h_{conv}^{E, W} \). Similar crosschecks have been performed and confirmed for all optimization problems presented in this study, however these studies have been omitted for space reasons.
6.2.2 Heat flux

The fourth numerical problem concerns the optimization of $f_Q$ which in implementation form is given by:

$$f_Q = L Q^T Q$$  \hspace{1cm} (39)

With reference to (20) and (21), $\nabla_x f_Q$ and $\nabla_x f_T$ can now be computed as:

$$\nabla_x f_Q = L Q^T V Q$$  \hspace{1cm} (40)

$$\nabla_x f_T = \left\{ \begin{array}{c} L Q^T V Q \\ L Q^T V J \end{array} \right\}$$  \hspace{1cm} (41)

The design solutions for the $f_Q$ optimization problem for various magnitudes of $h_{conv}$ have been plotted in Fig. 13.

The spike-shaped transitions seem to be propagating over a shorter distance and the transitions between the material phases occur at different $h_{conv}$ compared to the designs in Sections 6.1.1 and 6.1.2. In Fig. 13 we find bands in the small band of Material A placed at $T^E$ for all magnitudes of $h_{conv}$. The design feature occurs because $Q$ is related to $\nabla_x T$, and Material A has a relatively large $\alpha$ compared to Material B, which combined adds a contribution to $Q$ and hereby a cost effective contribution to $f_Q$. The design feature is from now on referred to as the band design feature.

6.2.3 Coefficient of performance

In the fifth numerical example we investigate $f_\mu$ which in implementation form is given by:

$$f_\mu = \frac{L Q^T Q}{(L Q^T V) (L Q^T J)}$$  \hspace{1cm} (42)
A density-based topology optimization methodology...

Fig. 13 Design solutions for the $f_Q$ optimization problem

Fig. 14 Optimized designs for the $f_\mu$ optimization problem

6.3 Asymmetric boundary conditions

1D boundary conditions problems refer to this paper to problems where the temperature and electric potential boundary conditions are imposed only on parallel boundaries, such as $F^E$ and $F^W$. Asymmetric boundary conditions problems refer to problems where the boundary conditions are imposed on perpendicular and parallel boundaries, such as $F^N$, $F^S$, $F^E$ and $F^W$. The designs presented so far in Sections 6.1–6.2 have been limited to 1D boundary conditions. Asymmetric boundary conditions may yield a deeper solutions space of the design problems, which may constitute more topological complex design solutions. Design solutions optimized for asymmetric boundary conditions are not likely to produce more efficient designs that the one dimensional boundary conditions. However, for physical or manufacturing reasons such designs may be desirable despite interior performance. The sixth numerical example concerns asymmetric boundary conditions and the design problem is primarily serving as an example of the versatility and application of the approach. We use Yang et al. (2012) material parameters, and consider the two sets of boundary conditions listed in Table 5.

A design optimized for $f_P$ and a design optimized for $f_\eta$ have been plotted in Fig. 15a–b and c–d, respectively. The design solutions indeed show very different and complex topological designs, and the example demonstrates that the
Table 5 Boundary conditions for the asymmetric boundary condition problems

<table>
<thead>
<tr>
<th>Boundary</th>
<th>( \Gamma^N )</th>
<th>( \Gamma^S )</th>
<th>( \Gamma^E )</th>
<th>( \Gamma^W )</th>
</tr>
</thead>
<tbody>
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<td>330</td>
<td>1000</td>
<td>0</td>
</tr>
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<td>( T_{fl} )</td>
<td>1000.0000</td>
<td>4.5 · 10^4</td>
<td>4.5 · 10^4</td>
<td>10^4</td>
</tr>
<tr>
<td>( h_{conv} )</td>
<td>--</td>
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<td>--</td>
<td>--</td>
</tr>
<tr>
<td>( V )</td>
<td>--</td>
<td>( V )</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>( \sigma_{per} )</td>
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</tr>
<tr>
<td>( \tau_{zimp} )</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>( \tau_{zimp} )</td>
</tr>
<tr>
<td>Set 2</td>
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<td>1000</td>
<td>0</td>
</tr>
<tr>
<td>( T_{fl} )</td>
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<td>10^5</td>
<td>10^5</td>
<td>10^5</td>
</tr>
<tr>
<td>( h_{conv} )</td>
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<td>10^5</td>
<td>10^5</td>
<td>10^5</td>
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<tr>
<td>( V )</td>
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<td>( \sigma_{per} )</td>
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<tr>
<td>( \tau_{zimp} )</td>
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<td>--</td>
<td>( \tau_{zimp} )</td>
</tr>
</tbody>
</table>

framework actually is capable of optimizing an arbitrary set of boundary conditions.

6.4 The p-n generator

The seventh and last numerical example concerns the so-called p-n generator (PNG) problem. The problem and the material parameters are inspired by the work of Angst (2016). P-n generators (PNGs) have – compared to conventional configurations of TEGs – an advantage in high temperature applications, as the electrodes in PNGs are disconnected from the heat input surfaces, which may reduce the thermal stress and wear on the electrodes. In conventional TEGs the electrodes are directly connected to the heat input surfaces, please confer Fig. 3, where the electrodes on PNGs are connected to thermally insulated surfaces, please confer Fig. 16. Due to lower temperatures on the insulated surfaces this configuration reduces the thermal stresses in the electrodes during operation. PNGs are prone to relatively poor theoretical performance compared conventional TEGs, however with topology optimization and the framework presented in this study we are able to reduce the performance gap between PNGs and conventional TEGs. The design problem takes basis in the schematic in Fig. 16. The material parameters used in the problem are academic, however, they are adequate for this specific design problem as Material A and B are equal in magnitude for \( \alpha \), \( \sigma \) and \( \kappa \), but with opposing operational sign in \( \alpha \).

The boundary conditions of the optimization problem has been listed in Table 6, and the corresponding design optimized for \( f_P \) have been plotted in Fig. 17. Several complicated topological design features occur in the optimized design such as asymmetry around \( (x, y) = (L_x/2, y) \), spike-shaped transitions and isolated islands of different material phases. The unintuitive and complex design features and comparisons with design solutions in Angst (2016), en-light that the proposed topology optimization approach is an effective strategy to optimize such problems.
A density-based topology optimization methodology for thermoelectric energy conversion problems has been proposed. The versatile framework supports physically realistic convective boundary conditions, temperature dependent material parameters and objective functions relevant to thermoelectric generators and coolers.

The framework is based on a fully coupled non-linear thermoelectric finite element model. The framework distributes two different thermoelectric active materials in a two dimensional design space in order to optimize for some performance measure. The study reveals new insight in physical and topological effects and shows potential performance improvements in the field of thermoelectric energy conversion. The design solutions depend on the boundary conditions, the material parameters and the objective functions. To obtain high performing thermoelectric generators and coolers, it is therefore critical to take the device application into consideration in the design phase.

The design solutions are physically realizable and the framework can easily be applied on physical realistic material parameters and model dimensions. Relevant implementation details with respect to the framework are stated.

The study demonstrates that the proposed approach indeed is well-suited for thermoelectric energy conversion problems. The study may provide guidance for future research in the pursuit at achieving large-scale commercial applications of thermoelectric generators and coolers.

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Topology optimization of segmented thermoelectric generators

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the date of receipt and acceptance should be inserted later

Abstract The thermoelectric (TE) power output, $f_P$, and conversion efficiency, $f_\eta$, for segmented thermoelectric generators (TEGs) are optimized by spatially distributing two TE materials (BiSbTe and Skutterudite) using a numerical gradient-based topology optimization approach. The material properties are temperature dependent and the segmented TEGs are designed for various heat transfer rates at the hot and cold reservoirs. The topology optimized design solutions are characterized by spike-shaped design features which enable the designs to operate in an intermediate state between the material phases. Important design parameters, such as the device dimensions, objective functions and heat transfer rates, are identified, investigated and discussed. Comparing the topology optimization approach with the classical segmentation approach, the performance improvements of $f_P$ and $f_\eta$ design problems depend on the heat transfer rates at the hot and the cold reservoir, the objective function and the device dimensions. The largest performance improvements for the problems investigated are $\approx 6\%$.

Keywords: Topology optimization, thermoelectric energy conversion, electric power output, conversion efficiency

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1 Introduction
Thermoelectric generators (TEGs) are used to transform thermal energy into electric energy by utilizing the Seebeck effect \cite{1}. TEGs are applicable in converting thermal energy from numerous sources such as exhaust gases of combustion engines, heat exchangers and solar devices. The increasing demand on green and sustainable energy resources, and the capability of TEGs to convert waste heat into electric energy, have positioned TEGs as a possible focal entrant in the global green energy source changeover. However, the unrolling of large-scale industrial applications of TEGs are limited by the performance of the technology \cite{2}, thus these performance limitations have attracted a considerable amount of scientific attention in recent decades.

High performing TEGs are characterized by maintaining a high ratio between the electric energy output and the thermal energy input. At least three measures are important in relation to the performance of TEGs: The thermoelectric figure-of-merit, $ZT$, the electric power output, $f_P$, and the conversion efficiency, $f_\eta$. In this study we will discuss the latter two.

It has previously been shown that the performance of TEGs can be significantly increased by segmentation \cite{3, 4}. Segmentation approaches take basis in finding materials which are compatible. Compatible materials operate optimally under the same external electrical resistance and are therefore suited for operation thermally and electrically in series. The segmentation approach is characterized by design solutions where the material phases are separated by one dimensional line interfaces. We will in this paper refer to this type of approaches as classical segmentation.

The density-based topology optimization approach utilized in this study is related to the classical segmen-
tation approach, as the design problems take basis in distributing two different thermoelectric active materials in order to optimize for some performance measure. The main difference between the two approaches is, that the topology optimization approach takes two dimensional features in the design solutions into consideration, where the classical segmentation approach is limited to one dimensional features.

The topology optimization approach [5, 6] is based on a finite element formulation of the generalized Ohm’s and Fourier’s law [7] and the topology optimization methodology described in Lundgaard and Sigmund [8]. Compared to analytic approaches, the finite element formulation makes it possible to take more advanced physical modelling concepts into consideration such as temperature dependent material parameters, complex geometries and advanced boundary conditions. The objective of the design problems is to optimize \( f_p \) and \( f_q \), which both are measures that reflect the practical applications of TEGs. In comparison to optimization approaches which aim to maximize the thermoelectric figure-of-merit of the material phases over the device [9], this optimization strategy may be better suited for real applications of TEGs. Thermoelectric materials are governed by three material parameters: the Seebeck coefficient, \( \alpha \), the electric conductivity, \( \sigma \), and the thermal conductivity, \( \kappa \). For real materials, the material parameters are temperature dependent and some materials degenerate for temperatures above specific magnitudes. These relationships are all taken into consideration in this study.

TEGs utilize the temperature difference between a hot and a cold reservoir to convert thermal energy into electric energy. The performance of TEGs is among other parameters governed by the size of the reservoirs and the magnitude of the thermal heat transfer at the boundaries [8, 10–12]. Studies of TEGs with limited heat transfer have been investigated for various problems such as micro-heat exchangers [13–15], air-to-air heat exchangers [16–19], as well as fluid-based heat exchangers [20–25].

The heat transfer rate between the TEG and the thermal reservoirs is characterized by the governing thermal energy convection mechanisms, and depends on the fluid type and the flow type in the thermal reservoirs. The heat transfer rate is quantified by heat transfer coefficients, \( h^H \) (\( H \) refers to hot) and \( h^C \) (\( C \) refers to cold) for the hot and the cold reservoirs, respectively. The heat transfer coefficients are related to the thermal resistance of the contact between the TEG and the source as \( R_T = \frac{1}{h} \) where \( A \) is the area of the contact.

With basis in real temperature dependent materials, realistic boundary condition and model parameters, we demonstrate that a density-based topology optimization approach can be utilized to optimize \( f_p \) and \( f_q \) for TEGs. The design solutions are driven by spatially determining the layout of two different thermoelectric materials in a two dimensional domain. We demonstrate that the topology optimized design solutions are never worse and may outperform the classical segmentation approach design solution for some choices of model parameters. Furthermore, we state and discuss several important parameters which influence the design solutions and should be taken into consideration when designing TEGs.

2 The optimization problem

In this section we briefly present the concept of the density-based topology optimization framework which is utilized to optimize the TEGs. We introduce several variables throughout the paper and for readability purposes, we have summarized the most important ones in Tab. 1.

2.1 Physical model

The optimization problem takes basis in the sketch in Fig. 1. A thermoelectric module, \( \Omega_D \), is separated by

<table>
<thead>
<tr>
<th>Table 1: List of important variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variable</td>
</tr>
<tr>
<td>( T^H )</td>
</tr>
<tr>
<td>( T^C )</td>
</tr>
<tr>
<td>( T^{HC} )</td>
</tr>
<tr>
<td>( h^H )</td>
</tr>
<tr>
<td>( h^C )</td>
</tr>
<tr>
<td>( h^{HC} )</td>
</tr>
<tr>
<td>( T )</td>
</tr>
<tr>
<td>( V )</td>
</tr>
<tr>
<td>( Q_x, Q_y )</td>
</tr>
<tr>
<td>( J_x, J_y )</td>
</tr>
<tr>
<td>( f_P )</td>
</tr>
<tr>
<td>( f_\eta )</td>
</tr>
<tr>
<td>( \Omega_D )</td>
</tr>
<tr>
<td>( L_x )</td>
</tr>
<tr>
<td>( L_y )</td>
</tr>
</tbody>
</table>
where \( T \) denotes the spatial derivative with respect to Cartesian directions \( x \) and \( y \); \( \nabla \cdot Q = Q_x + Q_y \) is the heat flow density in \( x \) and \( y \) \( [W/m^2] \); \( \dot{q} = J \cdot E \) is the Joule heating term \( [W/m^3] \); \( E = -\nabla V \) is the electric field \( [V/m] \); \( V \) is the electric potential and \( J = \{J_x, J_y\} \) is the electric current density in \( x \) and \( y \) \( [A/m^2] \). In thermoelectric analysis, the thermal and electric energies are coupled by the constitutive equations:

\[
\begin{align*}
\nabla \cdot Q &= \dot{q} \quad \text{in} \quad \Omega_D \quad (1) \\
\nabla \cdot J &= 0 \quad \text{in} \quad \Omega_D \quad (2)
\end{align*}
\]

where \( \nabla \) denotes the spatial derivative with respect to Cartesian directions \( x \) and \( y \); \( Q = \{Q_x, Q_y\} \) is the heat flow density in \( x \) and \( y \) \( [W/m^2] \); \( \dot{q} = J \cdot E \) is the Joule heating term \( [W/m^3] \); \( E = -\nabla V \) is the electric field \( [V/m] \); \( V \) is the electric potential and \( J = \{J_x, J_y\} \) is the electric current density in \( x \) and \( y \) \( [A/m^2] \). In thermoelectric analysis, the thermal and electric energies are coupled by the constitutive equations:

\[
\begin{align*}
Q &= \nabla \cdot J - \kappa \cdot \nabla T \\
J &= \sigma \cdot (E - \alpha \cdot \nabla T)
\end{align*}
\]

where \( T \) is the temperature \( [K] \), \( \alpha \) is the Seebeck coefficient, \( \kappa \) is the electric conductivity and \( \sigma \) is the electric conductivity.

Table 2: Heat transfer due to convection coefficients for various flow types and flow conditions

<table>
<thead>
<tr>
<th>Flow type</th>
<th>Flow condition</th>
<th>( h ) [W/m(^2)K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forced convection</td>
<td>Air over a surface</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Air over a cylinder</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Water in a pipe</td>
<td>3000</td>
</tr>
<tr>
<td>Free convection</td>
<td>Water and liquids</td>
<td>50-3000</td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>100-1200</td>
</tr>
<tr>
<td></td>
<td>Air</td>
<td>10-100</td>
</tr>
<tr>
<td></td>
<td>Various gases</td>
<td>5-37</td>
</tr>
</tbody>
</table>

2.1.1 Resistive load

The electric current in the external resistive load (see Fig. 1) is given by:

\[
\mathbf{n} \cdot \mathbf{J} = R_{\text{ext}}(V - V_C) \quad (5)
\]

where \( \mathbf{n} \) is a vector normal to the surface, \( R_{\text{ext}} \) is the resistance of the resistive load \( [\Omega/m^2] \) and \( V_C \) is the reference electric potential \( [V] \) on \( I_C \).

2.1.2 Newton's law of cooling

With reference to the simple rectangular design and the relatively small length scales of TEG modules in Fig. 1, we assume that an adequate modeling approach for the heat transfer between the hot and the cold reservoirs and the TEG module is Newton's law of cooling. Newton’s law of cooling assumes that the thermal heat transfer between thermal hot and cold reservoirs and the module is proportional to the difference in temperatures between these:

\[
\mathbf{n} \cdot \mathbf{Q} = h_{HC}(T - T_{HC}) \quad (6)
\]

where \( h_{HC} \) denotes the convection coefficient \( [W/m^2K] \) on \( I_H (h_H) \) and \( I_C (h_C) \), respectively, and \( T_{HC} \) denotes the temperatures of the thermal reservoirs \( [K] \) in \( I_H \) \( (T_H) \) and \( I_C \) \( (T_C) \), respectively.

By utilizing Eq. (6), it is assumed that the thermal heat transfer between the thermal hot and cold reservoirs and the module is proportional to the difference in temperatures between the body and its surroundings and that the temperatures of the reservoirs are constant along \( I_H \) and \( I_C \). We believe that these assumptions are adequate for this specific problem, however, in detailed computations the thermal heat transfer should be modeled taking local convection, diffusion and radiation into account. \( h_{HC} \) in Eq. 6 can be experimentally determined and some values for different flow types and flow conditions are listed in Table 2.
2.1.3 Material parameters

The TEGs are optimized with respect to \( f_P \) and \( f_\eta \) by spatially determining the distribution of BiSbTe \([26]\) and NdFe\(_{52.5}\)Co\(_{47.5}\)Sb\(_{12}\) (skutterudite) \([27]\) in \( \Omega_D \) (see Fig. 1). BiSbTe and skutterudite are p-type semi-conducting and temperature dependent materials. The relationships between \( \alpha \), \( \sigma \), \( \kappa \), and the temperature for both materials are plotted in Fig. 2. BiSbTe has a maximum operation temperature of 540 K, because it is chemically unstable for higher temperatures. To ensure that the BiSbTe material phases is not subjected to a too large operating temperature, we impose a temperature constraint on the BiSbTe material phase. Details on the implementation of the temperature constraint can be found in Sec. 6. BiSbTe and skutterudite are compatible materials \([28]\), and have previously been shown to have an increased efficiency in a classically segmented configuration compared to the constitutive materials \([4, 29]\). Compatible materials operate optimally under the same external resistance and are therefore suited for classical segmentation. According to \([28]\), thermoelectric materials are compatible if their so-called compatibility factor does not exceed a ratio larger than 3. BiSbTe and skutterudite in Fig. 2 have a compatibility factor of 2.1 for the plotted temperature range.

2.1.4 Finite element model

To set up the topology optimization framework, we introduce a spatial design field \( 0 \leq \rho \leq 1 \), such that Eqs. (1)-(4) become functions of the design field, i.e. \( \alpha(T) = \alpha(T, \rho) \), \( \sigma(T) = \sigma(T, \rho) \) and \( \kappa(T) = \kappa(T, \rho) \).

By doing so, it is possible to obtain the discretized finite element equations suited for topology optimization by multiplying the strong forms of Eqs. (1)-(4) with a suitable test function; integrating over the domain; performing integration by parts of higher dimensions on relevant terms \([7, 30, 31]\); and introducing the design field dependent interpolation functions. After introduction of the design variable field, it is now possible to control whether an element represents the skutterudite or the BiSbTe material phase. The material phase is determined by computing the gradients of the objective function with an analytic adjoint sensitivity analysis.

This outlines the fundamental concept of the topology optimization framework. Interested readers are referred to the detailed description of the implementation and concept of the density-based topology optimization framework in \([8]\).

Fig. 2: The Seebeck coefficient and electric conductivity (a) and the thermal conductivity and figure-of-merit (b) as function of the temperature, \( T \). The markers are experimental values and the continuous lines are the corresponding fitted interpolation functions.

2.1.5 The optimization problem

The optimization problem sketched in Fig. 1 has dimensions \( L_x = 5 \) [mm] and \( L_y = 5 \) [mm], and we aim to optimize \( f_P \) and \( f_\eta \). To optimize \( f_P \) and \( f_\eta \) we need to compute the electric power output of the thermoelectric module:

\[
f_P = \frac{1}{E_y} \int_{T_H} V \, dS \int_{T_H} J_x \, dS
\]  

This is simply an integral expression for the electric potential and the electric current density at the hot reservoir-electrode of the TEG. In one dimensional analysis, the expression is often written as: \( P = JV \), where
Topography optimization of segmented thermoelectric generators

The design solutions for the BiSbTe and skutterudite material phases of the thermoelectric module in Fig. 1 are determined for \( h^{HC} \in [100; 2000] \) [W/K·m\(^2\)] in the design solutions presented in this section. These coefficient values correspond to a large range of different flow types and flow conditions in Tab. 2, and turn out to provide topologically interesting and different design solutions.

3 Results

The optimized spatial distributions of the BiSbTe and skutterudite material phases of the thermoelectric module in Fig. 1 are determined for \( h^{HC} \in [100; 2000] \) [W/K·m\(^2\)] in the design solutions presented in this section. These coefficient values correspond to a large range of different flow types and flow conditions in Tab. 2, and turn out to provide topologically interesting and different design solutions.

3.1 Electric power output

The design solutions for the \( f_P \)-problem optimized for various \( h^{HC} \) have been plotted in Fig. 3. The plots suggest that the optimized topologies of the design solutions are dependent on \( h^{HC} \). As \( h^{HC} \) is increased, the extent of the “spike”-shaped design features are decreased. For higher magnitudes of \( h^{HC} \) the temperature constraint is active, which pushes the BiSbTe material phase towards \( I^C \) in order to match the temperature requirements of the BiSbTe material phases. The spike-shaped design features are gradually rounded when \( h^{HC} \) is increased and the design solutions are approaching the one-dimensional design solutions which is seen in classic segmentation when \( h^{HC} \to \infty \).

A discussion of the state fields (e.g. the temperature and electric potential) of the design solutions is given in Sec. 3.3.

The design solutions in Fig. 3 are two dimensional and the parasitic losses between the material phases are neglected. With an offset in an analytic optimization approach, [35] manufactured and experimentally tested design solutions which consisted of two materials with a considerable amount of transitions between material phases. Despite the neglect of the parasitic losses and the large area between the different materials, [35] found excellent agreements between the analytic predictions and the experimentally tested designs.

The complexity of the design solution presented in this study may be comparable to the complexity of the design solutions manufactured by Sakai and coworkers, for which reason we therefore assess that the design solutions are manufacturable with methodologies available today. However, if this is not the case we refer to the rapid advances in additive manufacturing and material science, and hereby predict that the design solutions such as the ones in Fig. 3 are realizable in the near future. Until that time, the design solutions presented in this study can serve as a theoretical benchmark for what is achievable by allowing two dimensional features in segmented thermoelectric legs. Even though it is general practice in many mathematical optimization approaches of thermoelectric energy conversion problems to neglect parasitic losses, see e.g. the work in [3, 36, 37], we emphasize the importance of taking parasitic losses into consideration in detailed computations.

Figure-3a-

3.2 Conversion efficiency

The \( f_P \)-design solutions for various \( h^{HC} \) have been plotted in Fig. 4. The same trends in design solutions are observed as for the \( f_P \)-design solutions in Sec. 3.1, however, the BiSbTe material phases are generally pushed toward \( I^R \) for the \( f_P \) design compared to the \( f_P \) design. This design feature may be due to the low \( \kappa \) of the BiSbTe material phase which is cost effective for \( f_P \) problems.

The design solutions in Fig. 3-4 are all solved for the temperature constraint stated in Eq. (10). For small
$h^{HC}$, the temperature constraint is inactive because $\Delta T \to 0$ as $h^{HC} \to 0$ and hence $T < T_{\text{max}}$ at $\Gamma^{HC}$. The temperature constraint becomes active when the magnitude of $h^{HC}$ is large enough to push the temperature at $\Gamma^H$ above $T_{\text{max}}$. In such problems, the BiSbTe material phase is pushed toward $\Gamma^C$ to fulfill the constraint. The constraint of the design problem ensures that the optimized TEG do not degenerate during operation. For more information and comparisons between design solutions, please consult Sec. 6.

3.3 State fields of a specific design

The temperature, the electric potential, the heat flux and current density for the $f_P$-design solution in Fig. 3c have been plotted in Fig. 5. The temperature field and the electric potential field are almost smoothly distributed with only small gradients in the $y$-direction despite the two dimensional features of the design solutions. As both Ohm’s and Fourier’s generalized laws, see Eq. (1)-(4) are diffusion equations, the small $y$-directional gradients in the state fields may be explained by the differences in the material parameters between the material phases and the length scales of the design solutions. These parameters are simply not large enough to generate a considerable difference in the state fields in the two material phases. However, by increasing the length-scale of the design problem and the difference in the material parameters, the $y$-directional gradients of temperature and electric potential fields will also increase.

The temperatures at $\Gamma^H$ and $\Gamma^C$ are not exactly $T^H$ and $T^C$ due to the finite $h^{HC}$. As $h^{HC}$ is increased, the temperatures at boundaries $\Gamma^H$ and $\Gamma^C$ will approach $T^H$ and $T^C$. The almost straight streamlines of the electric current density and the heat flux on Figs. 5c-5d suggest that only minor two dimensional effects are affecting the design solutions. However, the gradients in $Q$ and $J$ between the spike-shaped designs features are large, which indicate that the design features indeed affect the performance of the design.

The framework can straightforwardly be extended such that thermal heat transfer rates on the horizontal boundaries of the design solutions are taken into consideration. Taking such effect into consideration would change the design solutions considerably, however thermoelectric modules are almost always thermally insulated or periodically assembled for which reason the thermal heat transfer rates on $\Gamma^{HC}$ are many magnitudes larger than the thermal heat transfer rates on the vertical boundaries. With basis in this argument, we hence argue that the isolation assumption is physically realistic, which is a shame from the topology optimization perspective, as a considerable amount of thermal heat transfer on vertical boundaries may cause much more topological interesting and complex design solutions and increase the difference in performance between the topology optimized and segmented design solutions.

The appearance of the spike-shaped design features may be explained by the following two reasons: (1) They increase the heat flux and electric conductivity in the skutterudite material regions. (2) They enable the design to operate in an intermediate state between the two different material phases. In optimization approaches with functionally graded materials, the material parameters are determined as function of the spatial coordinates of the design domain in order to optimize for some performance measure (see e.g. the work by Seifert et al. [38], Gerstenmaier and Wachutka [39]). The design problems presented in this work are related to functionally graded materials design problems, though the topology optimized design solutions consist of two distinct material phases, where the design solutions of functionally graded material design approaches conceptually consist of infinitely many.
3.4 Performance of the designs

The performance of the design solutions in Sec. 3.1 and 3.2 are quantified in Fig. 6, where the normalized performances, $f_P$ and $f_H$, are plotted as function of $h_{HC}$ for the designs in Figs. 3-4. To clarify the differences between design performances, we have normalized the objectives with respect to the performance of a TEG consisting of a stand-alone skutterudite material phase. The $h_{HC}$ values next to the lines indicate the $h_{HC}$ at which the design was optimized. To present a fair comparison between the topology optimized design solutions and the classical segmentation approach, we computed the optimal segmented design solutions for the same $h_{HC}$ as the topology optimized designs. The design performances of the classical segmentation approach are determined by finding the optimal ratio between skutterudite and BiSbTe while fulfilling the temperature constraints for each magnitude of $h_{HC}$. The performance of the classical segmented design solutions is identified by the “segmented” legend in Fig. 6. The performances of the design solutions are computed by the following approach: The design solutions in Fig. 6a are evaluated for a sequence of $h_{HC}$ and each line in Fig. 6 refers to the design performances with respect to the performance measure indicated on the plots. For guidance we provide an example to read the graph: The red curve in Fig. 6a is the $f_P$-optimized design solution for $h_{HC} = 141$ (see Fig. 3a) evaluated for $h_{HC} = [100; 2000]$. With reference to Fig. 6, we notice that the design solutions perform equivalently or outperform design solutions optimized for other convection coefficients, the standalone skutterudite and the classical segmented design solutions. The best relative improvement of the topology optimized and classical segmented design solutions are obtained for $h_{HC} \rightarrow 0$.

Crosschecks are important to determine how much significance we may attribute to the features of the optimized designs in Fig. 3-4. The relationship between the performance and the design solutions in Fig. 6, demonstrates that the spike shaped design features indeed provide design improvements compared to the classical segmentation approach.

By comparing the performance of the topology optimized and the classical segmented design solutions (black curves with label “Segmented” in Fig. 6), we notice that the difference between the optimization approaches is decreased as $h_{HC} \rightarrow \infty$.

The maximum design improvements for the parameters investigated in this study are $\approx 5\%$ and $\approx 6\%$ for the $f_P$ and $f_H$ designs optimized for $h_{HC} = 141$, respectively. The difference between the two optimization approaches is decreasing as $h_{HC} \rightarrow \infty$. As $h_{HC}$ reaches a specific magnitude, the two optimization approaches provide the same design solutions and hereby also the same performances. The topology optimization approach is therefore only advantageous for low $h_{HC}$ problems for this set of material parameters and model parameters.

3.5 The relationship between design performance and leg length

The finite convection coefficients on $\Gamma^H$ and $\Gamma^C$ entail that the thermal heat transfer between the hot and the cold reservoir is limited by the heat transfer rate. In finite element simulations or analytic studies where the temperature boundary conditions are fixed or where the heat inputs are imposed as a heat flux, the size of the thermal hot and cold reservoirs and the heat transfer rate at $\Gamma^H$ and $\Gamma^C$ are assumed infinitely large. Optimization problems solved for fixed temperature boundary conditions may therefore provide non-physical and meaningless design solutions. To investigate the importance of device thickness, $L_x$, in the design problems, we have plotted the $f_P$ and $f_H$-design solutions for $L_x = [10, 20, 30, 40, 50] \text{[mm]}$ in Fig. 7-8. With reference to the figures, we notice that the design
Fig. 5: The temperature field [K] (a), the electric potential field [V] (b), the heat flux field [W/m²] (c) and the electric current density field [A/m²] (d) for the design solution solved for \( f_P \) and \( h^{HC} = 821 \) in Fig. 3c.

Fig. 6: The design solutions solved for \( f_P \) (a) and \( f_\eta \) (b) (see Figs. 3 and 4, respectively) evaluated for different \( h^{HC} \). The solutions are dependent on \( L_x \). Furthermore, the design feature tendencies with respect to the amount of the two material phases in the \( f_P \) and \( f_\eta \)-design solutions are similar to the design features tendencies discussed in Sec. 3.2.

The relationships between the normalized electric power output, \( \bar{f}_P = f_P / \max(f_P|_{h^{HC}=10000}) \), and device length, \( L_x \), for the design solutions in Fig. 7 have been plotted in Fig. 9. For readability purposes, we have normalized the objectives with respect to the largest measured value of \( f_P \) for \( h^{HC} = 10000 \). The design solutions are optimized with the temperature constraint as in Sec. 3.1-3.2. The relationships between \( f_P \) and \( L_x \) are obtained by sweeping \( L_x \) in 100 equally sized steps in the interval \( L_x \in [1; 10] \) [mm]. The largest \( f_P \) at the optimal thermoelectric module length, \( L^{opt}_x \), for each \( h^{HC} \) has been marked with black dots in the plot. The design solutions
Fig. 7: Designs solutions solved for $f_P$ and length of the design domain, $L_x$ [mm], equal to $L_x = 1$ (a), $L_x = 10$ (b), $L_x = 20$ (c), $L_x = 30$ (d), $L_x = 40$ (e) and $L_x = 50$ (f).

Fig. 8: Designs solutions solved for $f_\eta$ and length of the design domain, $L_x$ [mm], equal to $L_x = 1$ (a), $L_x = 10$ (b), $L_x = 20$ (c), $L_x = 30$ (d), $L_x = 40$ (e) and $L_x = 50$ (f).

Fig. 9: The relationship between the normalized electric power output, $\bar{f}_P = f_P / \max (f_P | h^{HC} = 10000)$ and device length, $L_x$, for various values of $h^{HC}$. The black dots indicate the largest electric power output for a specific $h^{HC}$.

for different $L_x$ illustrate several important relationships for the topology-optimized design solutions for TEGs: If $h^{HC} \to \infty$ and $L \to 0$ then $f_P \to \infty$. Furthermore, if $h^{HC} < \infty$ then there exists an optimum between $f_P$ and $L_x$.

The relationship between $f_P$ and $L_x$ is an interaction between the Seebeck effect, the Joule heating effect and the finite thermal reservoirs at $T^H$ and $T^C$. For finite magnitudes of $h^{HC}$ and $L_x < L^{opt}_x$, the available thermal energy at $T^{HC}$ is not effectively converted to electric energy, as the temperature difference between $T^H$ and $T^C$, $\Delta T$ is decreased as $L_x \to 0$. As the temperature difference is decreased, the work done by the Seebeck effect is decreased entailing that $f_P \to 0$. For $h^{HC} = \infty$, which is equivalent to fixed temperature boundary conditions, we notice that $f_P \to \infty$ for $L_x \to \infty$. As $L_x \to \infty$ the temperatures at $T^H$ and $T^C$ approach $T^H$ and $T^C$, however the Joule heating is also increased due to the larger internal electric resistance in the module. The compromise between the increasing work of the Seebeck effect and the Joule heating for $L_x \to \infty$ constitutes the interaction between $L_x$ and $f_P$, and causes the optima for $f_P$ and $L_x$ for finite $h^{HC}$.

With reference to the design solutions in Figs. 7 and 8, we notice that $L_x$ stretch out two extremes with respect to the shapes of the spike-shaped design features: Design solutions solved for low $L_x$ consist of sharp design features, whereas the design solutions solved for large $L_x$ consist of rounded design features. The transitions between the material phases can be quantified by the function $\nu(x)$, which relates the $y$-directional averaged volume ratio of the materials along the spatial direction, $x$. The sharp design features, see e.g. Fig. 8c, constitute an almost linear relationship of $\nu(x)$ in the transition, whereas the rounded design features, see e.g. Fig. 7f, constitute a non-linear relationship of $\nu(x)$ in the transition.

The shapes, the extent and the position of the spike-shape design features are dependent on the temperatures of the reservoirs, the length of the design domains, the
magnitude of the temperature constraint, the convection coefficients and the material parameters. It may be possible to derive analytic expressions which relate all these parameters to the performance of the thermoelectric generators, however such study goes beyond the scope of this paper.

To conclude the section, we emphasize with reference to Figs. 7, 8 and 9 and the discussion above that $L_x$, the objective function and $h^{HC}$ should be taken into account when designing TEGs.

3.6 Asymmetric hot and cold sides

As the final numerical example, we consider what we in this study denote asymmetric boundary conditions. Asymmetric boundary conditions are inspired by TEG applications where the flow type and flow conditions on $\Gamma^H$ and $\Gamma^C$ are different. Such applications are e.g. seen in applications where $\Gamma^H$ is subjected to forced convection by water and $\Gamma^C$ is subjected to natural convection by air or vice versa (confer with Tab. 2).

The importance of the design problem parameters is demonstrated in the design solutions in Figs. 10-11. The $f_P$-design solutions optimized for $h^C = 367$ and various $h^H$ have been plotted in Fig. 10, and the $f_P$-design solutions optimized for $h^H = 367$ and various $h^C$ have been plotted in Fig. 11.

We notice that the design feature tendencies of the design solutions are similar to the design feature tendencies discussed in Sec. 3.2. However, when comparing Figs. 10-11, we emphasize one new and important design feature tendency: The design solutions for these asymmetric boundary conditions are indeed very different, for which reason it is critical to take the asymmetric heat transfer mechanisms into consideration when designing TEGs.

With reference to Figs. 10-11, we notice that the Skutterudite material phase is either pushed towards $\Gamma^H$ or $\Gamma^C$ when $h^C$ and $h^H$ are changed. This interplay occurs due to the interaction between the temperature constraint and the heat transfer rates. The heat transfer rates are related to the convection coefficients, and the convection coefficients govern the temperature distribution in $\Omega_0$. Depending on the temperature distributions, the material phases are either pushed toward $\Gamma^H$ or $\Gamma^C$ to fulfill the temperature constraint and to maximize the performance of the device.

Similar to the design solutions solved for symmetric boundary conditions in Sec. 3.1 and 3.2, the spike-shaped design features are decreased as the convection coefficients are increased. The smaller absolute temperature difference between $\Gamma^H$ and $\Gamma^C$ in asymmetric design problems may explain that the transitions occur for larger convection coefficients for asymmetric design problems than symmetric design problems.

Nevertheless, the main message of this study is that asymmetric boundary conditions considerably change the design solutions, for which reason it is critical to take such model parameters into consideration when designing thermoelectric generators.
4 Discussion

In Figs. 3, 4, 7, 8, 10 and 11, we have demonstrated that density-based topology optimization can be utilized to improve the performance of segmented TEGs by introducing two-dimensional design features. We have presented an application of a density-based topology optimization framework, which takes real material parameters, device dimensions and realistic boundary conditions into account. The study has demonstrated that topology optimization may be used to increase the performance of TEGs.

Due to the two-dimensional and spike-shaped design features, the topology optimized design solutions require significantly more effort to manufacture compared to the design solutions of the classical segmentation approach. However, the additional manufacturing effort and the fact that the predicted performance improvements only yield a maximum of 5-6% for the parameters investigated in this study, may indicate that the topology optimization approach may have minor practical application for this specific problem and material parameters.

Topology optimization may provide larger design improvements for other materials and/or thermoelectric coolers. We are currently working on a study which aims to report on this topic.

The contact resistance in the interface between the material phases is neglected in the finite element modelling. The thermal and electrical contact resistance has been shown to decrease the performance of both conventional and segmented thermoelectric modules in Bjørk [4]. Some topology optimized design solutions presented in this paper have a much greater contact area between the material phases than classically segmented design solutions, for which reason the predicted improvements may actually be smaller.

We include the following suggestions to future work:

1. A three dimension implementation of the methodology may provide larger design improvements as the design solutions may take advantage of three-dimensional design features.
2. Multiple material phases may provide more advanced design features and performance improvements.
3. Other combinations of materials may provide larger performance improvements of the design solutions.
4. Deriving analytic expressions which relate the length of the spike-shaped design features, the choice of materials, the convection coefficients and the length of the designs may provide new and more insight in the pursuit of improving the performance of thermoelectric generators.

5 Conclusion

A density-based topology optimization approach for TEGs has been utilized to design the spatial layout of two real thermoelectric material phases, BiSbTe and...
skutterudite, in order to optimize the electric power output and the conversion efficiency of thermoelectric generators. The study demonstrates that the spatial layout of the material phases depends on a large number of model parameters such as the length of the design domain and the convection coefficients at the surfaces at the hot and cold reservoirs. The topology optimized design solutions provide maximum performance improvements compared to classical segmented design solutions of 5-6% for low convection coefficients. The performance improvements are decreasing as the convection coefficients are increased, and for convection coefficients larger than a specific limit the topology optimized design solutions and the classical segmented design solutions have similar performance. Design problems solved for different convection coefficients on the surfaces of the hot and the cold reservoirs are significantly different, for which reason such effects should be taken into consideration when designing thermoelectric generators.

A temperature constraint on the BiSbTe material phase ensures that the temperature in this phase does not exceed 540 K. BiSbTe degenerates for temperatures not exceeding a specific magnitude,

$$T_{\text{max}} \leq T_{\text{max}} \forall \in \Omega_{\text{BiSbTe}},$$

where \(\Omega_{\text{BiSbTe}}\) is the set of elements to be constrained, \(p\) is the temperature norm parameter and \(T^e\) is the temperature in the center of element \(i\). To consider \(T^e\) instead of the nodal temperatures is convenient implementation-wise and the connection between the objective function and the temperature constraint is laid out straightforwardly. For very large temperature gradients, the element-wise evaluation of the temperatures may impose an unacceptable large error in the \(T_{\text{max}}\) approximation. However, for the boundary conditions and finite element discretizations considered in this study, the approximation is acceptable. \(\Omega_{\text{C}}\) could in principle be a subset of \(\Omega_D\), however for the problems presented in this study, all elements in \(\Omega_D\) are included in \(\Omega_{\text{C}}\). The function \(g(\rho)\) in Eq. (12) is given by:

$$g(\rho) = \frac{(-1 + \rho)}{(1 + q) \max - \min \rho}$$

where \(\max\) and \(\min\) are the upper and lower bounds of \(\rho\), and \(q\) is the penalization parameter. The magnitudes of \(p\) and \(q\) are a compromise between numerically stability, well-posedness of the design problem, penalization of intermediate design variables and the precision of the \(T_{\text{max}}\) approximation in Eq. (12). The design solutions presented throughout this work are obtained for \(p = 12\) \([\cdot]\), \(q = 100\) \([\cdot]\), \(T_{\text{max}} = 540\) \([\text{K}]\), \(\min = 10^{-8}\) \([\cdot]\) and \(\max = 1\) \([\cdot]\). The magnitude of \(g_{\text{min}}\) is a small number instead of zero to ensure numerical stability of the algorithm. The function \(g\) in Eq. (13) interpolates between \(g_{\text{min}}\) and \(g_{\text{max}}\) for \(\rho \in [0; 1]\):

$$g = 0 \text{ if } \rho = 1 \text{ and } g = 1 \text{ if } \rho = 0.$$
The temperature constraint formulation in Eqs. (12)-(13) is inspired by the stress constraint work in [40], and Eq. (12)-(13) can in implementation form be written as:

$$f_C = \left( L_Q \circ (T^C \circ g)^\beta \right)^\gamma$$

(14)

where $\circ$ denotes the Hadamard product (element-wise multiplication), and $L_Q$ is a vector consisting of zeros except for the positions $i \in \mathcal{Q}$ which have the value unity. Eq. (14) is differentiated with respect to $\rho$ and $T$.

To simplify notation, we introduce the following terms:

$$\nabla f_C^L = L_Q \circ (T^C \circ g)^\beta \quad \nabla g = (T^C \circ g)^\beta$$

(15)

$$\nabla _f f_C^L = L_Q \circ (T^C \circ g)^\beta \quad \nabla \rho T = (T^C \circ g)^\beta \frac{\partial g}{\partial T}$$

(16)

$$\nabla _f f_C^L = pL_Q \circ (T^C \circ g)^\beta$$

(17)

and $\nabla T f_C^L$:

$$\nabla T f_C^L = L_Q \circ (T^C \circ g)^\beta \nabla T$$

(18)

$$\nabla T f_C^L = (pT^C \circ g)^\beta \nabla \rho T$$

(19)

$$\nabla T f_C^L = pL_Q \circ (T^C \circ g)^\beta$$

(20)

$\nabla f_C$ and $\nabla S f_C$ are now given by:

$$\nabla f_C = \nabla f_C^L \circ \nabla f_C^L$$

(21)

$$\nabla S f_C = \begin{vmatrix} \nabla f_C^L \\ \nabla T f_C^L \\ \nabla T f_C^L \\ \nabla T f_C^L \\ \nabla T f_C^L \end{vmatrix}$$

(22)

which hereby provide all relevant terms in the adjoint sensitivity analysis. All division operators should be interpreted as element-wise divisions.

Fig. 12: $f_\eta$-design solutions solved for $h^{HC} = 1502$ with and without an active temperature constraint.

References


Publication [P3]:

Design of segmented off-diagonal thermoelectric generators using topology optimization

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Abstract

A density-based topology optimization methodology is used to optimize the off-diagonal figure-of-merit and off-diagonal electrical power output of thermoelectric generators by distributing two different thermoelectric active materials in a two dimensional design space. Off-diagonal thermoelectric generators are characterized by converting a vertical thermal heat flux into a horizontal electric current, and may be useful in applications where the electrodes connected to the generator are prone to thermo-mechanical stress and wear.

With basis in the topology optimization framework and a sequence of numerical examples, we discuss critical and important model parameters such as objective functions, heat transfer rates and device lengths. All results are supported by exhaustive crosschecks and validations, and it is shown that the off-diagonal figure-of-merit and the off-diagonal electrical power output may be improved by 233% and 229%, respectively, compared to other optimization approaches available in the literature.

Keywords: Topology optimization, thermoelectric energy conversion, figure-of-merit, electric power output, thermoelectricity, renewable energy

1. Introduction

Thermoelectric generators exploit the Seebeck effect to convert thermal energy into electric energy [1]. This type of device is especially useful in waste heat recovery applications as 55-75% of the fuel consumption in conventional combustion engines is converted into waste heat [2]. By using thermoelectric generators in waste heat recovery applications, it is possible to increase the overall efficiency which may be profitable even for small performance improvements. With a point of departure in thermoelectric generators, we present and solve a numerical design problem which aims at increasing the performance of a special type of thermoelectric generators called off-diagonal thermoelectric generators.

With reference to the sketch in Fig. 1, off-diagonal thermoelectric generators convert a vertical heat flux into a horizontal electrical current. As the electrodes are disconnected from the thermal reservoirs, the thermo-mechanical stress and wear of the electrodes are reduced, which makes off-diagonal thermoelectric generators suitable in e.g. applications where the temperature difference between the hot and the cold reservoirs varies considerably during operation.

The present study is inspired by the work of Sakai et al. [3] and takes point of departure in an optimization problem of an off-diagonal thermoelectric generator serving in a realistic application. Sakai et al. [3] demonstrated that it is possible to increase the off-diagonal figure-of-merit and electrical power output for this type of device, by determining the optimal tilting angle and volume fraction between two thermoelectric active materials placed in a layered configuration.

As we point our attention to the layered configuration of Sakai and coworkers’ design solutions, we presume that the performance of the design solutions can be increased further by allowing geometrically free distribution of the two materials. Such a design problem can be powered by a numerical optimization approach called topology optimization [4, 5] which we use in the present study.

With basis in the schematic of the design problem in Fig. 1, the goal of the topology optimization problem is to increase the figure-of-merit and electrical power output of the off-diagonal thermoelectric generators by distributing two different thermoelectric materials, Material A and Material B, in the two dimensional design space, $\Omega_D$. The material parameters of Material A and B...
have been listed in Tab. 1.

The work of Sakai et al. [3] is particularly interesting for our endeavor, as the theoretically obtained design solutions were both manufactured and experimentally verified. Despite the neglect of parasitic losses between the layers of different types of materials, Sakai and coworkers found excellent agreement between the analytical predictions and experimental testing. Due to these observations, we find it reasonable to assume that Sakai and coworkers overcame challenges concerning manufacturability and minimization of parasitic losses. This topic is further discussed in Secs. 3.1 and 3.2.

The topology optimization methodology used in the present study is powered by the finite element method [7, 8], adjoint sensitivity analysis [9] and the method of moving asymptotes [10]. The finite element method is a discretization approach used to estimate the solution to the governing partial differential equations. Adjoint sensitivity analysis provides the gradients of the objective function with respect to the design variable field, which are used in the deterministic gradient-based optimization solver called the method of moving asymptotes. The method of moving asymptotes is an approach used to solve the design problem and ensure convergence of the design routine within a couple of hundred design iterations despite solving problems with more than 10,000 design variables. Interested readers are referred to Lundgaard and Sigmund [6] who provide a detailed introduction to the methodology.

The topology optimization approach is related to well-accepted studies in the thermoelectric literature such as functionally graded materials [1, 11], the compatibility approach [12], genetic sizing approaches [13] and homogenization [3, 14, 15, 16], however the methodology takes a completely different off-set and modeling approach, and converges to very different design solutions and hereby opens a hole new branch of optimization approaches for off-diagonal thermoelectric generators.

1.1. Physical model

The topology optimization framework is based on the temperature independent and steady state form of Fourier’s and Ohm’s generalized equations which are given by [7, 1]:

\[
\frac{\partial Q_i}{\partial x_i} = q \quad \text{in} \quad \Omega_d \quad (1a)
\]

\[
\frac{\partial J_i}{\partial n} = 0 \quad \text{in} \quad \partial \Omega_d \quad (1b)
\]

\[
Q_i = T \sigma_{ij} J_j - \kappa_i \frac{\partial T}{\partial x_i} \quad (1c)
\]

Figure 1: A sketch of the off-diagonal thermoelectric generator design problem. The temperature difference between the hot exhaust gas from, e.g., a combustion engine and the cold ambient air generates a heat flux from \( T^h \) to \( T^c \). The heat flux is converted into a vertical electrical current by exploiting the Seebeck effect. By spatially distributing Material A and B (see Tab. 1) in the two dimensional design space, \( \partial \Omega_d \), the off-diagonal figure-of-merit or electrical power output are optimized. The thermal heat transfer between the thermal hot and cold reservoirs and the thermoelectric generator are modeled by Newton’s law of cooling, see Sec. 1.3.

\[
J_i = \sigma_{ij} (E_j - \alpha_i \frac{\partial T}{\partial x_i}) \quad (1d)
\]

where \( Q_i \) is the heat flow density; \( x_i \) is the spatial coordinates; \( q = J_i E_i \) is the Joule heating term; \( T \) is the temperature; \( \alpha_{ij} \) is the Seebeck coefficient; \( J_i \) is the electric current density; \( \kappa_i \) is the thermal conductivity of the medium; and \( E_i = -\nabla V / \partial x_i \) is the electric field. The tensor indices, \( i \) and \( j \), have two entries, \( x \) and \( y \), which are corresponding to the spatial directions in a Cartesian coordinate system.

1.2. External resistive load

The electric current in the external resistive load is given by:

\[
n_i J_i = \bar{Z}_i (V - V_{i3}) \quad (2)
\]

where \( \bar{Z} \) indicates the surface on which the boundary condition is imposed (north, south, east, west, see Fig. 1 for definitions), \( Z_i \) is the impedance of the external resistive load, \( n_i \) is the unit vector normal and \( V_{i3} \) is a reference electric potential.

1.3. Newton’s law of cooling

With reference to the simple rectangular design and the relatively small length scales of the thermoelectric generator problem sketches in Fig. 1, we assume that the
The material parameters are similar to the material parameters used in [3].

Table 1: The Seebeck coefficient, $\alpha$, the electric conductivity, $\sigma$, and the thermal conductivity, $\kappa$, for Material A and B used in the design problems. The material parameters are similar to the material parameters used in [3].

<table>
<thead>
<tr>
<th>Color in plots</th>
<th>$\alpha$ [V/K]</th>
<th>$\sigma$ [S/m]</th>
<th>$\kappa$ [W/(m-K)]</th>
<th>$Z$ [1/K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material A</td>
<td>$210 \cdot 10^{-6}$</td>
<td>$8.333 \cdot 10^{4}$</td>
<td>$1.1$</td>
<td>$3.3409 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>Material B</td>
<td>$-20 \cdot 10^{-6}$</td>
<td>$588.2 \cdot 10^{5}$</td>
<td>$51.0$</td>
<td>$0.0461 \cdot 10^{-3}$</td>
</tr>
</tbody>
</table>

heat transfer between the hot and the cold reservoirs and the thermoelectric generator is governed by Newton's law of cooling.

By modeling heat transfer with Newton's law of cooling, it is assumed that the thermal heat transfer between the thermal hot and cold reservoirs and the module is proportional to the temperature differences between these. Mathematically, Newton's law of cooling is given by:

$$ q_i = h(T_i - T_{ci}) $$

where $q_i$ is the heat flux due to convection, $h(T_i - T_{ci})$ is the convection coefficient and $T_{ci}$ is the temperature of the reservoir.

### 1.4. Finite element formulation

To set up the topology optimization framework, we introduce a design field, $\rho$, such that Eqs. (1) become functions of $\rho$, i.e. $\alpha = \sigma(\rho)$, $\sigma = \sigma(\rho)$ and $\kappa = \kappa(\rho)$. The discretized finite element equations suited for the topology optimization framework can now be obtained by multiplying the strong forms of Eqs. (1) with suitable test functions; integrating over the domain; performing integration by parts of higher dimensions on relevant terms and introducing the design field dependent interpolation functions [7, 17, 8].

The design variable field makes it possible to compute the gradients of the objective functions with an analytic adjoint sensitivity analysis. The gradients of the objective function contain the information which describe how Material A and Material B should be spatially distributed to maximize the objective functions.

A detailed description of the derivation and implementation of the optimization framework is provided [6].

### 1.5. The design problem

To provide the best comparison between the optimization approaches, we decided to take basis in the same pair of objective functions as the main references of the present study, the works of Yang et al. [14] and Sakai et al. [3]. The objective functions are the off-diagonal figure-of-merit and the off-diagonal electrical power output.
Table 3. The boundary conditions used to evaluate the figure-of-merit, \( f_Z \), in Eqs. (5). To compute the figure-of-merit, it is necessary to solve three different finite element problems with the boundary conditions listed below.

<table>
<thead>
<tr>
<th>Load-case</th>
<th>Boundary</th>
<th>( \Gamma^N )</th>
<th>( \Gamma^E )</th>
<th>( \Gamma^S )</th>
<th>( \Gamma^W )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma )</td>
<td>( T )</td>
<td>( 10^{-3} )</td>
<td>0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( V )</td>
<td>-</td>
<td>-</td>
<td>0</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>( \sigma )</td>
<td>( T )</td>
<td>-</td>
<td>-</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>( V )</td>
<td>-</td>
<td>-</td>
<td>0</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>( \kappa )</td>
<td>( T )</td>
<td>( 10^{-3} )</td>
<td>0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>( V )</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

With reference to Fig. 1, we denote the northern, southern, eastern and western surfaces of the design domain \( \Gamma^N \), \( \Gamma^S \), \( \Gamma^E \), \( \Gamma^W \), respectively. The design domain is rectangular with length, \( L_x \), and height, \( L_y \), length-to-height ratio \( \Lambda = L_x/L_y \); and an outer electric impedance, \( Z \), is imposed on boundary \( \Gamma^N \). For readability purposes we have listed the most used abbreviations and variables used throughout the paper in Tab. 2. The model parameters are similar to the model parameters used in [3].

1.5.1. Figure-of-merit

The thermoelectric off-diagonal figure-of-merit, \( f_Z \), is computed by the following composite objective function:

\[
 f_Z = \frac{f^2 \kappa^f}{f^s \kappa^s} \tag{4}
\]

where \( f^s \) is the objective function for the Seebeck coefficient, \( f^f \) is the objective for the electric conductivity and \( f^\kappa \) is the objective for the thermal conductivity. In the following we will account for how to compute these objective functions.

The off-diagonal figure-of-merit is computed by solving three different finite element problems or load cases, computing the corresponding objective functions and multiplying them as stated in Eq. (4). The boundary conditions for the \( \sigma \)-load case, the \( \kappa \)-load case and the \( \kappa \)-load case have been listed in Tab. 3.

By computing the objective functions in Eq. (4) with small differences in the state fields as listed in Tab. 3, the governing equations remain in the linear regime where the Joule heating is negligible. By including the surface electrodes and ensuring that the governing equations stay in the linear regime, the evaluation of the objective functions are consistent with the analytic and experimental approaches seen in e.g. Rowe [1], Yang et al. [14, 18] and Sakai et al. [3].

The objective functions in Eq. (4) can now be computed by following the surface integrals, please cf. Fig. 1.

\[
 f_a = \frac{L_x}{L_x} \left[ \frac{1}{L_y} \int_{\Gamma^N} V \, dS - \frac{1}{L_y} \int_{\Gamma^W} V \, dS \right] \tag{5a}
\]

\[
 f_a = \frac{1}{L_y} \int_{\Gamma^N} T \, dS - \frac{1}{L_y} \int_{\Gamma^W} T \, dS \tag{5b}
\]

\[
 f_a = \frac{L_y}{L_y} \left[ \frac{1}{L_x} \int_{\Gamma^S} Q \, dS \right] \tag{5c}
\]

As a reference, the integral expressions above are often in one dimensional modeling written as \( f_a = \Delta V/\Delta T \), \( f_a = J/\Delta V \) and \( f_a = Q/\Delta T \), where \( \Delta T \) and \( \Delta V \) denote the temperature and electric potential difference between the boundaries, respectively.

The reporting of the intricated integral expressions in Eq. (5) is serving as guidance for future research, as the expressions explicitly state the approach for computing the objective functions in Eq. (4).

1.5.2. The electrical power output

The off-diagonal electric power output, \( f_p \), is given by:

\[
 f_p = \frac{1}{L_y} \int_{\Gamma^N} V \, dS \int_{\Gamma^N} J \, dS \tag{6}
\]

which is simply an integral expression, where the average electric potential along \( \Gamma^N \) is multiplied with the integral of the electric current density along \( \Gamma^N \). The corresponding objective function in one dimensional modeling is often written as \( P = VJ \), where \( P \) is the electrical power output, \( V \) is the electrical potential and \( J \) is the electric current.

By assuming that a highly conductive surface electrode is connected to \( \Gamma^N \), the boundary conditions can be written as listed in Tab. 4. The height of the design domain (\( L_y = 0.004 \, [m] \)) and temperatures of the hot and cold reservoirs are equivalent to the design problems investigated in Sakai et al. [3].
### Table 4: The boundary conditions used to evaluate the electrical power output, $f_P$, for off-diagonal thermoelectric generators.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>$\Gamma^\kappa$</th>
<th>$\Gamma^\theta$</th>
<th>$\Gamma^\omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T^{(2)}$ [K]</td>
<td>85</td>
<td>0</td>
<td>–</td>
</tr>
<tr>
<td>$h^{(2)}$ [W/m.K]</td>
<td>$10^4$</td>
<td>$10^4$</td>
<td>–</td>
</tr>
<tr>
<td>$V^{(2)}$ [V]</td>
<td>–</td>
<td>–</td>
<td>0</td>
</tr>
<tr>
<td>$\varepsilon^{(2)}$ [S/m]</td>
<td>–</td>
<td>–</td>
<td>$\varepsilon^E$</td>
</tr>
</tbody>
</table>

#### 1.5.3. Sensitivities, filter operations and optimizer

The gradients of the objective functions in Eqs. (5) and (6) with respect to the design variable field are computed by the discrete adjoint approach (see Bendsoe and Sigmund [5]). To ensure length-scale control and robustness toward manufacturing variations, the optimization problem is formulated in a min/max form for three different projected realizations of the design variable field [19]. The physical design variables used for the finite element analysis are obtained by a density filter and a Heaviside projection filter operation [20, 21] and the optimization problem is solved with the method of moving asymptotes [10]. Readers interested in implementation details of the framework are referred to Lundgaard and Sigmund [6].

### 2. Results

To demonstrate that the topology optimization framework is suited for optimizing the figure-of-merit and the electrical power output for off-diagonal thermoelectric generators, we present a sequence of different numerical examples throughout this section.

The framework is benchmarked against the analytical predictions and frameworks in Sec. 2.1, design problems solved for the figure-of-merit are presented in Sec. 2.2 and design problems solved for the electric power output are presented in Sec. 2.3. The performance of off-diagonal, diagonal thermoelectric generators are compared in Sec. 2.4 and the thermal heat transfer modeling with Newton’s law of cooling is discussed in Sec. 2.5.

#### 2.1. Benchmark examples

The topology optimization framework used in the present study is validated with basis in the analytic optimization approach presented in Sakai et al. [3]. The objective of the analytical approach is to increase the off-diagonal figure-of-merit, $f_z$, and the off-diagonal electric power output, $f_P$, by determining the optimal tilting angle between two thermoelectric materials placed in a layered configuration.

The analytical approach by Sakai et al. [3] is derived under the assumption of infinite periodicity and negligible boundary effects. Design solutions of infinite periodicity are assumed to consist of layered, and infinitely narrow channels. Boundary effects refer to the disturbances in the state fields that occur in the transitions between the material phases and near the outer boundaries of design solutions.

As infinite periodic design solutions are a purely mathematical concept, we have to distinguish between design solutions with finitely and infinitely small design features. Equivalent to the design solutions manufactured and tested by Sakai et al. [3], our design solutions with finite length scales have an enforced minimum physical length-scale relative to the design domain height of 0.05. The corresponding design solutions for infinitely small design features do not have such minimum length-scale.

With reference to Figs. 3a and 3b, layered designs with finite and infinite periodicity are here called finite layered designs and infinite layered designs, respectively. To validate the numerical framework, we have plotted the relationship between the figure-of-merit and the tilting angle for the different optimization approaches in Fig. 2.

The entries in Fig. 2 are computed with basis in the three different analytical design solutions in Fig. 3: (A) The infinite layered design without boundary effects in Fig. 3a, (B) the infinite layered design with boundary effects in Fig. 3b and (C) the finite layered design with boundary effects in Fig. 3b. The design solutions are all solved for $A = 10$, $V = 0.5$ and $\theta \in [0; 90]$ and the positions of the integration domains in Eq. (5) have been marked by black, green and blue encircled rectangles on the design solutions plots.

With reference to Fig. 2, the relationship between $f_z$ and $f_P$ for the infinite layered designs without boundary effects and the analytical predictions in Sakai et al. [3] show excellent agreements, as the numerical simulations and the analytical derivations are carried out under the same assumptions: Infinite periodicity and negligible boundary effects. As the analytical and numerical optimization frameworks show excellent agreement, we confidently conclude that the topology optimization framework and underlying finite element model are suited for solving off-diagonal thermoelectric generator design problems seen in Fig. 1.

The influence of the boundary effects and the variations in the state fields over the layers cause the relationship between $f_z$ and $f_P$ for the different designs to deviate. The differences between the numerical and analytical
The optimization framework can be minimized by narrowing the channels, increasing the length-to-height ratio, and placing the integration domains “sufficiently far” from the outer boundaries.

The physically realizable design solutions with finite layered design with boundary effects obtained with the approach presented in Sakai et al. [3] are in the remaining part of the paper simply denoted analytical design solutions.

The length-to-height ratio of the design domain, \( \Lambda \), is an important model parameter so we have solved 100 different and equally spaced steps in the interval \( \theta \in [0; 90] \) for each value of \( \Lambda \).

By comparing Fig. 4 and Fig. 5, we point out that the numerical and analytical approach converge to very different design solutions. The large difference is also reflected in performance of the design solutions which have been plotted in Fig. 6.

The plot shows the relationship between \( f_2 \) and \( \Lambda \) for the design solutions solved for \( f_2 \) and \( f_6 \) (see Sec. 2.3 for more information). The important message of the plot is the following: The design solutions solved for \( f_2 \) with the numerical approach outperform the design solutions solved for other objectives and other optimization approaches with up to 233%. With basis in this, we hereby conclude that the numerical optimization approach is suited for solving design problems of off-diagonal thermoelectric generators.

2.2. Figure-of-merit

The goal of the first numerical design problem is to optimize the off-diagonal figure-of-merit, \( f_2 \). To demonstrate what can be achieved in performance improvements with the proposed methodology, we have decided to use the design solutions obtained with the analytical approach as benchmarks for the numerical approach.

The length-to-height ratio of the design domain, \( \Lambda \), is an important model parameter so we have solved 100 different design problems for \( \Lambda \in [0.1; 10] \), and plotted a selection of the design solutions in Fig. 4. A selection of the corresponding design solutions solved with the analytical approach have been plotted in Fig. 5. The design solutions solved with the analytical optimization approach are obtained by a simple and computational expensive parameter study over \( \theta \) which is swept in 100 different and equally spaced steps in the interval \( \theta \in [0; 90] \) for each value of \( \Lambda \).

As seen in the state field plots for the design solutions in Fig. 7, this specific length-to-height ratio provides the ideal interplay between a high electric conductivity in the horizontal direction, a low thermal conductivity in the vertical direction and a high Seebeck coefficient in the off-diagonal direction.

2.2.1. The features of the design solutions

In this section we explain why there occurs an optimum between \( f_2 \) and \( \Lambda \) in Fig. 6 and how we can use this knowledge to increase the performance of thermoelectric generators. With reference to the figure, we start this discussion by pointing out that the largest \( f_2 \) is achieved for \( \Lambda = 1.3 \).

As seen in the state field plots for the design solutions in Fig. 7, this specific length-to-height ratio provides the ideal interplay between a high electric conductivity in the horizontal direction, a low thermal conductivity in the vertical direction and a high Seebeck coefficient in the off-diagonal direction.

It is possible to tweak the design process so that one diagonal channel is obtained for larger \( \Lambda \), cf. Fig. 4d with Fig. 4e, but doing so will, according to our experience, not provide better design solution performances than already presented.

Apparently, the design solutions prefer only one simple diagonal channel of Material A, as more channels cause Material B to connect between \( \Gamma^1 \) and \( \Gamma^2 \) and hence causing a “thermal short circuit” which results in a high \( f_3 \) and hereby a low \( f_2 \), please cf. Eq. (4).

As \( f_2 \) has a squared weight in the objective function, the main feature of the design solutions is therefore to generate a high average electric potential along \( \Gamma^2 \) in the \( \alpha \)-load case. This attribute is maximized by the following two design features: (1) maximizing the heat flux normal to Material A in the diagonal channel and (2) choosing an adequate diagonal channel width to ensure that a sufficient amount of Material A is available for powering the Seebeck effect.
Figure 3: The best performing design solutions obtained with the analytical optimization approach layout in Sakai et al. [3]. The design solutions are used to validate the topology optimization framework. The performances of the design solutions are compared in Fig. 2. The green, blue and black encircled squares indicate the integration domains in Eq. (5).

Figure 4: Design solutions solved for $f_Z$ and various length-to-height ratios, $\Lambda$. The corresponding design solutions obtained with the analytical optimization approach in Sakai et al. [3] are plotted in Fig. 5. The performance of the design solutions are compared in Fig. 6, where it is seen that the best performing design solution is obtained for $\Lambda \approx 1.3$.

Figure 5: The analytical designs solutions solved for $f_Z$ and various length-to-height ratios, $\Lambda$. The corresponding topology optimized design solution are plotted in Fig. 4. The performance of the design solutions are compared in Fig. 6.
By comparing the design solutions in Fig. 4 and 5, we observe that the relative differences between the design solutions of the two optimization approaches are decreased as \( \Lambda \) is increased. As the relative differences between the design solutions are decreased, the relative performance differences are also decreased, please cf. Fig. 6.

As a final remark, we call attention to that topology optimization is especially suited for off-diagonal problems, as trivial designs solutions, i.e. standalone Material A or B, have \( f_0 \neq 0, f_1 \neq 0 \) and \( f_2 = 0 \). The segmented configuration of off-diagonal thermoelectric generators is therefore necessary, because trivial design solutions don’t generate any electric current.

2.3. Electrical power output

The goal of the second design problem is to optimize the electric power output, \( f_P \), and again we use the design solutions obtained by the analytical optimization approach by Sakai and coworkers as benchmarks for the topology optimized designs solutions.

The design solutions solved with the analytical approach are obtained by a simple and computational expensive parameter study where both \( \theta \) and \( \varepsilon^d \) are swept in 100 equally sized steps in the intervals \( \theta \in [0; 90] \) [degrees] and \( \varepsilon^d \in [10; 15000] \) [1/S], respectively.

The design solutions solved for \( f_P \) and \( \Lambda = \{0.5, 1, 2, 5, 10\} \) have been plotted in Fig. 8. By comparing these design solutions with the solutions solved for \( f_Z \) in Fig. 4, we notice that the choice of objective function has a considerable influence on the topology of the design solutions.

This difference is also reflected in the performances of the design solutions obtained with the different optimization approaches and objective functions. In Fig. 9 we have plotted the relationship between \( \Lambda \) and \( f_P \) for the different design solutions. The important point of the graph is the following: the design solutions solved for \( f_P \) outperform all other design solutions, for which reason we confidently conclude that the choice of objective function is a critical parameter of the design problems and that the topology optimization methodology outperforms the analytical optimization approach.

Another interesting and important study is seen in Fig. 9b, where the electrical power output has been normalized with respect to \( L_x \). This is done to demonstrate than an optimal choice for \( \Lambda \) exists, if the designer’s goal is to generate as much electrical power output as possible for a constrained length of the thermal hot and cold reservoirs. The maximal \( f_P/L_x \) is obtained for \( \Lambda \approx 1 \) for reasons similar to those already discussed in Sec. 2.2.1.

2.3.1. The features of the design solutions

The main differences between the design solutions solved for \( f_Z \) and \( f_P \) can be characterized by two attributes: (1) the volume ratio of the materials and (2) the topology of the diagonal channels.

Design solutions solved for \( f_P \) generally have a larger amount of Material A in the diagonal than design solutions solved for \( f_Z \). This design feature is advantageous as an increased amount of thermoelectric active material powers the Seebeck effect and hereby increases the average electric potential difference on \( \Gamma^E \).

The diagonal channels of Material A in the design solutions solved for \( f_P \) tend to meet \( \Gamma^T \) and \( \Gamma^S \) at a perpendicular angle which is not the case for the design solutions solved for \( f_Z \). This design feature results in reduced temperature gradients near \( \Gamma^T \) and \( \Gamma^S \), which increases the Peltier heat load and hereby contributes negatively to the electric current and the objective function. As the overall temperature variations are small for these problems, the state field plots for the design solutions solved for \( f_Z \), this design feature is not advantageous for these problems.

The state field plots for the design solutions solved for \( f_P \) and \( \Lambda = 1 \) in Fig. 8b have been plotted in Fig. 10. The interplay between the design solution and the state fields are similar to those already discussed in Sec. 2.2.1.
Figure 7: The relevant state field plots of the $\alpha$-load case, (a) and (b), the $\sigma$-load case, (c) and (d), and the $\kappa$-load case, (e) and (f), for the design solution solved for $f_Z$ and $\Lambda = 1.3$ in Fig. 4b. With reference to the large gradients of the electric potential field in the diagonal channel, the surrounding metal is working as a thermal and electric conductor and the diagonal channel is powering Seebeck effect and hereby the thermoelectric energy conversion.
2.3.2. The impedance of the outer resistive load

The impedance of the outer resistive load is part of the design problem, and to demonstrate the importance of the model parameter, we have plotted the design solutions solved for \( f_P \), \( z_E = \{150, 8000, 15000\} \) and \( \Lambda = 2 \) in Fig. 11. The design solutions are considerably different, which is also reflected in the corresponding relationships between \( f_P \) and \( z_E \) for the three design solutions plotted in Fig. 12.

The relationships between \( f_P \) and \( z_E \) show that a design solution solved and evaluated for a specific \( z_E \) has superior performance compared to design solutions solved and evaluated for another \( z_E \). The impedance of the outer resistive load is therefore a critical model parameter and should be taken into account for design problems involving off-diagonal thermoelectric generators.

2.4. Diagonal and off-diagonal problems

In previous sections we have demonstrated that topology optimization can be used to outperform other optimization approaches in the literature. However, we have not discussed the performance difference between off-diagonal and diagonal thermoelectric generators. Diagonal thermoelectric generators convert a vertical heat flux into a vertical electric current, and this configuration is the most standard and applied configuration of thermoelectric generators.

Tab. 5 shows that diagonal thermoelectric generators outperform off-diagonal thermoelectric generators for both \( f_Z \) and \( f_P \), however the performance loss incurred by using the off-diagonal thermoelectric generators may be acceptable when taking into account that the electrodes on \( \Gamma_E \) and \( \Gamma_W \) are not required to be in contact with the heat source. By decoupling the electrodes and the heat source, the probability of damaging the electrodes with thermo-mechanical stresses and wear during operation is decreased and this may be game changing in applications where the temperature difference between the hot and the cold reservoirs are changing considerable during operation.

2.5. Boundary conditions

We claimed in Sec. 1.3 that adequate modeling for the thermal heat transfer between the hot and cold reservoirs and the thermoelectric generator is constituted by Newton’s law of cooling. The plot in Fig. 13 is key to support this claim.

With basis in a diagonal thermoelectric generator, the plot shows the relationship between the height of the design domain, \( L_y \), and the electric power output, \( f_P \), for various heat transfer rates. For finite heat transfer rates there exist an optimum between the electrical power output and the height of the design domain. However, as the heat transfer rate goes to infinity, the optimal height of the design domain goes to zero, and the electric power output goes to infinity. This singularity is indeed non-intuitive and non-physical and it is therefore concluded that finite heat transfer rates between the hot and cold reservoirs and the thermoelectric generator are required for carrying out adequate physical modeling for thermoelectric generators.
Table 5: A comparison between the figure-of-merit, \( f_Z \), electrical power output, \( f_P \), and the normalized electrical power output, \( f_P/L_x \), for design solutions of standalone materials in diagonal and off-diagonal configurations. The topology optimized design solution solved in the diagonal configuration (not shown in the paper) outperform the design solutions solved in the off-diagonal configurations. However, thermoelectric generators in off-diagonal configurations may be less prone the thermo-mechanical stresses and wear.

<table>
<thead>
<tr>
<th>Description</th>
<th>Type</th>
<th>( f_P/L_x )</th>
<th>( f_Z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standalone Material A</td>
<td>Diagonal</td>
<td>1444.18</td>
<td>3.341 ( \times 10^{-3} )</td>
</tr>
<tr>
<td>Standalone Material B</td>
<td>Diagonal</td>
<td>85.17</td>
<td>0.046 ( \times 10^{-3} )</td>
</tr>
<tr>
<td>Design solution</td>
<td>Diagonal</td>
<td>4378.62</td>
<td>3.302 ( \times 10^{-3} )</td>
</tr>
<tr>
<td>Design solution in Fig. 8b</td>
<td>Off-diagonal</td>
<td>3896.19</td>
<td>2.110 ( \times 10^{-3} )</td>
</tr>
</tbody>
</table>

Figure 9: The relationships between the length-to-height ratio, \( \Lambda \), the electrical power output, \( f_P \), and the normalized electrical power output, \( f_P/L_x \), for the design solutions solved for \( f_P \) and \( f_Z \). The design solutions solved for \( f_P \) with topology optimization outperform design solutions solved for other objectives and optimization approaches, for which reason we conclude that the topology optimization approach is suited for optimizing the off-diagonal electric power output of thermoelectric generators.
Figure 10: The state field plots for the design solution solved for electrical power output, $f_P$, and length-to-height ratio, $\Lambda = 1$, in Fig. 8b. The design features of the design solution are equivalent to what already discussed in the caption in Fig. 7 and in Sec. 2.3.1.

Figure 11: Design solutions solved for electrical power output, $f_P$, and different electrical impedances of the outer resistive load, $z^E$. The performance of the design solutions are plotted in Fig. 12. As the performance and topology of the design solutions are dependent on $z^E$, we conclude that $z^E$ is an important model parameter.

Figure 12: The relationship between the electrical power output, $f_P$, and the electrical resistance in the outer load, $z^E$, for the design solutions plotted in Fig. 11. Design solutions solved for one $z^E$ outperform design solutions solved for other $z^E$ for which reason we conclude that we can attribute importance to the features to the design solutions.
Figure 13: The relationship between the normalized electrical power output, $f_P/L_x$, the length of the design domain, $L_y$, and various convection coefficients, $h^{NS}$. For trivial design solutions consisting of standalone Material A. As the convection coefficients are increased, the electric power output are increased and the optimal design domain length is decreased. Dirichlet type boundary conditions are equivalent to $h^{NS} \to \infty$, which due to the singularity between $f_P/L_x$ and $L_y$ is concluded to be non-physical.

3. Discussion

All results presented in the present paper are supported by validation studies, benchmark examples and cross-checks, for which reason we confidently conclude that the topology optimization approach is a promising methodology for optimizing the performance of segmented off-diagonal thermoelectric generators. However, there are three issues that need to be discussed in relation to the presented results:

1. The neglection of parasitic losses
2. The manufacturability of the design solutions
3. The assumption of temperature independent material parameters

These topics are discussed in the following.

3.1. Parasitic losses

The thermal and electric parasitic losses in the transitions between the material phases are neglected in the underlying finite element model. The work presented is hence purely theoretical and the design solutions have not been tested experimentally.

The losses should indeed be included in detailed computations, however we argue that the methodology and design solutions are relevant despite neglecting the losses.

Our main argument can be divided in three subarguments:

(A) [3] presented an analytical optimization approach which was used to optimize the figure-of-merit and the electric power output. This study is especially interesting because the design solutions were manufactured and tested experimentally. Even though the design solutions consisted of a high number of transitions between material phases, Sakai and coworkers found good agreement between the experimental measurements and the analytical predictions. Since our designs have less interface regions, we therefore argue that it is reasonable to assume that the thermal and electrical parasitic losses are smaller for the design solutions presented in this study than the design solutions tested in by Sakai and coworkers.

(B) Off-diagonal thermoelectric generators are required to be segmented with two or more different materials to produce thermoelectric energy, please confer the discussion in Sec. 2.2.1. As segmentation is necessary to ensure the functionality of off-diagonal thermoelectric generators, designers are therefore forced to accept parasitic losses which make the topology optimization approach, used in the present study, suitable.

(C) With performance improvement beyond $\approx 200\%$ compared to analytical design solutions, we argue that these performance improvements are so large that they may dominate the parasitic losses.

3.2. Manufacturability of the design solutions

The manufacturability of the design solutions can be assessed with basis in three characteristics of the design solutions: (A) the topology of the design features (B) the number of transitions between the material phases and (C) the minimum length scale.

(A) The analytical design solutions tested and manufactured by [3] were quite similar to the design solutions presented in the present study as the design solutions obtained with the numerical and the analytical approach both consisted of simple geometrical structures such as triangles and parallelograms, see e.g Figs. 4b and 8b.

(B) With respect to the number of transitions between the material phases, the analytical design solutions consisted of a considerably amount of diagonal channels compared to the design solutions with only one diagonal channel seen in the present study. The transitions between the material phases are a critical part in relation to the manufacturability, as poor connections between the material phases result in poor transfer of thermal and electrical energy and hereby high parasitic losses. However, with reference to the good agreements between the analytical predictions and experiments in Sakai and coworkers, it seems that they overcame this challenge.
The design solutions presented in the present paper are solved with a requirement on the minimum length scale and the design solutions do therefore not contain design features which are smaller than a prescribed value. This approach provides a road to tailor the design solutions such that they are suited for additive manufacturing techniques as the minimum length-scales of the design features are matched to the available printing resolution.

With reference to the study by Sakai and coworkers, we point out that the topology optimized design solutions are simpler or equally simple in topology, have smaller amount of transitions between the material phases, and the same minimum length scale, for which reason we assess that the design solutions presented in the present paper are less or equally complicated to manufacture compared to the design solutions presented in the work of Sakai and coworkers.

3.3. Temperature independent materials

The design problems were solved for temperature independent material parameters, which indeed is an inadequate assumption for many physical materials. We decided to limit the design problems to temperature independent materials to ensure a frame of reference with respect to the design solutions presented in Sakai et al. [3]. The topology optimization methodology can straightforwardly be extended such that temperature dependent material parameters in taking into consideration. Implementation details are provided in Lundgaard and Sigmund [6].

4. Conclusion

We have used a density-based topology optimization methodology to optimize the figure-of-merit and the electric power output for off-diagonal thermoelectric generators. The objectives are optimized by spatially distributing two different thermoelectric materials in a two dimensional design space.

With basis in a fully coupled thermoelectric model with temperature independent materials, we use the framework to identify and discuss several important design model parameters. The most important findings have been listed in the following:

1. With reference to the excellent agreements between the analytic predictions in Yang et al. [14], Sakai et al. [3], the experimental validations in [3] and the topology optimization framework, we confidently conclude that we can rely on the underlying mathematical model of the framework.

2. The topology optimized design solutions outperform the analytical design solutions by 233% for design problems solved for figure-of-merit and by 229% for design problems solved for electric power output. The topology optimization approach is therefore concluded to be excellently suited for optimizing off-diagonal thermoelectric generators.

3. Design solutions solved for figure-of-merit do not necessarily provide large electrical power outputs and design solutions solved for electric power output do not necessarily provide large figure-of-merits. The choice of objective function is therefore concluded to be a critical design parameter and designers should therefore carefully consider the interplay between the end-goal application of the devices and the optimization problem.

4. By solving three different realization of the design problems in a min/max formulation, it is possible to control the length-scales of the design solutions, such that they are supported by the resolution of the manufacturing techniques available.

5. To ensure adequate physical modeling, the heat transfer rates between the cold reservoir, the hot reservoir and the thermoelectric generator are finite to ensure physical realistic modeling. Surfaces with Dirichlet type temperature boundary conditions are subject to infinite heat transfer rates, for which reason these type of boundary condition may result in non-physical physical modeling and therefore useless design solutions.

6. With basis in the state fields of the design solutions, we conclude that the spatial distribution and the volume ratio between the materials are the primary design features for maximizing the figure-of-merit and the electric power output.

7. By analyzing crosscheck studies, we identify the length of the thermoelectric generator and the impedance in the outer electrical load as critical design parameters for maximizing the figure-of-merit and the electric power output.

8. Diagonal thermoelectric generators outperform off-diagonal thermoelectric generators for both electric power output and figure-of-merit, however off-diagonal thermoelectric generators may be less prone to wear and/or thermo-mechanical stresses.

The methodology can easily be extended to incorporate temperature dependent materials, multiple materials phases, other objective functions and different boundary conditions. However, for now, the study serves as a demonstration that topology optimization is a suitable
method for optimizing off-diagonal thermoelectric generators.

5. Acknowledgements

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6. Bibliography

Publication [P4]:
Design of segmented thermoelectric Peltier coolers with topology optimization

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Abstract
A density-based topology optimization approach is used to optimize the cooling power and efficiency (coefficient of performance) of thermoelectric coolers by spatially distributing two different thermoelectric materials in a two dimensional design space. With basis in three numerical examples we identify important model parameters, such as the choice of objective function, the temperatures of the thermal reservoirs, the heat transfer rates and the available electrical energy. By using the topology optimization approach, we demonstrate that the cooling power and efficiency of thermoelectric coolers can be improved with 48.7% and 11.4%, respectively, compared to optimization approaches available in the literature.

Keywords: Topology optimization, thermoelectric energy conversion, Peltier coolers, segmentation

1. Introduction
Thermoelectricity is a physical phenomenon which concerns the interaction between electric and thermal energy in semi-conducting materials. Thermoelectricity can be characterized by two separately identified effects, the Seebeck effect which concerns the conversion of thermal energy into electric energy, and the Peltier effect which concerns the conversion of electric energy into thermal energy [1]. With reference to the sketch in Fig. 1, a thermoelectric cooler is a solid-state heat pump which uses the Peltier effect to convert electrical energy into a thermal energy flux and thereby providing cooling power at a specified surface.

Compared to vapor-compression refrigeration systems, thermoelectric coolers are so far limited to niche applications due to their relatively low operational cooling power and efficiency (coefficient of performance). Despite a considerable amount of scientific efforts, performance improvements of thermoelectric coolers are still required to increase the range of applications [4, 3]. The main efforts to increase the performance of thermoelectric coolers have so far been a broad search for identification and development of advanced thermoelectric materials [5, 6], however, in this paper we address a purely mathematical optimization approach aiming at finding the best spatial distributions of available materials in order to optimize a specified performance measure.

In the literature, the performance of thermoelectric coolers has been characterized in different ways, see e.g. Seifert et al. [7] or Bian et al. [8]. As we see it, the performance measures can be divided into four categories: (A) the temperature at the compartment surface, \( f_T \), (B) the heat flux at the compartment surface, \( f_Q \), (C) the coefficient of performance at the compartment surface, \( f_\mu \), (D) and the dimensionless figure-of-merit of the device, \( f_ZT = \alpha \sigma / \kappa \), where \( \alpha \) is the Seebeck coefficient, \( \sigma \) is the electric conductivity, \( \kappa \) is the thermal conductivity and \( T \) is the temperature. In this study we address objectives (A), (B) and (C).

Only a minor part of the scientific efforts concerned with improving thermoelectric energy conversion takes
basis in mathematical optimization approaches. The available approaches can generally be sorted in three categories: (a) functionally graded material studies, (b) compatibility and segmentation approaches, and (c) geometrical optimization approaches. The topology optimization approach proposed in present thesis is a subclass of (b).

Functionally graded material studies are aiming at identifying spatial profiles of relevant material parameters which optimize a prescribed performance measure of thermoelectric coolers and generators. The design solutions of functionally graded material studies are characterized by macroscopic gradients in the material parameters, which may be linked to the composition (including doping) or microstructures of the functional properties of the material [9].

In the works of Müller et al. [10], Bian and Shakouri [11, 12] and Bian et al. [8], the coefficients in arbitrary interpolation functions for the spatial profiles of \( \alpha(x) \) and \( \sigma(x) \) were optimized with basis in parameter studies and non-gradient algorithms. Parameter studies and non-gradient algorithms are inadequate for design problems with many design variables such as the density-based topology optimization approach used in this study [13].

Later, a gradient-based optimization approach for functionally graded materials was introduced in [14] and later extended to physically realistic boundary conditions in Gerstenmaier and Wachutka [15]. The topology optimization methodology [16, 17, 18, 19] used in this study is also gradient-based and supports the same type of boundary conditions as Gerstenmaier and Wachutka, however, the two methodologies take completely different offset and modeling approaches and hereby result in completely different design solutions.

Compatibility approaches were originally suggested for thermoelectric generators in the work of Ursell and Snyder [20] and have later been developed in a series of studies in e.g. Seifert et al. [21], Snyder et al. [22], Seifert et al. [23]. By identification of compatible materials, it has been shown that the performance of thermoelectric generators and thermoelectric coolers can be considerably improved by segmentation. Compatible materials operate optimally under the same external electrical resistance and are therefore suited for being segmented, i.e. connected thermally and electrically in series. The design solutions of the compatibility approach are generally characterized by one dimensional (1D) line interfaces between the materials phases, where the design solutions of the topology optimization approach support arbitrary two dimensional (2D) features. The compatibility approach is, as the functionally graded material approach, related to the topology optimization methodology, however the approaches take very different offsets and converge to different design solutions.

By studying the volume fraction between two materials connected thermally and electrically in series, Yang et al. [24] presented a mathematical optimization approach aiming at increasing the effective figure-of-merit of two segmented materials. It was shown that the figure-of-merit of the composite medium could exceed the figure-of-merit of the constitutive materials, if the electric potential difference was chosen sufficiently large when evaluating the electric conductivity. A related approach was utilized to optimize the conversion efficiency in Yang et al. [25].

System configurations where a vertically directed heat flux is converted into a horizontally directed electric current are often referred to as off-diagonal problems. These problems were addressed in Sakai et al. [26], who studied the tilting angle and volume fraction between two segmented materials in order to optimize the device figure-of-merit. The approach, which has been theoret-
ically improved and discussed in [27], was limited to fixed temperature boundary conditions, simple topological design solutions and constant material parameters.

In the work of Schilz et al. [9], Müller et al. [10], the cooling power of thermoelectric coolers were optimized by maximizing the local figure-of-merit with respect to the local temperature conditions of the device during operation. The interaction between figure-of-merit and electric power output for thermoelectric generators was addressed in [27], and we do therefore not consider this measure in the present paper.

The topology optimization approach used in this study uses a completely different offset and modeling approach and converges to different design solutions compared to the functionally graded material, compatibility and homogenization approaches. The topology optimized design solutions are characterized by two separately identified material phases and two dimensional features, and if the design problems are solved for physical material parameters, the design solutions can straight-forwardly be interpreted and manufactured without any consideration of the local functional properties of the materials.

2. The design problem

The topology optimization methodology [16, 17] used in this study is based on a finite element formulation of the generalized Ohm’s and Fourier’s law [28], the method of moving asymptotes [29], adjoint sensitivity analysis [30], and various filter operations [31, 32]. The framework supports advanced physical modeling concepts such as temperature dependent material parameters, complex geometries and advanced boundary conditions. A detailed description and implementation details of the framework can be found in Lundgaard and Sigmund [19], however we will briefly discuss the most important features of the framework in the following. In this connection we introduce several variables which we have summarized in Tab. 1.

2.1. Physical model

The design problem takes basis in the sketch in Fig. 2, where a single leg of a single module of a single thermoelectric cooler is considered. The boundary conditions and the model parameters are inspired by a household refrigerator being powered by thermoelectric cooling. The hot ambient with temperature, $T^H$, and the cold compartment, $T^C$, are separated by the leg with dimensions $\{L_x, L_y\} = \{0.005, 0.005\}$ [m].

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma^H$</td>
<td>Boundary at the ambient (thermal hot reservoir)</td>
</tr>
<tr>
<td>$\Gamma^C$</td>
<td>Boundary at the compartment (thermal cold reservoir)</td>
</tr>
<tr>
<td>$T^H$</td>
<td>Temperature of the ambient at $\Gamma^H$</td>
</tr>
<tr>
<td>$T^C$</td>
<td>Temperature of the compartment at $\Gamma^C$</td>
</tr>
<tr>
<td>$T^{HC}$</td>
<td>Abbreviation of $T^H$ and $T^C$ combined</td>
</tr>
<tr>
<td>$h^H$</td>
<td>Convection coefficient at $\Gamma^H$</td>
</tr>
<tr>
<td>$h^C$</td>
<td>Convection coefficient at $\Gamma^C$</td>
</tr>
<tr>
<td>$h^{HC}$</td>
<td>Abbreviation of $h^H$ and $h^C$ combined</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>Temperature difference between $T^H$ and $T^C$</td>
</tr>
<tr>
<td>$\Delta V$</td>
<td>Electric potential difference between $T^H$ and $T^C$</td>
</tr>
<tr>
<td>$f$</td>
<td>The temperature field [K]</td>
</tr>
<tr>
<td>$\nabla v$</td>
<td>The electric potential field [V]</td>
</tr>
<tr>
<td>$Q_x, Q_y$</td>
<td>The thermal heat flux [W/m$^2$] in x and y, respectively</td>
</tr>
<tr>
<td>$J_x, J_y$</td>
<td>The electric current density [A/m$^2$] in x and y, respectively</td>
</tr>
<tr>
<td>$f_T$</td>
<td>Temperature average at $\Gamma^C$</td>
</tr>
<tr>
<td>$f_Q$</td>
<td>Heat flux at $\Gamma^C$</td>
</tr>
<tr>
<td>$f_P$</td>
<td>Electric power input at $\Gamma^C$</td>
</tr>
<tr>
<td>$f_\mu$</td>
<td>Coefficient of performance, $f_\mu = f_Q/f_P$, at $\Gamma^C$</td>
</tr>
<tr>
<td>$\Omega_D$</td>
<td>Design domain</td>
</tr>
<tr>
<td>$L_x$</td>
<td>Length of $\Omega_D$ in x</td>
</tr>
<tr>
<td>$L_y$</td>
<td>Length of $\Omega_D$ in y</td>
</tr>
</tbody>
</table>
Material A and B (see Fig. 2) are assumed temperature independent, similar to the material parameters used in the analytic derivations in the work of [24], and listed in Tab. 2. We decided to limit the design problems to linear materials, as the design features of the counterpart design solutions with non-linear materials are more challenging to interpret. However, the framework could easily be extended to support temperature dependent materials, see Lundgaard and Sigmund [19], and could easily be extended to support temperature dependent materials, see Lundgaard and Sigmund [19], and researchers with ambitions to manufacture the design solutions should definitely take temperature-dependent effects into account.

2.1.1. Equations

The basic partial differential equations of thermoelectricity are constrained by Fourier’s and Ohm’s generalized law. The continuity of thermal energy and electric charge are in \( \Omega_D \), see Fig. 2, given by [1]:

\[
\begin{align*}
\nabla \cdot \vec{\dot{q}} &= \dot{q} \quad \text{in} \quad \Omega_D \\
\nabla \cdot \vec{\dot{f}} &= 0 \quad \text{in} \quad \Omega_D
\end{align*}
\]

where \( \nabla \) denotes the spatial derivative with respect to Cartesian directions \( x \) and \( y \); \( \vec{\dot{q}} = [\dot{Q}_x, \dot{Q}_y] \) is the heat flow density in \( x \) and \( y \) [W/m²]; \( \dot{q} = \vec{\dot{q}} \cdot \vec{E} \) is the Joule heating term [W/m³]; \( \vec{E} = -\nabla V \) is the electric field [V/m]; \( V \) is the electric potential and \( \vec{f} = [\dot{J}_x, \dot{J}_y] \) is the electric current density in \( x \) and \( y \) [A/m²]. In thermoelectric analysis, the thermal and electric energies are coupled by the constitutive equations:

\[
\begin{align*}
\vec{Q} &= T \sigma \cdot \kappa \cdot \nabla T \\
\vec{f} &= \sigma \cdot (\vec{E} - \alpha \cdot \nabla T)
\end{align*}
\]

where \( \vec{Q} \) is the heat flux density [W/m²], \( \vec{f} \) is the electric current density [A/m²], and \( T \) is the temperature [K].

2.1.2. Newton’s law of cooling

With reference to the simple rectangular geometry of the thermoelectric cooler in Fig. 2 and the relatively small length scales of the modules, we assume that the heat transfer between the module, the ambient and the compartment can be modeled by Newton’s law of cooling. Utilizing Newton’s law of cooling, it is assumed that the thermal heat transfer rate at \( \Gamma^D \) and \( \Gamma^C \) is proportional to the temperature difference between the ambient, the compartment and the module:

\[
\vec{n} \cdot \vec{\dot{q}} = b^{HC}(T - T^{HC})
\]

where \( b^{HC} \) denotes the heat transfer coefficient [W/m²K] on \( \Gamma^D \) and \( \Gamma^C \), respectively, \( \vec{n} \) is the normal vector to the surface, and \( T^{HC} \) denotes the temperatures of the thermal reservoirs [K] in \( \Gamma^D \) and \( \Gamma^C \), respectively.

In Newton’s law of cooling, the heat transfer rate between the leg and the thermal reservoirs is governed by the fluid and the flow types at the boundaries. The flow rate is quantified by the so-called convection coefficient, which is denoted \( h^f \) and \( h^c \) for the ambient and the compartment, respectively. Convection coefficients of various flow types and flow conditions have been listed in Tab. 3 for reference.

2.2. Finite element model

The governing equations in Eqs. (1)-(4) are solved numerically by discretizing the equations into finite elements [33, 28, 34]. The topology optimization framework is set up by introducing a design field \( 0 \leq h \leq 1 \), such that the material parameters in the governing equations become functions of the design field, i.e. \( \sigma = \sigma(h) \), \( \alpha = \alpha(h) \) and \( \kappa = \kappa(h) \). By introducing the design variable field, it is possible to control whether a finite element represents Material A or Material B. This functionality can be used to optimize a specific performance measure, i.e. objective function, of the device.

2.3. The optimization problems

We believe that three objective functions are important in TE cooling applications: The average temperature over the boundary \( \Gamma^C \), \( f_2 \); the \( x \)-directional heat flux through \( \Gamma^C \), \( f_3 \); and the \( x \)-directional heat flux divided by the \( x \)-directional electric energy through \( \Gamma^C \), \( f_4 \).
Table 2: The Seebeck coefficient, $\alpha$, the electric conductivity, $\sigma$, and the thermal conductivity, $\kappa$ for Material A and B used in the design problem sketched in Fig. 2. The material parameters are copied from Yang et al. [24].

<table>
<thead>
<tr>
<th></th>
<th>Color in plots</th>
<th>$\alpha$ [V/K]</th>
<th>$\sigma$ [S/m]</th>
<th>$\kappa$ [W/(m·K)]</th>
<th>$Z^*$ [1/K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material A</td>
<td></td>
<td>$200 \cdot 10^{-6}$</td>
<td>$110 \cdot 10^0$</td>
<td>1.60</td>
<td>2.75 · $10^{-3}$</td>
</tr>
<tr>
<td>Material B</td>
<td></td>
<td>$270 \cdot 10^{-6}$</td>
<td>$22 \cdot 10^0$</td>
<td>0.77</td>
<td>2.10 · $10^{-3}$</td>
</tr>
</tbody>
</table>

Table 3: List of convection coefficients for various flow types and flow conditions.

<table>
<thead>
<tr>
<th>Flow type</th>
<th>Flow condition</th>
<th>$h_{HC}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forced convection</td>
<td>Air over a surface</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>Air over a cylinder</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>Water in a pipe</td>
<td>3000</td>
</tr>
<tr>
<td>Free convection</td>
<td>Water and liquids</td>
<td>50-3000</td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>100-1200</td>
</tr>
<tr>
<td></td>
<td>Air</td>
<td>10-100</td>
</tr>
<tr>
<td></td>
<td>Various gasses</td>
<td>5-37</td>
</tr>
</tbody>
</table>

Objective function $f_e$ is in the literature often denoted Coefficient Of Performance and abbreviated COP.

The average temperature objective function, $f_T$, is defined as:

$$f_T = \frac{1}{L_T} \int_{V_T} T \, dS,$$  \hfill (6)

The heat flux objective function, $f_Q$, is given by:

$$f_Q = \int_{V} Q \, dS,$$  \hfill (7)

where the lowercase $x$ denotes that the $x$ directional component of the field is being considered. The COP objective function, $f_C$, is given by:

$$f_C = \frac{f_Q}{f_T}$$  \hfill (8)

where $f_T$ is the $x$-directional electric energy (the power consumption of the module) given by:

$$f_T = \frac{1}{L_T} \int_{V_T} V \, dS \int_{V_T} J_x \, dS$$  \hfill (9)

In one dimensional problems in the literature, Eq. (9), is often simply written as $P = V J$.

The optimization framework is powered by discrete adjoint sensitivity analysis which provides gradients of the objective functions, see Michaleris et al. [30], Bendsoe and Sigmund [17], Lundgaard and Sigmund [19] for more information.

3. Results

Five numerical examples are presented to demonstrate that the topology optimization methodology is suitable for optimizing thermoelectric coolers. By identifying and discussing important model parameters such as the objective functions, Sec. 3.1; the temperatures of thermal reservoirs, Sec. 3.2; the electric power supply, Sec. 3.3; the heat transfer rates, 3.4; and the features of the design solutions, Sec. 3.5.

The design solutions presented throughout the paper are dependent on the applied electric potential difference, $\Delta V$, between $\Gamma^V$ and $\Gamma^C$, and unless otherwise stated all design solutions are solved for the specific magnitude of $\Delta V$ that provides the best performing design solution.

3.1. The objective function

In the first numerical example we investigate the relationship between the objective functions and the design solutions. The study takes basis in the design solutions solved for average temperature, $f_T$, heat flux, $f_Q$, a sequence of different convection coefficients, $h_{HC}$, and thermal reservoir temperatures of $T_{HC} = 300$ in Fig. 3.

With reference to Fig. 3, the design solutions can generally be characterized by three attributes: (A) the volume ratio between the material phases, (B) the length of the spike-shaped transitions between the material phases, and (C) the position of the transition between the material phases. The attributes (A), (B) and (C) are all governed by the convection coefficients and the choice of objective function.

By comparing the design solutions solved for $f_T$ and $f_Q$, we notice that for a specific set of convection coefficients, the design solutions are almost similar, compare e.g. Figs. 3c and 3h. As design problems solved for $f_T$ and $f_Q$ result in almost similar design solutions, we will only solve maximum cooling problems for $f_Q$ throughout the remaining part of the paper. The equivalence between $f_T$ and $f_Q$ design problems were also observed in the work by Müller et al. [10]. The equivalence between the design problems solved for $f_T$ and $f_Q$ is after all not surprising, as the temperature difference and heat flux between the same two surfaces basically are the same.
Design solutions solved for $f_Q$ and $f_{\mu}$ (coefficient of performance), a sequence of different convection coefficients, $T_H = 300$ and $T_C = 260$ have been plotted in Figs. 4. By comparing the designs solutions solved for a specific set of convection coefficients, we observe that the two objective functions result in very different design solutions, compare e.g. 4d and 4i.

Three important differences of the design solutions solved for $f_Q$ and $f_{\mu}$ are identified: (A) the spike-shaped transitions between the material phases occur for larger convection coefficients in design problems solved for $f_{\mu}$. (B) design solutions solved for $f_{\mu}$ have generally a lower ratio between Material A and B which is cost function effective due to the low thermal conductivity of Material B and (C) the position of the transition between the material phases is different for design problems solved for $f_Q$ and $f_{\mu}$.

With basis in these observations, we hereby conclude that the magnitude of the convection coefficients and the objective functions are important model parameters in design problems of thermoelectric coolers.

3.1.1. Objective function cross-checks

To make probable that the design solutions in Sec. 3.1 indeed have superior performance for the model parameters they were optimized for, we have carried out a so-called cross-check. Cross-checks are very important in many aspects of optimization, as they enlight how much significance we can attribute to the features of the design solutions.

The design solutions in Fig. 3 and 4 are compared with design solutions obtained with the classical segmentation approach. Design solutions solved with the classical segmentation approach are characterized by a one dimensional line interface between the material phases. The main difference between the classical segmented design solutions and the topology optimized design solutions is therefore the two dimensional spike-shaped design features seen in e.g. Fig. 4i.

In Figs. 5 we have plotted the relationship between $f_Q$ and $\Delta V$ for the design solutions solved for $f_T$, $f_Q$, $h_{HC} = 412$ and $T_{HC} = 300$ in Figs. 3c and 3h. With reference to the plot, we see that the designs solutions solved with topology optimization outperform the design solutions solved with the classical segmentation approach when $\Delta V$ is tuned such that the highest possible device performances are achieved. Furthermore, we notice that the performance of the design solutions solved for $f_T$ and $f_Q$ are almost identical which supports what already discussed in Sec. 3.1.

In the sake of completeness, we have cross-checked the design solutions solved for $f_\mu$, $h_{HC} = 2500$, $T_{HC} = 260$ in Fig. 6. The important features of the cross-check plot are identical to what was already discussed for the cross-check plot in Fig. 5 and we will therefore not discuss this further. However with basis in the cross-
Design solutions solved for $f_Q$, $T_C = 260$, and $T_H = 300$. The design solutions are dependent on $h_{HC}$ and the choice of objective function, for which reason we conclude that these parameters are important in design problems of thermoelectric coolers.

![Figure 4: Design solutions solved for the heat flux objective function, $f_Q$, and the coefficient of performance objective function, $f_{\mu}$, compartment temperature of $T_C = 260$, ambient temperature of $T_H = 300$ and various convection coefficients, $h_{HC}$. The design solutions are dependent on $h_{HC}$ and the choice of objective function, for which reason we conclude that these parameters are important in design problems of thermoelectric coolers.](image)

Check plots we confidently conclude that (A) we may attribute features to the design solutions, (B) that the objective function is an important model parameter and that (C) the topology optimization approach outperforms the classical segmentation approach.

### 3.2. The temperatures of the thermal reservoirs

The second numerical example is concerned with the relationship between the design solutions and the temperature difference between the ambient and the compartment, $\Delta T$. The study takes basis in the design solutions solved for $f_{\mu}$, $\Delta T = \{0, 10, 20, 30, 40\}$, and $h_{HC} = \{191, 446, 530, 700, 2500\}$ in Fig. 7.

The design solutions can generally be characterized by two attributes: (A) the ratio between Material A and B is increased when $T_C$ is increased, because an increased $\Delta T$ results in an increased thermal heat transfer rate between the compartment and the ambient. To reduce this heat transfer, the effective thermal conductivity of the design solutions is reduced by increasing the relative amount of Material A. (B) length and positions of the spike-shaped transitions between the material phases and the increased ratio between Material A and B for increasing $h_{HC}$ is equivalent to what was already discussed in Sec. 3.1.

As the design solutions are dependent on $h_{HC}$ and $\Delta T$, we conclude that these model parameters are important for design problems of thermoelectric coolers.
3.2.1. Temperatures of the thermal reservoirs cross-check

The design solutions solved for $h^\text{HC} = 666$ and $\Delta T = \{0, 10, 20, 30, 40\}$ in Fig. 7d, 7l, 7n and 7x have been cross-checked with the classical segmentation approach in Fig. 8. The corresponding cross-check for the design solutions solved for $f_{Q}$, $h^\text{HC} = 2500$ and $\Delta T = \{0, 10, 20, 30, 40\}$ has been plotted in Fig. 9. Please notice that these design solutions are not shown in the paper.

With reference to the cross-check plots in Figs. 8 and 9, we notice that the design solutions solved with topology optimization outperform the design solutions solved with classical segmentation by 48.7% and 11.4% with respect to $f_{Q}$ and $f_{Q}$, respectively. We therefore confidently conclude that topology optimization is suited for optimizing thermoelectric cooling problems.

3.3. The electric energy supply

The third numerical example is concerned with the relationship between the design solutions and the electric potential difference between the ambient and the compartment, $\Delta V$. The design solutions solved for $f_{Q}$, $h^\text{HC} = 615$, $T^C = 280$, $T^H = 300$ and $\Delta V = \{0.0169, 0.0386, 0.0483, 0.0579, 0.0700\}$ have been plotted in Fig. 10.

The design solutions are obviously dependent on the electric potential difference, and we emphasize the importance of taking this model parameter into consideration in the design problems. The magnitude of $\Delta V$ which result in the best performing design solution is a compromise between the Peltier effect and the Joule heating effect. Design problems solved for too large $\Delta V$ are subject to an objective-ineffective amount of Joule heating, where design problems solved for too low $\Delta V$ are subject to a too low amount of electric energy for powering the Peltier effect. Design solutions solved for insufficiently large $\Delta V$ are also seen in the cross-check plot in Fig. 6.

The relationships between $\Delta V$ and $f_{Q}$ for the design solutions solved $f_{Q}$, $T^C = 280$, $T^H = 300$ and $h^\text{HC} = \{242, 327, 463, 564\}$ have been plotted in Fig. 11. The plot demonstrates that the cooling power and the electric potential difference are coupled with the convection coefficient. We emphasize three important features of the plot: (A) the maximum cooling power is increased as $\Delta V$ is increased. This continues until a specific threshold where the Joule heating effect becomes too dominating and the maximum cooling power begins to decrease. (B) the electrical potential difference necessary to obtain the maximum cooling power is increased as the convection coefficients are increased. (C) The heat flux on $\Gamma^C$ is positive for small electric potential differences. Due to the temperature difference between $\Gamma^C$ and $\Gamma^H$ and the small electric potential difference, the Seebeck effect dominates over the Peltier effect and the thermoelectric cooler is actually working as a thermoelectric generator for these model parameters.

The relationships between $\Delta V$ and $f_{Q}$ for the design solutions solved $f_{Q}$, $T^C = 260$, $T^H = 300$ and $h^\text{HC} = \{530, 649, 1000, 2500\}$ have been plotted in Fig. 12. The same features as already discussed in points (A), (B) and (C) are also evident for this study and we will therefore not discuss them further.

3.4. The convection coefficient

The fourth numerical example is a cross-check study which concerns the relationship between the convection coefficients and the design solutions. The study takes basis in Fig. 13, where the relationships between $f_{Q}$ and $h^\text{HC}$ for the design solutions solved for $f_{Q}$, $T^C = 280$, $T^H = 300$ and $h^\text{HC} = \{175, 276, 412, 530, 1000\}$ have been plotted. The performance of the design solutions has been computed for $h^\text{HC} \in \{0; 1000\}$ to demonstrate that the design solutions have superior performance for the convection coefficients at which they were optimized.

As guidance to understand the plot, we point the attention to the teal/cyan line which illustrates the relationship between $h^\text{HC}$ and $f_{Q}$ for the design solution solved for $h^\text{HC} = 1000$. As the design solutions are evaluated for $h^\text{HC} = 1000$ we notice that the design solutions solved...
Design solutions solved for $T_C = 260$ and $T_H = 300$.

Design solutions solved for $T_C = 270$ and $T_H = 300$.

Design solutions solved for $T_C = 280$ and $T_H = 300$.

Design solutions solved for $T_C = 290$ and $T_H = 300$.

Design solutions solved for $T_C = 300$ and $T_H = 300$.

Figure 7: Design solutions solved for the temperature objective function, $f_T$, various compartment convection coefficients, $h^C$, and various compartment temperatures, $T^C$. Due to the dependency between the $h^C$ and $T^C$ and the design solutions, we conclude that these model parameters indeed are important for design problems of thermoelectric coolers.
The design solutions solved for $f_Q$ with topology optimization outperform the design solutions solved for other convection coefficients.

The same tendency is evident for all the design solutions in Fig. 13, and we thereby conclude that the convection coefficient is an important model parameter and that the topology optimization approach is suited for taking this model parameter into account.

### 3.5. The design features

Throughout the numerical examples presented in Secs. 3.1, 3.2 and 3.3, we have seen that some design solutions are characterized by spike-shaped transitions between the material phases. This is indeed a key feature of the design solutions and to understand its functionality better, we take basis in the design solution in Fig. 7m and the corresponding state field plots in Fig. 14.

Despite the two dimensional features of the design solution, the state fields are only varying slightly in the $y$-direction, for which reason we argue that the design solution can be decomposed into horizontally segmented channels with varying width along $x$. With reference to the sketch in Fig. 15, the two dimensional designs are decomposed into one dimensional designs by defining a local $x$-directional volume ratio between the materials, $\nu = \nu(x)$.

The decomposition is initiated with basis in the finite layered 2D design in Fig. 15a. This design is then decomposed into an infinite layered 2D design in Fig. 15b, and finally decomposed into an infinite layered 1D design in Fig. 15c.

By considering the intermediate design variables in Fig. 15c as horizontal channels where the $x$-directional volume ratio between the materials is determined by the function $\nu(x)$, the material parameters can be interpolated with the following interpolation functions [26]:

$$
\sigma(x) = \frac{(1 - \nu(x))\sigma_A + \nu(x)\sigma_B}{(1 - \nu(x))\nu_A + \nu(x)\nu_B}
$$

(10a)

$$
\sigma(x) = (1 - \nu(x))\sigma_A + \nu(x)\sigma_B
$$

(10b)

$$
\sigma(x) = (1 - \nu(x))\nu_A + \nu(x)\nu_B
$$

(10c)

To demonstrate that this is a suitable approach, we have plotted the state fields along $x$ for the infinitely layered 2D design and infinitely layered 1D design in Fig. 16. With reference to the excellent fits of the state fields of the two modeling approaches, we confidently conclude that the two dimensional spike-shaped transitions of the design solutions actually account for a one dimensional feature. If the interpolation functions in Eqs. (10) are used to interpolate intermediate design variables, it is therefore sufficient to consider the equivalent one dimensional optimization problem, compare with Fig. 2.
Figure 10: Design solutions solved for $f_{\mu}, h_{HC} = 615, T^c = 280, T^H = 300$ and various electric potential differences, $\Delta V$. The plots illustrate that the design solutions are dependent on the electric potential difference and this model parameter should be taken into consideration in the design problem.

Figure 11: The relationships between $f_Q$ and $\Delta V$ for design solutions solved for $f_{\mu}, T^c = 280, T^H = 300$ and $h_{HC} = \{242, 327, 463, 564\}$. The plot shows that an increase of the convection coefficients results in an increase of the cooling power. The electric potential difference which results in the largest cooling power is increased as the convection coefficients are increased.

Figure 12: The relationships between $f_{\mu}$ and $\Delta V$ for the design solutions solved for $f_{\mu}, T^c = 260, T^H = 300$ and $h_{HC} = \{530, 649, 1000, 2500\}$. The two plots show two important features of the design problems: (1) Due to a compromise between the Joule heating and the Peltier work, there exist an optimum between $\Delta V$ and $f_{\mu}$ and (2) an increase of the convection coefficients results in an increase in the coefficient of performance.
The equivalence between the two dimensional infinitely layered and one dimensional infinitely layered design solutions is also observed for temperature dependent material parameters. These observations may be basis for the derivations of analytic optimization approaches in the future. However, it is important to clarify that the infinitely small feature of the design solutions in Fig. 16b may be challenging to manufacture and may cause large parasitic losses, for which reason designers may consider to impose a minimum length scale as in the design solutions presented in present paper. If this is the case, the 1D and 2D models may deviate and it is therefore necessary to consider the full two dimensional optimization problem.

Figure 13: The relationships between \( f_Q \) and \( h_{HC} \) for the design solutions solved for \( f_Q \) and \( T^C = 280, T^H = 300 \) and \( h_{HC} = \{175, 276, 412, 530, 1000\} \), where some of the design solutions are shown in Fig. 7. As the design solutions solved for one specific magnitude of \( h_{HC} \) outperform the design solutions solved for different \( h_{HC} \), we confidently conclude that we may attribute importance of the features of the design solutions with respect to \( h_{HC} \).

Figure 14: The temperature and electric potential fields for the design solution solved for \( f_Q, T^C = 280, T^H = 300 \) and \( h_{HC} = 497 \) in Fig. 7m. Despite the two dimensional features of the design solution, the state fields have relatively small gradients in the \( y \)-direction.
Figure 15: Schematic of the steps in the decomposition of a Two Dimensional (2D) finite layered design into an One Dimensional (1D) infinite layered design. It is shown that the state fields of the design in (b) is equivalent to the state fields of the design in (c) if the interpolation functions in Eqs. (10) are used to interpolate intermediate design variables.

Figure 16: Comparison between the state fields of the infinite layered two dimensional design and infinite layered one dimensional design in Figs. 15b and 15c. The two modeling approaches provide identical results for which reason it is concluded that the one dimensional optimization problem is adequate if the interpolation functions in Eq. (10) are used to interpolate intermediate design variables.
Discussion

The topology optimization approach for thermoelectric coolers presented in this paper is related to well-accepted work in the literature such as functionally graded materials [35], the compatibility approach [20], the thermoelectric homogenization approach [24, 26] and sizing approaches [36], however the methodology takes a completely different offset and modeling approach and therefore opens a complete new branch for optimization of thermoelectric coolers.

3.6. Neglecting parasitic losses between material phases

The parasitic losses between the material phases are neglected in the finite element modeling. This assumption is justified with reference to the work of Sakai et al. [26], who manufactured and experimentally tested design solutions which consisted of two materials with a considerable amount of transitions between the material phases. These design solutions were manufactured and experimentally tested, and despite neglecting parasitic losses, good agreements between the analytic predictions and the experimentally tested and manufactured designs were shown. The parasitic losses could be included directly by formulating a more complex finite element model or indirectly through geometrical restrictions.

3.7. Temperature dependent materials

The material parameters are assumed temperature independent, which is a non-physical assumption for most applications of thermoelectric energy conversion devices. It was decided to limit the modeling to temperature independent materials to simplify the interpretation of the spike-shaped design features. By utilizing non-linear material parameters, it would be challenging to conclude whether the spike-shaped design features were occurring due to non-linear effects of the material parameters or to achieve intermediate effective material parameters of the stand-alone materials.

However, the topology optimization methodology can easily be extended to support temperature dependent material, see Lundgaard et al. [37] for more information.

3.8. Manufacturability of the design solutions

The level of geometrical complexity of the design solutions presented in this study is approximately similar to the design solutions manufactured and tested by Sakai and coworkers. With basis in this observation and with reference to advanced additive manufacturing methods [38], we assess that the design solutions are manufacturable with methodologies available today. Nevertheless, to manufacture and experimentally test the design solutions and hereby assess the difference between the numerical modeling and the experimental testing is a very important and interesting future study.

4. Conclusion

A density-based topology optimization approach is used to optimize the spatial distribution of two materials in order to optimize the performance of thermoelectric coolers. The design problems are solved for physically realistic boundary conditions and model dimensions, however, the design problems are purposely limited to temperature independent materials in order to ease the interpretation of the design features. The physical modeling is based on a fully coupled non-linear finite element model in two dimensions and steady state.

The most important findings are summarized in the following:

1. The topology optimization approach provides design solutions which outperform the classical segmentation approach with 48.7% and 11.4% for design problems solved for heat flux and coefficient of performance, respectively. We hereby conclude that topology optimization is a suited approach for optimizing thermoelectric coolers.

2. Design problems solved for average temperature and heat flux provide identical design solutions which is also concluded in the work of [10].

3. Design solutions solved for heat flux do not necessarily provide large coefficients of performance and design solutions solved for coefficients of performance do not necessarily provide large heat fluxes. The choice of objective function is therefore concluded to be a critical design parameter in design problems of thermoelectric coolers.

4. With basis in validation studies and cross-checks, it is shown that the applied electric potential difference, the temperatures of the thermal reservoirs and the convections coefficients are important model parameters and should be taken into consideration when optimizing thermoelectric coolers. Furthermore, we confidently conclude that the topology optimization approach is suited for taking these model parameters into account.

5. The design solutions are characterized by spike-shaped design features, which allow the designs solutions to operate locally in an intermediate state between the material phases. The two dimensional models can be decomposed into one dimensional models if interpolation functions of horizontally layered designs are used to define intermediate design
variables. This may provide a road for developing new optimization approaches for thermoelectric coolers in the future.

The study provides new insight in the field of thermoelectric coolers and may provide guidance for future research aiming on developing high performing thermoelectric coolers.

5. Acknowledgements

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6. References


[10] Martin Bogert and Daniel A Tortorelli. Topology optimization for segmented Peltier coolers and may provide guidance for future research aiming on developing high performing thermoelectric coolers.


Publication [P5]:
Abstract
This study revisits the application of density-based topology optimization to fluid-structure-interaction problems. The Navier-Cauchy and Navier-Stokes equations are discretized using the finite element method and solved in a unified formulation. The physical modeling is limited to two dimensions, steady state, the influence of the structural deformations on the fluid flow is assumed negligible, and the structural and fluid properties are assumed constant. The optimization is based on adjoint sensitivity analysis and a robust formulation ensuring length-scale control and 0/1 designs. It is shown, that non-physical free-floating islands of solid elements can be removed by combining different objective functions in a weighted multi-objective formulation. The framework is tested for low and moderate Reynolds numbers on problems similar to previous works in the literature and two new flow mechanism problems. The optimized designs are consistent with respect to benchmark examples and the coupling between the fluid flow, the elastic structure and the optimization problem is clearly captured and illustrated in the optimized designs. The study reveals new features of topology optimization of FSI problems and may provide guidance for future research within the field.

Keywords Topology optimization · Fluid-structure-interaction · Adjoint sensitivity analysis · The robust formulation · Objective functions · Flow mechanisms

1 Introduction
Fluid-structure-interaction (FSI) is a multi-physics problem which concerns the interaction between a moving fluid and an elastic or rigid, movable or constrained structure. FSI is a strongly coupled phenomenon, which means that the structural deformations depend on the fluid flow and the fluid flow may depend on the structural deformations. FSI is an interesting and important phenomenon as it is relevant for a large number of engineering applications and natural phenomena such as airfoils (Dowell and Hall 2001; Farhat et al. 1998), engines (Shangguan and Zhen-Hua 2004), compressors (Wu and Wang 2014), moving containers (Kolaei et al. 2016), the human blood flow system (Gerbeau et al. 2005; Gerbeau and Vidrascu 2003), the human lung system (Tezduyar et al. 2008), among many more.

Over the past decades, a considerable international research effort has been addressing FSI problems; in 2015 alone more than 400 FSI journal papers were published. Despite the large research effort, only a small number of papers has been concerned with structural topology optimization of FSI problems, see e.g. Yoon (2010), Kreissl et al. (2010), Yoon et al. (2014a, b), Jenkins and Maute (2015, 2016) and Picelli et al. (2015, 2017). The motivation and aim of the present study is to contribute to the development of the topology optimization approach for FSI problems, which in the future may be used to analyze and optimize industrially relevant problems, such as bridges, turbines or compliant component designs.

The optimization framework presented in this work is based on topology optimization which is a material distribution method for finding optimized structural layouts subjected to some specified design constraints. Topology optimization was originally suggested for elastic problems
by Bendsøe and Kikuchi (1988), and the methodology has ever since its introduction been developed and matured within structural elasticity and a large number of multiphysic problems. Topology optimization may have an advantage compared to other optimization approaches, such as sizing or shape optimization as topology optimization allows internal holes to occur in the structure during the optimization process, and a qualified initial guess is generally not required for obtaining well-performing designs.

Topology optimization can be utilized in all problems modeled by partial differential equations, and therefore the methodology has proven its relevance in a large range of multiphysics applications, such as acoustics (Dühring et al. 2008), electrostatics (Yoon and Sigmund 2008), fluid-structure-interaction in poroelasticity (Andreasen and Sigmund 2008), fluid-dynamics (Borrvall and Petersson 2003), thermal transport (Andreasen et al. 2009; Alexandersen et al. 2014) among many more. For an extensive introduction to topology optimization, please consult e.g. Sigmund and Maute (2013), Chen (2016), and Bendsøe and Sigmund (2003).

Topology optimization of fluid dynamical problems was pioneered by Borrvall and Petersson (2003). Inspired by lubrication theory, Borrvall and Petersson introduced a Brinkman-type penalization term in the Stokes equations, which hereby allowed the amount of dissipated energy in a Stokes flow problem to be minimized using a topology optimization approach. Topology optimization for flow problems was later extended with a similar approach to the Navier-Stokes equations by Gersborg-Hansen et al. (2005). The Brinkman approach has within the last 10-12 years been used in a large sequence of multi-physic fluid flow problems such as transport problems (Andreasen et al. 2009), reactive flows (Oikkels and Bruus 2007), transient flows (Deng et al. 2011; Kreissl et al. 2011), flow driven by constant body force (Deng et al. 2013), among many more.

The field of topology optimization of FSI problems was initiated by Yoon (2010), who minimized the structural compliance of an elastic structure subjected to a fluid flow in a channel. Yoon solved the Navier-Stokes equations and the linear Navier-Cauchy equations in a unified formulation. This unified formulation employs that the deformations of the elastic structure and the velocity and pressure fields of the fluid flow are solved simultaneously in the hole modeling domain. The dependency between the structural deformations and the fluid flow (from hereon denoted the deformation dependency) was taken into account in the framework presented in Yoon (2010). The same author presented a topology optimization framework for a passive valve flap optimization problem in Yoon (2014a). The topology of a valve flap was optimized with deformation dependency for two different Reynolds numbers. In the papers by Picelli et al. (2015, 2017), a bi-directional evolutionary (BESO) topology optimization method was used to optimize structural compliance problems under design-dependent pressure loads. In this framework the deformation dependency was neglected. Most recently Jenkins and Maute (2016) demonstrated an optimization framework for an immersed method with explicit boundary representation (IMwEBR) method using the extended finite element method and an explicit level set method. In the works by Yoon (2010) and Jenkins and Maute (2016) the deformation dependency was taken into account, and full-scale topological changes were observed for compliance optimization problems. Furthermore, Jenkins and Maute (2016) studied a heart valve inspired problem where the objective was to minimize the average maximum shear stress in the fluid.

Topology optimization of FSI problems is to some extend related to pressure loaded acoustic problems (Yoon et al. 2007; Vicente et al. 2015) and FSI for porous flow problems (Andreasen and Sigmund 2013), though in structure-acoustic problems the structural forces are imposed by the acoustic pressure.

In this work, the deformation dependency is neglected, which means that the finite element analysis, sensitivity analysis and the optimization problem are carried out in the undeformed structural configuration. In this study, we devote our primary focus on various design problem formulations. We refine several aspects of the field of density-based topology optimization for FSI problems, which provide new insight and may provide guidance for future research within the field. The study takes basis in the work of Yoon (2010) however the study includes several new features and reveals several new findings in relation to TO of FSI problems. The new findings and features have been summarized in the following list:

1. The coupling between the fluid flow, the elastic structure and the optimization problem is clearly captured and demonstrated for six objective functions and three numerical examples. The optimized designs are consistent with respect to benchmark problems and cross-check tables. The presented framework is tested and compared with well-known problems from the literature and two new challenging problems are proposed that procure new insight in the field of topology optimization for FSI problems.
2. The derivation of the unified finite element formulation of the fluid-structure-interaction problem is elaborated, and an additional term in the coupling between the fluid and the structure is included in the TO and FSI formulations compared to the equivalent formulations in Yoon (2010).
3. A robust optimization formulation is added, which ensures length-scale-controlled well-performing and binary optimized designs, and may make the optimization process less sensitive to the choice of interpolation function parameters, model parameters, and penalization and continuation strategies.
4. The importance of choosing a “sufficiently” high structural impermeability is highlighted.
5. A methodology to ensure a monotonic relationship between the objective functions and the design variables. A monotonic relationship between the objective functions and the design variables may ensure well-performing designs and smooth and stable optimization processes.
6. Non-physical free-floating islands of solid elements (FFIOSE), which also have been encountered in other works, can be removed from the optimized designs by combining different objective functions with different features and weights.

The paper is organized as follows. The governing equations and assumptions are introduced in Section 2, the finite element formulation is introduced in Section 3, the implementation details is covered in Section 5, the topology optimization problem is introduced in Section 4, numerical examples are presented in Section 6, Section 7 contains discussions and Section 8 contains conclusions.

2 Governing equations

2.1 The Navier-Stokes and Navier-Cauchy equations

The weak form of the governing equations are defined in domain, $\Omega$. The domain $\Omega$ consists of a solid sub-domain $\Omega_S$ and a fluid sub-domain $\Omega_F$ which initially are clearly segregated and non-overlapping with the interface $\Gamma_{SF}$. The segregated sub-domains fulfill that $\Omega \in \Omega_S \cup \Omega_F$. The Navier-Cauchy equations are assumed linear elastic, the Navier-Stokes equations are limited to constant and incompressible fluid properties, and the physics are modeled assuming steady state. Shear stresses on the interface between the fluid and the structure are neglected. The strong form of the partial differential equations can be written as (e.g. Cook et al. 1991, Farhat and Roux 2002, White and Corfield 1991)

\[
\begin{align*}
\frac{\partial \sigma_{ij}^f}{\partial x_j} + f_i &= 0 \quad \text{in} \quad \Omega_F \sigma_{ij}^f = C_{ijkl} \epsilon_{kl}^f \quad (1a) \\
\frac{\partial u_i}{\partial x_j} - \frac{\partial \sigma_{ij}^f}{\partial x_j} &= b_i \quad \text{in} \quad \Omega_F \sigma_{ij}^f = \frac{2}{Re} \epsilon_{ij}^f - \delta_{ij} p \quad (1b) \\
\epsilon_{ij} &= \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (1c) \\
\frac{\partial u_i}{\partial x_j} &= 0 \quad \text{in} \quad \Omega_F \\
\sigma_{ij}^s n_j &= 0 \quad \text{on} \quad \Gamma_{SF} \quad (1d)
\end{align*}
\]

where $\sigma^f$ is the Cauchy stress tensor, $\epsilon_{ij}^f$ is the spatial variables, $f_i$ is the external applied loads, $C_{ijkl}$ is the structural stiffness tensor, $\epsilon_{ij}^s$ is the structural strains, $d_i$ is the structural displacements, $u_i$ is the fluid velocity, $\sigma_{ij}^f$ is the fluid stress tensor, $b_i$ is the fluid body forces, $Re$ is the Reynolds number, $\epsilon^f$ is the fluid strain rate, $\delta_{ij}$ is Kronecker’s delta, $\rho$ is the fluid pressure and $n_j$ is the normal vector to the surface $\Gamma$. The tensor indices $i, j, k, l$ have two entries, $x$ and $y$, which refer to the spatial directions $x$ and $y$. The Reynolds number is defined as $Re = U_{max} \rho / \mu$, where $U_{max}$ is a maximum fluid velocity in the inlet, $\rho^f$ is the fluid density, $\mu$ is the fluid viscosity and $L$ is the width in the inlet.

The boundary conditions of the governing equations in (1a–d), are:

- No-slip fluid: $u_i = u_i^0 = 0$ on $\Gamma_{ud}$ (2a)
- Fluid inflow: $u_i = u_i^*$ on $\Gamma_{ui}$ (2b)
- Fluid outflow: $p = p^0 = 0$ on $\Gamma_{po}$ (2c)
- Structural displacement: $d_i = d_i^0 = 0$ on $\Gamma_{po}$ (2d)

where $\square$ indicates a boundary condition with a prescribed non-zero magnitude, and $\square^p$ indicates a boundary condition with a prescribed zero magnitude.

3 Finite element formulation

The segregated formulation of the governing equations in (1a–d) is inadequate for density-based topology optimization, so the equations are rewritten to a unified domain formulation, see Fig. 1.

The unified formulation is obtained by introducing a design variable field, $0 \leq \rho \leq 1$: adding a Brinkman penalization term, $b_i = -\alpha(\rho) u_i$, to the Navier-Stokes equations in (1b); and introducing design-dependent material parameters for the structural stiffness $E = E(\rho)$ and the permeability of the Brinkman penalization term, $\alpha = \alpha(\rho)$, see e.g. Borrvall and Petersson (2003) and Yoon

\[
\begin{align*}
\frac{\partial \sigma_{ij}^f}{\partial x_j} + f_i &= 0 \quad \text{in} \quad \Omega_F \quad (1a) \\
\frac{\partial u_i}{\partial x_j} - \frac{\partial \sigma_{ij}^f}{\partial x_j} &= b_i \quad \text{in} \quad \Omega_F \quad (1b) \\
\epsilon_{ij} &= \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (1c) \\
\frac{\partial u_i}{\partial x_j} &= 0 \quad \text{in} \quad \Omega_F \\
\sigma_{ij}^s n_j &= 0 \quad \text{on} \quad \Gamma_{SF} \quad (1d)
\end{align*}
\]

\[
\begin{align*}
\frac{\partial \sigma_{ij}^f}{\partial x_j} + f_i &= 0 \quad \text{in} \quad \Omega_F \quad (1a) \\
\frac{\partial u_i}{\partial x_j} - \frac{\partial \sigma_{ij}^f}{\partial x_j} &= b_i \quad \text{in} \quad \Omega_F \quad (1b) \\
\epsilon_{ij} &= \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (1c) \\
\frac{\partial u_i}{\partial x_j} &= 0 \quad \text{in} \quad \Omega_F \\
\sigma_{ij}^s n_j &= 0 \quad \text{on} \quad \Gamma_{SF} \quad (1d)
\end{align*}
\]
form of the equations, (1a), with a suitable test function; integrating over the domain; assuming that the forces on the structure and the fluid are in equilibrium, i.e. \( \sigma_f \) = 0, are mainly governed by the fluid equations; and intermediate design variables, 0 < \( \rho \) < 1, are in an intermediate state between the fluid and the solid structure.

The finite element discretized equations of the Navier-Cauchy equations are obtained by multiplying the weak form of the equations, (1a), with a suitable test function; integrating over the domain; and introducing the design dependent pressure-coupling filter function \( \psi = \psi(\rho) \) on the pressure coupling terms:

\[
\int_{\Omega} \frac{\partial w^h}{\partial x_j} \sigma_{ij}^h(\rho) dV = \int_{\Omega} \Psi(\rho) u_i^h \frac{\partial \rho}{\partial x_i} dV \\
+ \int_{\Omega} \Psi(\rho) \frac{\partial w^h}{\partial x_j} dV + \int_{\Omega} w^h f_i dV \tag{3}
\]

where \( \psi \) denotes the term that has been discretized and \( w^h \) denotes the basis functions. Details on the derivation of (3) can be found in Appendix A.1. The design dependent pressure-coupling filter function, \( \psi \), ensures that the unified formulation of the domain-integrals of the pressure load in (3) for 0/1 designs is equal to the segregated formulation of the pressure load in (1d). The pressure load is interpolated in intermediate designs for which reason the pressure load in the unified formulation may differ from the equivalent surface integral in the segregated formulation.

The Pressure-Stabilising Petrov-Galerkin (PSPG) and the Streamline-Upwind Petrov-Galerkin (SUPG) methods are used to suppress oscillations in the pressure and velocity fields due to first order shape functions which are used to descretize the fluid velocity and the fluid pressure field (Hughes et al. 1986; Tezduyar 1991; Brooks and Hughes 1982). The weak form of the momentum equations in (1b) are hereby written as:

\[
\int_{\Omega} \frac{\partial w^h}{\partial x_j} \frac{\partial \sigma_{ij}^h}{\partial x_j} dV + \int_{\Omega} \frac{\partial w^h}{\partial x_j} \frac{\partial f_i}{\partial x_j} dV \\
- \int_{\Omega} \frac{\partial w^h}{\partial x_j} \frac{\partial \rho}{\partial x_j} dV \tag{6a}
\]

\[
+ \sum_{c=1}^{N} \int_{\Omega_e} \frac{\partial}{\partial x_j} \left( \sum_{j=1}^{N} \alpha(\rho)u_j^h V_j \frac{\partial \rho}{\partial x_j} \right) dV + \sum_{c=1}^{N} \int_{\Omega_e} \tau_{PS} \frac{\partial w^h}{\partial x_j} \frac{\partial \rho}{\partial x_j} dV \tag{6b}
\]

\[
+ \sum_{c=1}^{N} \int_{\Omega_e} \tau_{SU} \frac{\partial w^h}{\partial x_j} \alpha(\rho) u_i dV = 0 \tag{6c}
\]

The symbol \( \| \) denotes the maximum of a parameter, \( \max \) denotes the minimum of the parameter, and \( \Omega_{\text{min}} \) denotes the maximum of a parameter.

4 Topology optimization

4.1 Problem definition

To ensure length-scale control and robustness with respect to manufacturing errors, the optimization problem is formulated in a min-max form for \( k = 1, 2, \ldots, N^t \) projected realizations of the design variable field (Wang et al. 2011b). The optimization problem reads:

\[
\min \max \left( f^k \right) \quad \text{s.t.} \quad \tilde{R}^k(\tilde{\rho}, \tilde{S}^k) = \tilde{\theta} \quad \text{g} \left( \tilde{\rho}^N \right) = \sum_{N} \tilde{e}_i^N \frac{v_i}{V} \leq V^f \quad \forall \rho_i \in \Omega_D \quad \forall \rho_i \in \Omega_D \quad \text{where} \quad \rho^k \quad \text{is the objective function of the} \ k \ \text{th realization of the design field (the superscripted} \ k \ \text{denotes the design realizations);} \ \tilde{R}^k \quad \text{is the residual equations;} \ \tilde{\rho} \quad \text{is the filtered and projected design field realization;} \ \tilde{S}^k \quad \text{is the state field vectors;} \ g \ \text{is the volume inequality constraint;} \ N^t \quad \text{is the number of elements in the design domain,} \ \Omega_D; \ v_i \quad \text{is the volume of element} \ i, \ V \quad \text{is the total volume of the} \ \Omega_D \quad \text{and} \ V^f \quad \text{is the volume fraction. The optimization problem in (7) is in the rest of this paper denoted as the robust formulation.
The optimization problem in (7) is solved for three projected realizations of the designs variable field which are denoted the eroded, the nominal and the dilated designs, respectively. Design solutions are throughout this paper plotted for the nominal design realization. The volume fraction for the dilated design is updated every 20 design iteration so the volume of the intermediate design becomes equal a prescribed value, please confer Wang et al. (2011b)

The robust formulation was suggested by Sigmund (2009) in linear elasticity problems to provide manufacturable designs, later the methodology was improved in (2009) for more details.

The physical design variables used in the finite element analysis, $\mathbf{\rho}$, are obtained by imposing the projection filter operation:

$$
\tilde{\mathbf{\rho}}_i = \frac{\sum_{j \in \mathcal{N}_i} w(\tilde{x}_j) v_j \mathbf{\rho}_j}{\sum_{j \in \mathcal{N}_i} w(\tilde{x}_j) v_j}
$$

where $v_j$ is the area of the $j$th element, $\mathcal{N}_i$ is the index set of the design variables which is within the radius $R$ of design variable $i$, $w(\tilde{x}_j)$ is the filter weighting function, $\mathbf{\rho}_j$ is the mathematical design variables and $\tilde{x}_j$ is the spatial location of the element $j$. The filter weighting function is given by:

$$
w(\tilde{x}_j) = \begin{cases} 
R - |\tilde{x}_j| & \text{if } \forall R \wedge \tilde{x}_j \in \Omega_D \\
0 & \text{otherwise} \end{cases}
$$

The field sensitivities are obtained by utilizing the chain rule twice:

$$
\frac{\partial f}{\partial \mathbf{\rho}_i} = \sum_{j \in \Omega_D} \frac{\partial f}{\partial \tilde{\mathbf{\rho}}_j} \frac{\partial \tilde{\mathbf{\rho}}_j}{\partial \mathbf{\rho}_i}
$$

4.2 Adjoint sensitivities

Gradients of the objective function with respect to the design variable field, in this study denoted sensitivities, are required in order to solve the optimization problem in (7). The sensitivities of the $k$’th design realization, $\frac{\partial L^k}{\partial \mathbf{\rho}_i}$, where $L$ is the general Lagrangian functional, are computed by the discrete adjoint approach, see Michaleris and Vidal (1994) and Bendse and Sigmund (2003), which reads:

$$
\left( \frac{\partial \mathbf{R}^k}{\partial \mathbf{\rho}_i} \right)^T \mathbf{\lambda}^k = \left( \frac{\partial f^k}{\partial \mathbf{\rho}_i} \right)^T
$$

where $\mathbf{\lambda}^k$ is the vector of adjoint variables and $\frac{\partial}{\partial \mathbf{\rho}_i}$ denotes the transpose. The sensitivities can now be computed by the following expression:

$$
\frac{\partial L^k}{\partial \mathbf{\rho}_i} = \frac{\partial f^k}{\partial \mathbf{\rho}_i} - \left[ \frac{\partial}{\partial \mathbf{\rho}_i} \right]^T \frac{\partial \mathbf{R}^k}{\partial \mathbf{\rho}_i}
$$

where $\frac{\partial}{\partial \mathbf{\rho}_i}$ denotes the total derivative and $\frac{\partial}{\partial \mathbf{\rho}_i}$ denotes the partial derivative.

4.3 Filters and projection strategy

The physical design variables used in the finite element analysis, $\mathbf{\rho}_i$, are obtained by imposing the projection filter operation (10):

$$
\tilde{\mathbf{\rho}}_i = \frac{\text{tanh}(\beta \eta^k) + \text{tanh}(\beta(\tilde{\mathbf{\rho}}_i - \eta^k))}{\text{tanh}(\beta \eta^k) + \text{tanh}(\beta(1 - \eta^k))}
$$

where $\beta$ is the Heaviside projection parameter, $\eta^k$ is the projection filter threshold value, $k$ is the design realization, and $\tilde{\mathbf{\rho}}_i$ is the density filtered design variables. The density filtered design variables $\tilde{\mathbf{\rho}}_i$ are obtained from the mathematical design variables by the following filter operation:

$$
\tilde{\mathbf{\rho}}_i = \frac{\sum_{j \in \mathcal{N}_i} w(\tilde{x}_j) v_j \mathbf{\rho}_j}{\sum_{j \in \mathcal{N}_i} w(\tilde{x}_j) v_j}
$$

4.4 Design-dependent loads

If a design problem takes design dependent loads into account, it implies that the interaction between the fluid and the structure depends on the topology of the design. This framework takes design dependent loads into account, as the pressure loads are transferred from the fluid to the structure through the pressure coupling terms in (3). The pressure coupling terms enter the sensitivity analysis in (8)–(9) entailing that the design problem and FSI problem are implicitly related though the sensitivities as $L = L(\mathbf{\rho})$. Design dependent loads are also seen in the work of Yoon (2010, 2014a), Jenkins and Maute (2016), Picelli et al. (2015, 2017).

5 Implementation

The finite element equations and the sensitivities for the TO FSI framework are derived in the mathematical software Maple and implemented in the scripting programming language Matlab. The Matlab framework is parallelized to the extend where multiple processors are used to evaluate the finite element matrices which may constitute a minor speed up for some problems.

5.1 Finite element formulation

The finite element equations are solved using rectangular elements and linear basis functions for the fluid velocity field, the fluid pressure field and the structural displacement field. Each finite element consists of one design variable
and four nodes with five degrees of freedom (DOF). The DOF are: Two structural displacements, one fluid pressure and two fluid velocities. The residual equation is written as: 
\[ \tilde{R}(\tilde{S}, \tilde{p}) = M(\tilde{S}, \tilde{p})\tilde{S} - \tilde{F} = 0, \]
where \( \tilde{R} \) is the residual vector, \( \tilde{F} \) is the force vector, \( \tilde{S} \) is the system matrix, \( \tilde{S} = \{ \tilde{U}, \tilde{P}, \tilde{D} \} \) is the state variable vector, where \( \tilde{U} \) is the fluid velocity vector, \( \tilde{P} \) is the fluid pressure vector, \( \tilde{D} \) is the structural displacements vector. The residual equation is solved by a combination between the undamped Newton’s method (see e.g. Deuflhard 2014) and Pichard iterations. Newton iterations have relative to Pichard iterations fast convergence for initial guesses close to the solution, where Pichard iterations have relatively to Newton steps fast convergence for initial guesses far away from the solution.

5.2 Optimization parameters

The optimization problem is solved using the method of moving asymptotes (MMA) (Svanberg 2006) with the standard settings and a move limit of 0.1. The Heaviside projection parameter, \( \beta \), is updated every 100th design iteration following the scheme: 
\[ \beta = \{4, 8, 16, 32, 64\}. \]
The optimization algorithm is stopped when the maximum difference between the design variables in iteration \( i \) and \( i - 1 \) is less than 0.1% and \( \beta = 64 \). The projection filter threshold values \( \eta \) for the eroded, nominal and dilated designs are, unless otherwise stated, \( \eta = \{0.3, 0.5, 0.7\} \), respectively. The initial density distributions for all design problems presented in this study are \( \rho = V^f \). The density filter radius \( R \) is chosen to be \( R = 4.75N_y^c \) where \( N_y^c \) is the number of elements in the \( Y \) direction. This density filter radius, combined with the robust formulation, corresponds to a length scale of \( \approx 0.05 \).

5.3 Brinkman penalization

The Brinkman penalization parameter (BPP) for void and solid are \( \{\alpha_{\text{min}}, \alpha_{\text{max}}\} = \{0, 10^5\} \), respectively. The BPP is chosen relatively large compared to previous work in the literature (Borrvall and Petersson 2003; Gersborg-Hansen et al. 2005; Yoon 2010, 2014a; Andreasen et al. 2009; Alexandersen et al. 2014), as it turns out that the correctness of the FE modeling of the pressure field and the validity of the optimized designs are conditioned by a large BPP. Designs optimized for e.g. \( \{\alpha_{\text{min}}, \alpha_{\text{max}}\} = \{0, 10^5\} \) may be unphysical and meaningless, however, design problems with low \( \alpha_{\text{max}} \) may be better posed compared to design problems optimized with high \( \alpha_{\text{max}} \). The pressure modeling issue was discovered during numerical studies with the TO FSI framework. It turned out that the optimization algorithm took advantage of the poorly resolved pressure field to provide physically meaningless but well-performing designs (note: well-performing with respect to the poor physical model) for some problems. To avoid a similar pitfall, we suggest researchers always to validate all designs with a body fitted mesh and a segregated solver configuration. This will ensure that the performances of the optimized designs are caused by the features of the optimized designs and not caused by poor physical modeling. Interested readers are referred to Appendix A.4, where a detailed description of the issue and numerical examples can be found.

5.4 Interpolation function parameters

The interpolation function parameters (IF) in(6a–c) are \( p_\Psi = 1, p_\delta = 1 \) and \( p_\alpha = \{5.25 \cdot 10^{-6}, 2.75 \cdot 10^{-6}, 1 \cdot 10^{-5}, 2.5 \cdot 10^{-7}, 9.2 \cdot 10^{-7}\} \) for problems with \( Re = \{1, 5, 10, 40, 100\} \), respectively. The pressure coupling filter function parameters are \( \{\Psi_{\text{min}}, \Psi_{\text{max}}\} = \{0, 1\} \) and the structural stiffness of the void and the solid are \( \{E_{\text{min}}, E_{\text{max}}\} = \{1 \cdot 10^{-5}, 1 \cdot 10^5\} \).

The degree of well-posedness of a density-based TO FSI design problem is very dependent of the choice of interpolation functions (IF) and IFP. Numerical studies with the TO FSI framework have suggested that a poor choice of IF and IFP provides ill-posed optimization problems and poorly performing optimized designs. However, a good choice of IF and IFP provides well-posed optimization problems and well-performing optimized designs.

The determinations of the IF and IFP take basis in a systematic comparison between the topology sensitivities and the shape sensitivities for a simple elastic problem and a simple FSI problem. By tuning the IF and IFP, such that the topology gradients resemble the shape gradients for intermediate design variables, we obtain well-performing and well-posed optimization problems. A detailed description and numerical examples of this approach can be found in Appendix A.3.

5.5 Units of physical parameters

All equations have been derived in non-dimensional form and all physical parameters are given in SI base units, e.g. pressure is given in [Pa], displacements in [m], velocity in [m/s], dissipated energy in the flow in [W/kg], structural compliance in [1/Pa], the BBP in [m²], and so forth. Optimization parameters such as \( \beta, \eta^2, p_\Psi, p_\delta \) and \( p_\alpha \) are given in non-dimensional form and are mesh independent.

5.6 The assumption of neglecting the shear stress

In Fig. 2, we have sketched what we call the Hungry Horse (HH) problem, which has been used to validate the unified FSI framework. The HH problem is a good benchmark
example due to its simple design and many focal FSI relevant features such as internal holes, boundaries with high pressure and low fluid velocity and boundaries with low fluid velocity and high pressures.

The HH problem is subject to the following BCs: A parabolic fluid flow with maximum velocity of unity enters the channel on $\Gamma^W$ and the fluid exits on $\Gamma^E$. No-slip boundary conditions are imposed on $\Gamma^N$ and $\Gamma^S$, and the structural deformations in all DOF are fixed on $\Gamma^S$. A prescribed $p = 0$ is imposed on the $\Gamma^E$ which models the outflow condition.

The pressure field, the velocity field and the flow streamlines for $Re = 1$ have been plotted in Fig. 3. The relationship between the pressure and shear stress along the outer boundary (sketched with the red line in Fig. 2) have been plotted in Fig. 4. The integrated absolute pressure and shear stress along the outer boundary of the HH problem are 411.15 N and 29.72 N, respectively. The shear stress is large compared to the pressure near boundaries where the velocity and its gradients are large and the pressure is low, such as in and between points F and G. The ratio between shear stress and pressure depends on the problem. However in detailed computations the shear forces should always be taken into account. Shear forces may be difficult to model with a density-based Brinkman penalization approach as the porous media in the intermediate design variables penalizes the fluid velocity and hereby the fluid shear stresses. Penalization of the fluid flow velocity implies that the shear stress may be poorly resolved during the optimization process when intermediate design variables are present. IMwEBR for FSI problems may be better suited for building frameworks in which effects such as shear stresses are taken into account.

6 Numerical examples

6.1 The wall

The first example concerns a well-known problem from the literature, which we call the wall problem. The wall problem
was originally suggested by Yoon (2010) and later revisited for slightly different problem layout and flow properties by Picelli et al. (2017), Jenkins and Maute (2015), and Jenkins and Maute (2016). The aim of the wall problem is to minimize the structural compliance of a wall subjected to a fluid flow in a channel.

In this work, the wall problem has, compared to the problem layout presented by Yoon, Picelli and Jenkins, a smaller ratio between the length and the height of the computational domain and a relatively larger design domain. We believe, that the larger design domain yields a higher level of design freedom, a more pronounced fluid-structure-interaction, and hence facilitates a more challenging optimization problem.

To provide guidance for future research within the field of TO of FSI problem and to demonstrate the new features and the stronger approximations of present framework, we have revisited the exact wall problems presented in Yoon (2010), Jenkins and Maute (2016) and Picelli et al. (2017) in Appendix A.2.

The problem layout and the corresponding boundary conditions are as illustrated in Fig. 5 for the wall problem investigated in this work. \( \Omega_D \) and the fixed domain, \( \Omega_I \), are non-overlapping, and the design variables in \( \Omega_I \) are all fixed to unity. The sub-domains \( I \) and \( D \) are non-overlapping for all problems but all sub-domains are part of the computational domain. The domain \( \Omega_I \) is referred to as the wall.

A parabolic fluid flow with maximum velocity of unity enters the channel on \( \Gamma^W \) and exits on \( \Gamma^E \). No-slip boundary conditions are imposed on \( \Gamma^N \) and \( \Gamma^S \) of the channel, and the structural deformations in all DOF are fixed on \( \Gamma^S \). A prescribed \( p = 0 \) is imposed on the \( \Gamma^E \) modeling the outflow condition.

The objective of the wall problem is to minimize the structural compliance, \( f_C \), in \( \Omega_D \) and \( \Omega_I \). The compliance function for the wall flow problem is given by:

\[
f_C = \int_{\Omega_D} \epsilon_{ij} \sigma_{ij} \, dV
\]  

\( \Omega \) is discretized into \( \{N^x_C, N^y_C\} = (300, 150) \) elements, where \( N^x_C \) and \( N^y_C \) refer to the number of elements in the \( x \) and \( y \) directions in the computational domain, respectively. The domain \( \Omega_D \) consists of \( \{N^x_D, N^y_D\} = (210, 120) \) elements, where \( N^x_D \) and \( N^y_D \) refer to the number of elements in the \( x \) and \( y \) directions in \( \Omega_D \), respectively. The total number of state DOF is 227,255 and the maximum allowed volume fraction is \( V_f = 0.1 \).

The problem is investigated for four Reynolds numbers, \( Re = \{1, 5, 10, 40\} \) and the optimized designs and relevant state fields are plotted in Figs. 6, 7, 8 and 9. The pressure coupling forces are the discrete vectors of the pressure coupling terms 1 and 2 in (3) obtained in the finite element discretization and are plotted in Figs. 6a, 7a, 8a and 9a. The blue arrows in the pressure force coupling plot illustrate the direction and the magnitude of the reaction forces of the structure against the fluid pressure. These are plotted in the FE nodes and each arrow has contributions from the neighboring elements for which reason they may appear non-perpendicular to the surfaces of the elements in some instances.
The fluid pressure field and the fluid flow streamlines, seeded along $\Gamma^W$, have been plotted in Figs. 6b, 7b, 8b and 9b. The normalized fluid flow velocity and the fluid flow streamlines, seeded along $\Gamma^W$, have been plotted in Figs. 6c, 7c, 8c and 9c. The scaled deformed and undeformed configuration of the optimized structures have been plotted in Figs. 6d, 7d, 8d and 9d. In plots with the deformed and undeformed configuration of the optimized designs, the deformation of the deformed configurations have been scaled so that the maximum deformation occur with the same magnitude in all plots. However, recall that the deformations of the designs are not taken into account in the optimization process, so the plots of the deformed configurations are only for illustrative purposes. The internal pressures of the holes in the optimized designs in Figs. 6a, 7a, 8a and 9a are physical reasonable, as we assume that the structures are leaking through the finite
permeability of the solid regions. The leaking features of the structure allow fluid to enter and pressurize internal holes. Optimized designs and relevant state field plots follow a similar setup as the wall flow presented in Figs. 6–9 in the rest of this paper.

The relationships between the normalized $f_D$ and iteration number, $k$, for the eroded, the dilated and the nominal designs in the design in Fig. 6 have been plotted in Fig. 10. Snapshots of the design evolution for every 100 iteration have been plotted in Fig. 11.

To determine how much significance one may attribute to the features of the optimized designs, one can consider a cross-check table, which contains the evaluations of the objective function for all combinations of model parameters (the Reynolds number in the present problem) and the optimized designs. A design optimized for one model parameter is required to outperform designs optimized for other model parameters if one shall attribute any significance to the features of the design solutions.

The objective values of the four designs for the four Reynolds numbers have been listed in Table 1. The design optimized for one Reynolds number outperforms the designs optimized for other Reynolds numbers (the lowest objective values are in the diagonal), confirming that the designs indeed have superior performance for the Reynolds number they are optimized for.

All objective functions in this work are evaluated for projected binary (0/1) designs using $\tilde{\rho} = 0.5$ as threshold value. This sharp thresholding is carried out to ensure that the improved performances of the optimized designs are not governed by nonphysical intermediate design variables that may be present. However, the difference between the thresholded designs and the design which contain intermediate design variables are less than 1% for all cases.

Visual inspection of Fig. 6–9 and analysis of the cross-check table shows that the optimized designs are dependent on the choice of $Re$ and that the coupling between the fluid flow, the elastic structure and the optimization problem is captured. The amount of material placed in the upstream area of the wall and the degree of asymmetry around the axis $(x, y) = (x = 1, y)$ increases as $Re$ increases.

The optimization process is governed by two main, and possibly conflicting, features: (1) Minimization of the drag of the structure and (2) maximization of the stiffness of the structure. To determine which of the features that
governs the design process is non-trivial, but an interesting observation is made when evaluating the design solutions in Figs. 6–9 for dissipated energy in the flow, $f_E$ (see (17)). Tables 1 and 2 suggest that $f_E$ for the designs placed in the diagonal is positively correlated with $f_C$; a small amount of dissipated energy in the fluid is connected to a small structural compliance and vice versa. The drag on the structure is not explicitly stated in $f_C$, but the correlation between $f_C$ and $f_E$ seems to be an inherent feature of this optimization problem.

Jenkins and Maute (2016) reported on FFIOSE during their optimization process. We did not observe such phenomenon in this optimization problem, which may be explained by the continuous relationship between the design variables and the element stiffnesses in the density-based topology optimization approach.

### 6.2 The flow obstacle

The idea of the second numerical example and optimization problem is to minimize the downstream deformations of the center of a plate in a channel by optimizing the material distribution in the proximity of the plate, see Fig. 12. A prescribed fluid flow with a parabolic velocity profile enters the computational domain at $\Gamma^W$ and the fluid exits through $\Gamma^E$. No-slip boundary conditions are imposed on $\Gamma^N$, $\Gamma^S$ and $\Gamma^E$ has a prescribed zero pressure condition. The domain $\Omega_\beta$ is placed in the center of the channel (light grey area) and contains a vertical solid domain with prescribed unity design variables, $\Omega_\gamma$, and a square volume, $\Omega_\delta$, which is circled by red lines. All structural DOF in $\Omega_\delta$ are supported by linear springs with stiffness $k_s = 10^5$ in both $x$ and $y$ directions. The springs in $\Omega_\gamma$ constitute the only structural constraints of the problem.

The symmetry around $(x, y) = (x, 0.5)$ is exploited in the state and optimization problems, to discretize $\Omega$ into $\{N_x^\Omega, N_y^\Omega\} = \{400, 100\}$ finite elements. The domain $\Omega_\beta$ consists of $\{N_x^\beta, N_y^\beta\} = \{240, 80\}$ finite elements. The total amount of state DOF is 202,505, the volume fraction is $V_f = 0.3$ and the Reynolds number is $Re = 1$. The volume constraint was chosen so high that it was inactive for all final optimized designs.

In FSI optimization problems, it may be non-trivial to determine which features of a design solution that have been

<table>
<thead>
<tr>
<th>Design</th>
<th>Evaluated for</th>
<th>$Re = 1$</th>
<th>$Re = 5$</th>
<th>$Re = 10$</th>
<th>$Re = 40$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Re = 1$</td>
<td>$2.8359 \cdot 10^{-7}$</td>
<td>$1.1579 \cdot 10^{-8}$</td>
<td>$3.1559 \cdot 10^{-9}$</td>
<td>$5.1549 \cdot 10^{-10}$</td>
<td></td>
</tr>
<tr>
<td>$Re = 5$</td>
<td>$2.8373 \cdot 10^{-7}$</td>
<td>$1.1411 \cdot 10^{-8}$</td>
<td>$3.0552 \cdot 10^{-9}$</td>
<td>$4.7432 \cdot 10^{-10}$</td>
<td></td>
</tr>
<tr>
<td>$Re = 10$</td>
<td>$2.9226 \cdot 10^{-7}$</td>
<td>$1.1478 \cdot 10^{-8}$</td>
<td>$2.9915 \cdot 10^{-9}$</td>
<td>$4.3669 \cdot 10^{-10}$</td>
<td></td>
</tr>
<tr>
<td>$Re = 40$</td>
<td>$3.8645 \cdot 10^{-7}$</td>
<td>$1.4423 \cdot 10^{-8}$</td>
<td>$3.5304 \cdot 10^{-9}$</td>
<td>$4.2497 \cdot 10^{-10}$</td>
<td></td>
</tr>
</tbody>
</table>
governed by maximizing structural stiffness, minimizing the fluid drag, or exploiting features of the fluid-structure-interaction. With basis in the flow obstacle problem and six different objective functions, we may find a road to a better understanding of the interaction between these possibly conflicting objectives.

### 6.2.1 Structural displacements in the spring-domain

The overall aim of the plate optimization problem is to minimize the average of the $x$-directional displacements in $\Omega_2$. The domain $\Omega_2$ is non-overlapping with $\Omega_I$ and $\Omega_D$, and the displacement objective function, $f_D$, is given by:

$$f_D = \frac{\int_{\Omega_2} dV}{\int_{\Omega_1} dV} \quad (15)$$

The optimized designs and the pressure coupling reaction forces, the pressure field and the fluid flow streamlines, and the deformed and undeformed configuration (from now on denoted the relevant state fields) for $f_D$ have been plotted in Fig. 13. The pressure fields of the flow obstacle problem are plotted on the same scale for easier comparison.

The optimized design for $f_D$ is non-physical due to the FFIOSE. The objective function $f_D$ does not put any requirements on the stiffness of the structure and nothing inherent in the optimization formulation removes the non-physical FFIOSE. The FFIOSE may or may not occur if the dependency of the structural deformations was taken into account. In the simplified model, the FFIOSE exploit several features of the interaction between the fluid and the structure, such as: The pressure difference between the upstream surface and the downstream surface of the $\Omega_I$ is reduced; the fluid flow is lead past the $\Omega_I$ to reduce the fluid dynamical drag force; and a high fluid pressure is build up in the proximity of the upstream FFIOSE which generates a negative $x$-directional pressure-force contribution on the structure.

<table>
<thead>
<tr>
<th>Table 2</th>
<th>Cross-check between $f_E$ and $Re$ for the designs optimized for $f_C$ in Figs. 6–9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Design</td>
<td>Evaluated for $Re$ = 1</td>
</tr>
<tr>
<td>$Re = 1$</td>
<td>23.366</td>
</tr>
<tr>
<td>$Re = 5$</td>
<td>23.670</td>
</tr>
<tr>
<td>$Re = 10$</td>
<td>24.001</td>
</tr>
<tr>
<td>$Re = 40$</td>
<td>26.454</td>
</tr>
</tbody>
</table>

Fig. 12 Schematic of the problem layout and the boundary conditions of the flow obstacle problem

Fig. 13 $f_D$ optimized designs and the state field plots

(a) Pressure coupling forces
(b) Pressure field and fluid flow streamlines
(c) Velocity field and fluid flow streamlines
(d) Deformed and undeformed configuration
Jenkins and Maute (2016) reported on a similar issue with FFIOSE in similar \( f_c \) optimization problems which included the deformation dependency. Jenkins and Maute dealt with the issue of FFIOSE by solving an additional heat transport problem. The FFIOSE were excluded from the finite element analysis based on the heat transport problem and the corresponding temperature field. A similar approach to ensure manufacturable designs in linear elastic topology optimization problems was presented in Liu et al. (2015).

Physically realistic designs are characterized by a connected topology where all solid elements are connected to \( \Omega_s \). As an alternative to the indicator models, we investigate several objective functions which put different requirements on the stiffness of the optimized structure. An appropriately chosen objective function may provide inherent features of the optimization process, which avoid FFIOSE, while the design maintains a good performance for \( f_D \).

Fig. 14 \( f_c \)-optimized designs and the state field plots

Fig. 15 \( f_E \)-optimized designs and the state field plots
6.2.2 Structural compliance

The problem in Fig. 12 is now optimized with respect to minimum structural compliance, \( f_C \), in the domain \( \Omega_{IDS} \). The objective function reads:

\[
 f_C = \int_{\Omega_{IDS}} \epsilon_{ij} \sigma_{ij} \, dV \tag{16}
\]

The optimized design and the state fields of the structural compliance problem are plotted in Fig. 14. This objective results in a connected structure since islands could result in very large strain energies in the void domains between \( \Omega_S \) and the islands. However, this objective does not provide a satisfactory performance in the original \( f_D \) objective.

6.2.3 Dissipated energy in the flow

The optimization problem in Fig. 12 is minimized with respect to the amount of dissipated energy in the fluid flow, \( f_E \), in the full domain \( \Omega \). The objective function reads:

\[
 f_E = \int_\Omega \frac{1}{Re} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \, dV + \int_\Omega \alpha u_i \, dV \tag{17}
\]

The \( f_E \)-optimized design and the state fields are plotted in Fig. 15. The optimized design corresponds to the minimum surface solution as \( f_E \) for highly viscous flows, \( Re = 1 \), are positively correlated with the surface area of the structure; a small surface area is connected with a small \( f_E \). The optimized design has the smallest surface area possible for this optimization problem.

6.2.4 Structural free body motion

The aim of the fourth optimization problem is to minimize the free-body-motion of the intermediate and solid elements (i.e. \( \rho > 0 \)) in the x and y-directions in \( \Omega_{IDS} \) (from now on denoted the free-body motion objective function). The free body motion objective function, \( f_F \), is given by:

\[
 f_F = \int_{\Omega_{IDS}} \rho d_i d_i \, dV \int_{\Omega_{IDS}} \rho \, dV \tag{18}
\]

The optimized design with respect to \( f_F \) and the corresponding state fields are plotted in Fig. 16.

The holes in the upstream part of the design have a relatively high internal pressure. The high internal pressure constitutes a negative x-directional pressure-load component which may explain the occurrence of the holes. The design optimized for \( f_F \) has, compared to the design optimized for \( f_C \) in Fig. 14, a lower drag force and exhibits a smaller pressure loss.

6.2.5 Structural displacement variance

The optimization problem in Fig. 12 is minimized with respect to the variance between the average of the x-directional structural displacements in \( \Omega_S \) and the x-directional structural displacements of the solid elements in \( \Omega_{ID} \). The objective function is denoted \( f_V \) and referred to as the structural displacement variance objective function. Designs optimized for \( f_V \) seeks a topology in which all non-zero density elements undergo the same structural
Revisiting density-based topology optimization for fluid-structure-interaction problems

displacement with respect to direction and magnitude. This formulation may provide a well performing \( f_D \) and a connected topology of the solid elements. The displacement variance function objective function is formulated as:

\[
f_V = \frac{\int_{\Omega_D} \rho (d_x - \bar{d}_x) (d_x - \bar{d}_x) \, dV}{\int_{\Omega_D} \rho \, dV} \tag{19}
\]

where \( d_x \) is the \( x \)-directional displacement and \( \bar{d}_x \) is the average of the \( x \)-directional displacements in \( \Omega_S \):

\[
\bar{d}_x = \frac{\int_{\Omega_S} d_x \, dV}{\int_{\Omega_S} dV} \tag{20}
\]

The optimized design and the state fields are plotted in Fig. 17. The upstream part of the design is a compromise between fluid dynamic properties (low drag force) and structural free-body motion of the solid elements in \( \Omega_D \). The fluid dynamical properties of the design (lower drag force) may be improved by increasing the amount of the material in the upstream part of \( \Omega_I \) and \( \Omega_S \). A larger amount of solid in the upstream part of \( \Omega_I \) and \( \Omega_S \) may cause a larger pressure drop over the design and thereby cause a larger imposed pressure-coupling force, which decreases the performance of the design.

The downstream part of the design is primarily serving fluid dynamical purposes, such as minimizing the drag force.

### 6.2.6 Multi-objective function

The objective functions in (16)–(18) provide physically meaningful optimized designs, but the introduction of new objective functions does not put any requirements on the performance of \( f_D \). The sixth optimization problem takes basis in a multi-objective function, which combines different objectives with different weights, \( a_1 \) and \( a_2 \). The multi-objective function may ensure that non-physical features of \( f_D \)-optimized designs are avoided, while the design maintains a good performance in \( f_D \). The multi-objective function, \( f_M \), contains a combination of (15) and a general version of (19) and is given by:

\[
f_M = (1 - a) \frac{\int_{\Omega_S} d_x \, dV}{\int_{\Omega_S} dV} + a \frac{\int_{\Omega_D} \rho (d_x - \bar{d}_x) (d_x - \bar{d}_x) \, dV}{\int_{\Omega_D} \rho \, dV} + a \frac{\int_{\Omega_D} \rho (d_y - \bar{d}_y) (d_y - \bar{d}_y) \, dV}{\int_{\Omega_D} \rho \, dV} \tag{21}
\]

where

\[
\bar{d}_x = \frac{\int_{\Omega_S} d_x \, dV}{\int_{\Omega_S} dV} \quad \text{and} \quad \bar{d}_y = \frac{\int_{\Omega_S} d_y \, dV}{\int_{\Omega_S} dV} \tag{22}
\]

The optimization problem seeks a design which fulfills two conditions: (1) \( f_D \) is minimized and (2) the \( x \) and \( y \) directional displacements variance are minimized. The \( f_M \)-optimized design and the relevant state fields have been plotted in Fig. 18. The optimized design is obtained for the weight of \( a = 0.01 \).

The \( x \) and \( y \) directional displacement variance terms in (21) penalize the free-floating island of solid elements in the displacement design in Fig. 13. The design optimized for
The optimized designs for the objective functions in (15)–(21) have been cross-checked in Table 3. The cross-check table reveals that all designs optimized for one objective have superior performance in that objective compared to designs optimized for other objectives. This demonstrates that the coupling between the fluid flow, the elastic structure and the optimization problem indeed is captured. The \( f_M \)-optimized design is not defined for the \( f_V \) objective due to division by zero as all design variables are equal to zero.

Multi-objective functions can be formulated from arbitrary combinations of (15)-(18). Different sets of multi-objective functions provide different characteristics of the optimized designs. We have tried several combinations of different objective functions, and to our experience, (21), provides the best results.

### 6.2.7 Comparison of the optimized design

The optimized designs for the objective functions in (15)–(18) have been cross-checked in Table 3. The cross-check table reveals that all designs optimized for one objective have superior performance in that objective compared to designs optimized for other objectives. This demonstrates that the coupling between the fluid flow, the elastic structure and the optimization problem indeed is captured. The \( f_M \)-optimized design is not defined for the \( f_V \) objective due to division by zero as all design variables are equal to zero.

Multi-objective functions can be formulated from arbitrary combinations of (15)-(18). Different sets of multi-objective functions provide different characteristics of the optimized designs. We have tried several combinations of different objective functions, and to our experience, (21), provides the best results.

### 6.3 The fluid gripper

The aim of the third numerical example is to optimize a gripper mechanism which is capable of converting the pressure load caused by the moving fluid into a structural force in a spring. The design problem is inspired by the linear elastic structural mechanism which was presented by Sigmund (1997), and later extended to include stress constraints (De Leon et al. 2015), manufacturing error tolerances (Schevenels et al. 2011), large structural displacements (Pedersen and Buhl 2001), among others.

The aim of the optimization problem is to maximize the structural \( y \)-directional displacement of a spring with spring stiffness \( k \) using only the pressure load caused by the fluid flow. The problem layout and the boundary conditions of the optimization problem have been sketched in Fig. 19. The objective function, \( f_P \), reads:

\[
f_P = \int_{\Omega_P} d_i \, dV
\]

(23)

The spring point (a single node) is denoted \( \Omega_P \) and is placed in the center of a squared domain, \( \Omega_T \), which has fixed unity design variables. The objective function is defined in a single node instead of a domain, as we aim on defining a problem which resembles as much as possible of the original gripper problem in Sigmund (1997). The fluid flow boundary conditions of the fluid gripper problem are similar to the boundary conditions presented for the flow obstacle problem in Fig. 12, but fixed structural boundary conditions in all DOF have been imposed along \( \Gamma^\text{s} \) and \( \Omega_D \) has been enlarged so solid elements can connect from \( \Omega_P \) to \( \Gamma^\text{s} \).

The domain \( \Omega \) is discretized into \( \{ N_x, N_y \} = (200, 100) \) elements. The total number of state DOF is 101,505 and the maximum allowed volume fraction is \( V_f = 0.2 \). The problem is investigated for \( Re = (1, 100) \) and for the spring stiffness of \( k = 10^{13} \).

The optimized design and the relevant state fields of the fluid gripper optimization problem in (23) have been plotted in Figs. 20 and 21.
The cross-check table in Table 4 confirms that the design optimized for one $Re$ indeed has superior performance compared to the design optimized for the other $Re$.

The optimized designs consist of four main parts: A horizontal superjacent bar; a pivot which converts positive $y$-directional fluid pressure loads working on the superjacent bar into negative $y$-directional motion in $\Omega_P$; a vertical bar which connects the pivot and the superjacent bar to $\Omega_P$; and a foundation structure which connects the pivot to the structural constraints along $\Gamma_S$.

The foundation structures are robust to ensure that the pressure load is converted into a force in $\Omega_P$. Designs optimized for a too low $k_s$ may cause a “fragile” optimized designs with poor conversion of pressure loads into spring forces.

The horizontal superjacent bars have two purposes: (1) the $y$-directional vertical pressure forces on the horizontal superjacent bars are converted into a clockwise moment around the pivot. The moment around the pivot is transferred to $\Omega_P$ through the vertical bar which connects $\Omega_P$ and the pivot. (2) the input velocity of the fluid flow is fixed, and the optimization problem does not put any requirements on the maximum allowed pressure drop. A large drag force of the optimized design causes a large pressure drop between $\Gamma_W$ and $\Gamma_E$ and hereby a large pressure load on the superjacent bar. The large pressure load

Fig. 19 Schematic of the problem layout and the boundary conditions of the fluid gripper

Fig. 20 Optimized designs and the state field plots for $Re = 1$
causes a large pivoting moment and hereby a large force on $\Omega_1$. The vertical superjacent bar of the $Re = 1$ design is longer than the vertical superjacent bar of the $Re = 100$ design. The difference in lengths between the superjacent bars may be explained by the difference in the pressure loss between the two optimized designs. Due to the difference in the viscous forces of the fluid, the pressure loss over the vertical superjacent bar of the $Re = 1$ design is significantly lower than the pressure loss over the vertical superjacent bar of the $Re = 100$ design. The lower pressure loss of the $Re = 1$ design makes the downstream part of the superjacent bar efficient, as it contributes to the clockwise moment around the pivot.

The superjacent bar for the $Re = 1$ design is straight, whereas the superjacent bar of the $Re = 100$ design has a small concave (with respect to an observer on $\Gamma_N$) feature in the upstream tip. The concave feature of the tip of the $Re = 100$ design generates a low pressure in the northern proximity of the superjacent bar which sucks the superjacent bar upwards and hereby contributes to the clockwise moment around the pivot.

The cross-checks in Table 4 indicate that the topology of the optimized designs and the fluid properties are significantly correlated and adequately captured by the optimization algorithm, and that a design optimized for one $Re$ indeed have superior performance compared to designs optimized for the other $Re$.

<table>
<thead>
<tr>
<th>Design evaluated for</th>
<th>$Re = 1$</th>
<th>$Re = 100$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Re = 1$</td>
<td>$-3.847 \cdot 10^{-5}$</td>
<td>$-9.294 \cdot 10^{-7}$</td>
</tr>
<tr>
<td>$Re = 100$</td>
<td>$-3.557 \cdot 10^{-5}$</td>
<td>$-9.767 \cdot 10^{-7}$</td>
</tr>
</tbody>
</table>

Fig. 21 Optimized designs and the state field plots for $Re = 100$

Fig. 22 Normalized sensitivity fields for the optimized fluid gripper designs
To provide guidance for future research within TO of FSI problems, we have plotted the normalized sensitivity fields and the 0/1 contour for the optimized fluid gripper designs in Fig. 22. Negative values of the sensitivities advice a decrease in design variable density and positive values of the sensitivities advice an increase in design variable density. The design evolution is solely driven by the convective response as the shear stresses of the flow are neglected in the physical model. High positive sensitivity values are observed in the pivots for the both $Re = 1$ and $Re = 100$ designs. This indicates the urge for thinner and more flexible pivots which, however, is hindered by the minimum length scale strongly imposed by the robust design formulation.

7 Discussion

7.1 Interaction between fluid, structure and the optimization problem

The passed cross-checks in Tables 1, 3 and 4 prove that the coupling between the fluid problem, the structural problem and the optimization problem is appropriately and consistently captured. The cross-checks strongly indicate that the various optimized designs are governed by the changes in the model parameters, and not caused by poor local minima.

7.2 The choice of interpolation functions and parameters

The choice of interpolation functions and their parameters is crucial in order to obtain well-posed optimization problems. For a specific set of discretized equations, the choice of interpolation functions and their parameters determine the relationship between the objective function and the design variables. Appendix A.3 demonstrates that a monotonic relationship between the design variables and the objective function may provide a better performing and smoother optimization process.

The density-based topology optimization approach is sensitive to the interactions between various interpolation functions. The introduction of the design field and poorly chosen interpolation functions may cause non-monotonic relationships between the objective function and the design variables. Appendix A.3 demonstrates that a monotonic relationship between the design variables and the objective function may provide a better performing and smoother optimization process.

7.3 The robust formulation

The robust formulation and the continuation scheme in the projection filter threshold may make the optimization framework, apart from providing manufacturing robustness and length-scale-control, less sensitive to non-monotonic relationships between the objective function and the design variables. The robust formulation uses several realizations of the designs, and the probability for the optimizer to find a non-physical, but well-performing, intermediate state is hereby reduced.

7.4 The choice of Brinkman penalization parameter

A very high Brinkman penalization parameter, e.g. $a_{\text{max}} = 10^9$, in the solid elements is crucial in order to model the pressure field correctly. The underlying physical model is incorrect (compared to the segregated approach) for problems in which the Brinkman penalization is too small as the pressure field is incorrectly modeled. Designs optimized for too low Brinkman penalization may perform poorly in segregated models, as the optimized designs may contain features which take advantage of the too permeable structure. The large Brinkman penalization is most important when the objective function or the optimization constraints are directly related to the fluid pressure field, such as in FSI problems.

7.5 Free floating island of solid elements

The multi-objective formulation for the $f_D$ optimization problem in (15) constitutes an alternative to the auxiliary indicator method presented in the work of Jenkins and Maute (2016). The multi-objective approach requires a tuning of an additional parameter as the choice of $a_2$ is important to obtain an adequate ratio between the influence of the multiple objective functions. The approach has shown promising results in removing FFIOSE from the flow obstacle problem, however comparison between the performance of the indicator method and the multi-objective approach requires more studies.

Jenkins and Maute (2016) reported on FFIOSE for compliance problems; such issues were not observed in compliance problems in this study. The absence of FFIOSE in compliance problems may be explained by the continuous nature of the design variables in the density-based topology optimization approach. Elements disconnected from the main structure are removed continuously during the optimization process as the void elements connected between
the FFIOSE and the structural constraints undergo large structural compliance. Void elements with large structural compliance are inefficient for the design performance for which reason the FFIOSE are removed.

### 7.6 The displacement dependency

The displacement dependency significantly increases the non-linearity of the design problem. A design framework which takes the displacement dependency into account could identify design concepts which may not be encountered when neglecting the displacement dependency. To demonstrate the influence of the deformation dependency, we suggest future research to include a comparison between an optimized design which complements the deformation dependency and an optimized design which neglects the deformation dependency.

### 7.7 Topology optimization with immersed versus density-based methods

Immersed methods with explicit boundary representation (IMwEBR) have a well defined boundary between the fluid and the structure, which resolves the physics correctly though the entire optimization process. Intermediate design variables in density-based methods rely in interpolation functions, which do not guarantee correct physical modeling during the optimization process unless a complete 0/1 design is present. We showed that adequate choice of interpolation function parameters provided well-posed optimization problems. IMwEBR may generally have an advantages compared to density-based topology optimization approaches for fluid-structure-interaction, as IMwEBR have a well defined boundary between the fluid and the structure whereas density-based methods are prone to a complex interplay between the fluid and the structure in the intermediate design variables.

### 7.8 Shear stress

In the Hungry Horse problem in Section 5.6, we demonstrated that the shear stress may be significant magnitude compared to the pressure for some problems. Shear stresses should therefore be taken into account in detailed computations. Shear forces may be difficult to model with a density-based Brinkman penalization approach as the porous media in the intermediate design variables penalizes the fluid velocity and hereby the fluid shear stresses. IMwEBR for FSI problems may be better suited for taking such effects into account as IMwEBR always have well-defined boundaries, which avoid issues with non-physical intermediate design variables.

### 7.9 Future work

Future developments in the field of topology optimization for FSI problems may concern: (1) Taking the deformation dependency in the finite element model and the sensitivity analysis into account to demonstrate the connection between optimized topology and the magnitude of the structural deformations. (2) Investigation of the dependency between the optimized topology of various mechanism problems and the choice of input spring stiffnesses, pressure drop constraints and Reynolds numbers. (3) A three dimensional and time dependent implementation of the framework in a parallel code to optimize for more realistic problems. (4) The influence of the shear stress for low Reynolds number flows.

### 8 Conclusion

The density-based topology optimization approach is revisited, and the framework is tested for low and moderate Reynolds numbers on benchmark problems, well-known design problems from the literature, and two new challenging design problems. The framework takes basis in the finite element discretization of the Navier-Cauchy and Navier-Stokes equations which are solved in an unified formulation. The physical modeling is limited to two dimensions, steady state, the influence of the structural deformations on the fluid flow is assumed negligible, and the structural and fluid properties are assumed constant.

The derivation of the unified finite element formulation is elaborated, where an additional term in the coupling between the fluid and the structure is included compared to the equivalent formulations in the literature. Critical implementation details concerning the Brinkman penalization parameter and the interpolation functions and parameters are provided.

The framework is built on basis of a robust formulation, which ensures length-scale-controlled well-performing and binary optimized designs and makes the optimization process less sensitive to the choice of interpolation function parameters, model parameters, and penalization and continuation strategies. The coupling between the fluid flow, the elastic structure and the optimization problem is clearly captured and demonstrated with comprehensive numerical studies and cross-check tables.

By combining different objective functions with different features and weights, non-physical free-floating islands of solid elements (FFIOSE) can be removed during the design process.

The study procures new insight in the field of topology optimization for fluid-structure-interaction problems, and...
may provide guidance for future research within topology optimization for fluid-structure-interaction problems.

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**Appendix**

A.1 Details on the derivation of (3)

The Navier-Cauchy equations are given by:

\[ \frac{\partial \mathbf{\sigma}}{\partial t} + \mathbf{f}_i = 0 \quad \text{in} \quad \Omega_s \]

\[ \mathbf{\sigma}_i = C_{ijkl} \mathbf{\varepsilon}_{kl} \]

\[ \mathbf{\varepsilon}_{kl} = \frac{1}{2} \left( \frac{\partial \mathbf{u}_i}{\partial x_j} + \frac{\partial \mathbf{u}_j}{\partial x_i} \right) \]

The coupling between the fluid and the structure is given by (Farhat and Roux 1991; Yoon 2014a)

\[ \sigma_{i} n_j = \sigma_{i}^{f} n_j \quad \text{on} \quad \Gamma_{SF} \] (25)

The weak form of (24) is given by:

\[ \int_{\Omega_s} u_i^h \frac{\partial \sigma_{i}^f}{\partial x_j} \, dV + \int_{\Gamma_{SF}} u_i^h \mathbf{f}_i \, dV = 0 \] (26)

where \( u_i^h \) is a suitable basis function. Integration by parts of higher dimensions on the first term of (26), yields:

\[ \int_{\Gamma_{SF}} u_i^h \mathbf{a}_{i} n_j \, dS - \int_{\Omega_s} \frac{\partial u_i^h}{\partial x_j} \mathbf{a}_{i} \, dV + \int_{\Gamma_{SF}} w_i^h \mathbf{f}_i \, dV = 0 \] (27)

Shear stresses on the interface between the fluid and the structure are neglected for which reason (25) can be written as \( \sigma_{i} n_j = -p n_i \) on \( \Gamma_{SF} \), where \( p \) is the pressure on the interface surface. Equation (27) is now rewritten as:

\[ \int_{\Gamma_{SF}} u_i^h \rho^h n_j \, dS - \int_{\Omega_s} \frac{\partial u_i^h}{\partial x_j} \sigma_{i}^f \, dV + \int_{\Gamma_{SF}} w_i^h \mathbf{f}_i \, dV = 0 \] (28)

Integration by parts of higher dimensions on the first term of (28), yields:

\[ \int_{\Omega_s} \frac{\partial u_i^h}{\partial x_j} \, dV + \int_{\Gamma_{SF}} w_i^h \frac{\partial p^h}{\partial x_i} \, dV - \int_{\Omega_s} \frac{\partial u_i^h}{\partial x_j} \sigma_{i}^f \, dV + \int_{\Gamma_{SF}} w_i^h \mathbf{f}_i \, dV = 0 \] (29)

Equation (29) may now be rewritten from the segregated domains \( \Omega_s \) to a unified domain \( \Omega \), by introducing a design variable field \( 0 \leq \rho \leq 1 \) and the following interpolation function:

\[ C_{ijkl} = E(\rho)C_{ijkl}^0 \] (30)

Correct integration of the fluid pressure on the elastic structure is ensured by introducing the filter function \( \Psi(\rho) \):

\[ \int_{\Omega} \mathbf{\Psi}(\rho) \left( \frac{\partial u_i^h}{\partial x_j} + u_i \frac{\partial p^h}{\partial x_i} \right) \, dV + \int_{\Omega} w_i^h \mathbf{f}_i \, dV = \int_{\Omega} E(\rho) \frac{\partial u_i^h}{\partial x_j} \sigma_{i}^f \, dV \] (32)

A.2 Benchmark examples

To demonstrate the features of the present framework, we have revisited the wall flow design problems presented in the works of Yoon (2010) and Picelli et al. (2017) and Jenkins and Maute (2016). These, what we call, benchmark design problems are solved with the same physical parameters as in the respective papers but with our framework. The design solution, obtained with the framework presented in this study, to the design problem presented in Jenkins and Maute (2016) has been plotted in Fig. 23. The design solution shown in Jenkins and Maute (2016) and our design solution in Fig. 23 are by visual comparison quite similar. The small difference in the design solutions suggests that the internal pressure, the displacement dependency and/or the shear stress may have minor effects for this specific optimization problem. However, more studies and other optimization problems are required to fully understand the influence of the different modeling approaches and assumptions.

In Figs. 24 and 25, the Yoon (2010) and Picelli et al. (2017) benchmark design problems, solved by our framework, have been plotted for \( Re = 0.004 \) and \( Re = 12 \). The designs have been optimized for the full pressure coupling formulation in (3). It is unclear whether the design solutions in Yoon (2010) are solved for pressure-coupling term 1 or pressure-coupling term 1 and 2. In Yoon (2010), it is seen that an increased Reynolds number causes the wall support to move to the downstream part of the design domain. This tendency is conflicting with the tendencies...
observed in Picelli et al. (2017) and in Figs. 24–25. In these design problems, it is observed that an increased Reynolds number causes the wall support to move to the upstream part of the design domain. As far as we are aware there does not exist any crosschecks between the Reynolds number and the optimized designs in the mentioned papers, for which reason it is challenging to assess how much significance we can attribute to the features of the optimized designs in Yoon (2010) and Picelli et al. (2017). However, please notice that our optimized designs in Figs. 24–25 pass a crosscheck.

A.3 Details on the determination of interpolation functions

TO for FSI problems are highly non-linear, ill-posed and non-convex. Several model parameters influences the design processes and the design solutions, which require a significant amount of parameter tuning due to the deepness of the design space. Numerical experiments with the framework presented in this work, have suggested that the design process is highly dependent on the choice of interpolation functions, $\alpha(\rho), E(\rho)$ and $\psi_1(\rho)$ (abbreviated: $H_{\alpha, E, \phi}$), and the choice of interpolation function parameters, $p_\alpha$, $p_E$ and $p_\psi$ (abbreviated: $p_{\alpha, E, \phi}$). It is our experience that adequate choices of $p_{\alpha, E, \phi}$ and $H_{\alpha, E, \phi}$ are critical to obtain well-performing and 0/1 design solutions. As $p_{\alpha, E, \phi}$ and $H_{\alpha, E, \phi}$ are key to carry out successful optimization problems, we will in this section present a methodology which can be used to determine adequate $p_{\alpha, E, \phi}$ and $H_{\alpha, E, \phi}$ and hereby formulate well-posed optimization problems.

IMwEBR are based on shape sensitivities which may be better suited for TO for some multi-physics problems. IMwEBR have a well-defined boundary between the
different types of physics, which ensures that the physics are resolved correctly throughout the entire design process, as no sub-domains are dependent on the quality of the interpolation functions of the intermediate design variables. In density-based methods the correctness of the physical modeling rely, among many other aspects, on the choice of $p\{\alpha,E,\Psi\}$ and $H\{\alpha,E,\Psi\}$. The hypothesis is that topology sensitivities, $\partial f/\partial \rho_d$, may obtain the same well-behaving features as shape sensitivities, $\partial f/\partial \rho_s$, if some adequate $H\{\alpha,E,\Psi\}$ and $p\{\alpha,E,\Psi\}$ are chosen.

To determine adequate sets of $H\{\alpha,E,\Psi\}$ and $p\{\alpha,E,\Psi\}$, we compare $\partial f/\partial \rho_s$ and $\partial f/\partial \rho_d$ for two different problems: (1) a purely elastic problem and (2) an FSI problem. The problem layouts and the boundary conditions have been sketched in Fig. 26. To carry out the study, we compare four different objective functions, $f_E$, $f_C$, $f_T$ and $f_P$ (abbreviated: $f\{E,C,T,P\}$):

1. Dissipated energy in the flow, $f_E$, see (17).
2. Structural compliance $f_C$, see (16).
3. The $y$-displacement of the tip of the beam in point $(x, y) = (2, 0.45)$:

$$f_T = \frac{1}{f_{\rho_d}} \int_{\Omega_T} dV \int_{\Omega_T} dV$$

(33)

The relationship between $f\{E,C,T,P\}$, $\rho_s$ and $\rho_d$ is determined with basis in a simple problem where a beam separates a channel into two regions of the same size. The problem is modeled in the unified framework. The beam separating the channel, $\Omega_1$, has fixed unity design variables and the tip of the beam is loaded with a force $f_y$. With reference to Fig. 26, we consider two different problems: (a) An elastic problem where $u^*_x = 0$ and $f_y = 10$, and (b) an FSI problem where $u^*_x = 1$ and $f_y = 0$.

With reference to Fig. 26a, the topology sensitivities of various objective functions are computed by changing the design variables of the lowest line of elements of the vertical beam. With reference to Fig. 26b, the shape gradients of various objective functions are computed by changing the position of the nodes on the lower boundary of the beam. The position of the boundary is varied over the length of one element, entailing that $\partial f/\partial \rho_d$ and $\partial f/\partial \rho_s$ are comparable in material usage.

The relationship between $f\{C,P\}$, $f\{C,T\}$, $\rho_d$ and $\rho_s$ for the elastic problem have been compared in Fig. 27. The relationships are different but can be characterized by the following attribute: $f\{C,T\}(\rho_s)$ and $f\{C,T\}(\rho_d)$ are strictly monotonic entailing that $\partial f\{C,T\}/\partial \rho_s$ and $\partial f\{C,T\}/\partial \rho_d$ are strictly monotonic. Well-versed and crisp 0/1 designs and smooth optimization processes are obtained for a large
number of TO for elastic problems, see e.g. (Bendsøe and Sigmund 2003). The hypothesis in this study is, that the well-posed properties of linear elastic problems are explained by the strictly monotonic features of the $\partial f_C/\partial \rho_d$.

We now point out attention to the FSI problem, where we investigate the monotonicity of $f_{E.C.T.P} (\rho_s)$ and $f_{E.C.T.P} (\rho_d)$. The relationships have been plotted in Fig. 28, and are characterized by:

1. $f_{E.C.T.P} (\rho_s)$ are strictly monotonic in all cases, which entail that $\partial f_{E.C.T.P}/\partial \rho_s$ are strictly monotonic in all cases.
2. $f_{E.C.T.P} (\rho_s)$ are strictly monotonic for some choices of $p_{\alpha, E, /Psi1}$ and $H_{\alpha, E, /Psi1}$.
3. The relationship between $f_{E.C.T.P} (\rho_d)$ seem to be very sensitive with respect to the choice of $p_{\alpha}$, as a small change in $p_{\alpha}$ may disrupt the monotonicity for all $f_{E.C.T.P}$.

To demonstrate the importance of the monotonicity of $f_{E.C.T.P} (\rho)$ we have included a numerical example where we compare two design optimized for two different $p_{\alpha}$. In Fig. 29, $f_D$ have been optimized for the flow obstacle problem (see Section 6.2) for $p_{\alpha} = 0.5 \cdot 10^{-6}$ and $p_{\alpha} = 10^{-6}$. The design optimized with a strictly monotonic $f_D$ perform much better than the design optimized for non-monotonic $f_D$. We notice that a small change in $p_{\alpha}$ significantly influences the topology and the performance of the design solutions.
We suggest that the correlation between the monotonicity of the objective functions and the well-posedness of the design problems is likely to generalize to all multiphysics topology optimization problems.

### A.4 Details on the Brinkman penalization parameter

Numerical experiments with the framework suggested that \( \alpha_{\text{max}} \) should be chosen high (e.g. \( \alpha_{\text{max}} = 10^9 \)) to model the pressure field correctly. A low \( \alpha_{\text{max}} \), e.g. \( \alpha_{\text{max}} = 10^5 \), provides a more well-posed optimization problem, however the pressure field is not modeled correctly. Modeling the pressure field incorrectly may provide unintuitive and physically meaningless optimized designs, as the coupling from the fluid to the structure is transferred through the pressure field. To demonstrate the relationship between the pressure field and the magnitude of \( \alpha_{\text{max}} \), we have plotted the pressure field along the line \( (x, y) = (x, 0.34) \) for the design shown in Fig. 30 in Fig. 31. The pressure fields for the COMSOL composite model and the unified model with \( a_{\text{max}} = 10^9 \) is closely correlated. However, for small \( \alpha_{\text{max}} \), a large difference between the composite model and the unified model is observed. As a final remark, the minor difference between the fields is caused by different finite element discretizations of the segregated and unified models.

To demonstrate the occurrence of unintuitive optimized topologies for design problems with too low \( \alpha_{\text{max}} \), we consider two different design problems. The design in Fig. 32a has been optimized for \( \alpha_{\text{max}} = 10^5 \) and the design

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**Fig. 29** Optimized designs for the flow obstacle problem in Fig. 12 for two different interpolation function parameters

(a) Monotonic gradients

(b) Non-monotonic gradients

**Fig. 30** Design used to evaluate the pressure

**Fig. 31** The pressure as function of \( x \) for various \( \alpha_{\text{max}} \)

**Fig. 32** Design solutions for the flow obstacle problem in Fig. 12 for various \( \alpha_{\text{max}} \)

(a) \( \alpha_{\text{max}} = 10^5 \)

(b) \( \alpha_{\text{max}} = 10^9 \)
in Fig. 32b has been optimized for $\alpha_{\text{max}} = 10^5$. The designs provide superior performance for the model parameters under which the designs were optimized. However, the design optimized for $\alpha_{\text{max}} = 10^5$ does not perform well in a segregated FSI formulation. The too low $\alpha_{\text{max}}$ causes poor resolution of the pressure field which causes unintuitive optimized designs. For comparison we have plotted the design optimized for $\alpha_{\text{max}} = 10^7$ in Fig. 32b. This design performs well in a segregated model.

The coupling between the structure and the fluid is carried out through the pressure field, for which reason adequate modeling of the pressure field is crucial in FSI problems. Previous work on topology optimization for fluid problems has used magnitudes of $\alpha_{\text{max}}$ which do not resolve the pressure field correctly. Non-intuitive designs may not have been observed in these studies because the pressure fields were not directly related to the objective functions or the constraints of the optimization problems.

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References

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