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Multi-Material Design Optimization of Composite Structures

— PREPRINT —

PhD Thesis

by

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You can add up the parts
but you won't have the sum
Leonard Cohen

Preface

This thesis has been submitted to the Faculties of Engineering, Science and Medicine at Aalborg University in partial fulfillment of the requirements for the Ph.D. degree in Mechanical Engineering. The underlying work has been carried out at the Department of Mechanical and Manufacturing Engineering¹, Aalborg University in the period from August 2007 to September 2010. The work is part of the project “Multi-material design optimization of composite structures” sponsored by the Danish Research Council for Technology and Production Sciences (FTP), Grant no. 274-06-0443, this support is gratefully acknowledged.

I would like to thank my supervisors Professor Erik Lund and Associate Professor Mathias Stolpe for their advice and support throughout this project.

I am glad to have been a part of the former Department of Mechanical Engineering. It has been a great place to work which most certainly is due to the pleasant atmosphere brought about by nice colleagues. I would like to thank Ph.D. Esben Lindgaard for sharing office with me as well as thoughts about life in general and as a PhD student in particular.

I would also like to thank Professor Kai-Uwe Bletzinger and his staff at the Technical University of Munich (TUM) for hosting me during a four month visit at their department in the Fall of 2008.

A special thanks goes to Ph.D. Eduardo Muñoz from the Technical University of Denmark (DTU) for the rewarding collaboration and good times we have had working together on multi-material optimization.

Finally I would like to thank my family, and in particular my wife Marie for her love and support throughout the period of this work and for cheering on me when times are difficult. Tak! Since our marriage in August 2010 my new name is Christian Frier Hvejsel and hence my former middle name Gram is now history.

Christian Frier Hvejsel
Aalborg, March 2011.

¹Former Department of Mechanical Engineering

Summary

This PhD thesis entitled “Multi-Material Design Optimization of Composite Structures” addresses the design problem of choosing materials in an optimal manner under a resource constraint so as to maximize the integral stiffness of a structure under static loading conditions. In particular stiffness design of laminated composite structures is studied including the problem of orienting orthotropic material optimally. The approach taken in this work is to consider this multi-material design problem as a generalized topology optimization problem including multiple candidate materials with known properties. The modeling encompasses discrete orientation of orthotropic materials, selection between different distinct materials as well as removal of material representing holes in the structure within a unified parametrization. The direct generalization of two-phase topology optimization to any number of phases including void as a choice using the well-known material interpolation functions is novel.

For practical multi-material design problems the parametrization leads to optimization problems with a large number of design variables limiting the applicability of combinatorial solution approaches or random search techniques. Thus, a main issue is the question of how to parametrize the originally discrete optimization problem in a manner making it suitable for solution using gradient-based algorithms. This is a central theme throughout the thesis and in particular two gradient-based approaches are studied; the first using continuation of a non-convex penalty constraint to suppress intermediate valued designs and the second approach using material interpolation schemes making intermediate choices unfavorable through implicit penalization of the objective function. The last contribution consists of a relaxation-based search heuristic that accelerates a Generalized Benders Decomposition technique for global optimization and enables the solution of medium-scale problems to global optimality. Improvements in the ability to solve larger problems to global optimality are found and potentially further improvements may be obtained with this technique in combination with cheaper heuristics.

Resume

Denne PhD-afhandling med titlen "Multi-materiale designoptimering af kompositte konstruktioner" omhandler designproblemet i optimalt at vælge materialer under begrænsede ressourcer således at konstruktionens stivhed maksimeres under statisk belastning. Især studeres stivhedsdesign af laminerede komposit konstruktioner inklusiv optimal orientering af orthotropt materiale. Den valgte i denne afhandling tilgang betragter dette multi-materiale designproblem som et generaliseret topologioptimerings-problem der inkluderer et antal materialer med kendte egenskaber. Denne modelering af problemet indbefatter diskret orientering af ortotrope materialer, valg mellem forskellige distinkte materialer såvel som fjernelse af materiale i een og samme parametrisering. Den direkte generalisering af to-fase topologioptimering til et arbitrært antal faser hvor huller inkluderes som en mulighed ved hjælp af de velkendte materiale-interpolationsfunktioner er ny.

For praktiske multi-materiale designproblemer fører parametriseringen til optimeringsproblemer med så mange designvariable at kombinatoriske eller tilfældighedsstyrede søgealgoritmer ikke er anvendelige. Derfor er spørgsmålet, hvordan det oprindeligt diskrete problem parametriseres så det kan løses ved hjælp af gradientbaserede algoritmer et centralt tema i afhandlingen. To gradient-baserede tilgange studeres; den første anvender en gradvis indsnævring af det tilladelige designrum til endeligt at fjerne ikke-heltallige løsninger, mens den anden tilgang anvender materiale-interpolation som implicit igennem objektfunktionen gør ikke-heltallige løsninger ufavorable. Det sidste bidrag er en relaksations-baseret søgeheuristik som accelererer en generaliseret Benders' dekompositions-algoritme til global optimering, og som muliggør løsning af middelstore problemer til globalt optimum. Det påvises at sådanne heuristikker kan øge størrelsen af problemer der kan løses til globalt optimum og potentielt kan der udvikles yderligere forbedringer ved hjælp af denne teknik i kombination med billigere heuristikker.

Publications

This dissertation consists of an introduction to the area of research and three papers submitted or to be submitted for refereed scientific journals.

Publications in refereed journals

- Hvejsel, C.F.; Lund, E.; Stolpe, M. (2011): “Optimization strategies for discrete multi-material stiffness optimization”, *Structural and Multidisciplinary Optimization*, DOI: 10.1007/s00158-011-0648-5.
- Hvejsel, C.G.; Muñoz, E. (2010): “Discrete Multi-material Optimization: Combining Discrete and Continuous Approaches for Global Optimization”, to be submitted.
- Hvejsel, C.F.; Lund, E. (2011): “Material Interpolation Schemes for Unified Topology and Multi-material Optimization”, *Structural and Multidisciplinary Optimization*, DOI: 10.1007/s00158-011-0625-z.

Publications in proceedings and monographs with review

- Hvejsel, C.G.; Muñoz, E.; Lund, E. (2010): “Multi-Material Optimization - Global Optimization and Relaxations”. In: *Abstract from The IV European Conference on Computational Mechanics* (Eds. Allix, O. et al.), Palais de Congrès, Paris, France, May 16 - 21 2010, 2 pages.
- Hvejsel, C.G.; Lund, E. (2009): “Failure Constraints for Discrete Material Optimization”. In: *DTU Mathematics Report nr. 2009-02 PLATO-N International Workshop “Advances in Topology and Material Optimization - Methods and Industrial Applications”*, DTU Lyngby, September 23 - 25 2009, Denmark, ISBN 0904-7611, 2 pages.
- Lund, E.; Hvejsel, C.G.; Lindgaard, E. (2009): “From Topology to Detailed Design of Multi-Material Laminated Composite Structures”. In: *DTU Mathematics Report nr. 2009-02 PLATO-N International Workshop “Advances in Topology and Material Optimization - Methods and Industrial Applications”*, DTU Lyngby, September 23 - 25 2009, Denmark, ISBN 0904-7611, 2 pages.
- Lund E.; Hvejsel C.G.; Lindgaard, E. (2009): “An Integrated Design Approach to Multi-Material Multi-Criteria Optimization of Laminated Composite Structures”. In: *Book of Abstracts. 8th World Congress on Structural and Multidisciplinary Optimization* (Eds. H.C. Rodrigues et al.), 1 - 5 June 2009, Lisbon, Portugal, 1 page.
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 - Hvejsel, C.G.; Lund, E.(2008): “Towards Local Design Criteria in Discrete Material Optimization”. In: *Proc. 8th World Congress on Computational Mechanics WCCM8, 5th European Congress on Computational Methods in Applied Science and Engineering ECCOMAS 2008* (Eds. B.A. Schrefler and U. Perego), Venice, June 30 - July 5 2008, Italy, 2 pages.
 - Lund, E.; Johansen, L.S.; Hvejsel, C.G.; Lindgaard, E. (2008): “Multi-Criteria Multi-Material Topology Optimization of Laminated Composite Structures”. In: *Proc. 12th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference*, 10 - 12 September 2008, Victoria, Canada, British Columbia, AIAA Paper 2008-5897, 14 pages.
 - Lund, E.; Johansen, L.S.; Hvejsel, C.G.; Lindgaard, E. (2008): “Multi-Material Topology Optimization of Geometrically Nonlinear Multi-Layered Composite Shell Structures”. In: *Proc. 8th World Congress on Computational Mechanics WCCM8, 5th European Congress on Computational Methods in Applied Science and Engineering ECCOMAS 2008* (Eds. B.A. Schrefler and U. Perego), Venice, June 30 - July 5 2008, Italy, 2 pages.

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- Hvejsel, C.G.; Lund, E. (2007): “Efficient Shell Element Formulation for Use in Discrete Material Optimization”. In: *Proceedings of the 20th Nordic Seminar on Computational Mechanics* (Eds. Larsson, R.; Runesson, K.), Chalmers Tekniska Högskola, November 23 - 24 2007, Göteborg, Sweden, 2 pages.
- Hvejsel, C.G.; Hansen, H. F.; Lund, E. (2007): “Shell Element for Efficient Analysis and Optimization of Laminated Composite Shell Structures”. In: *Book of Abstracts 2nd GACM Colloquium on Computational Mechanics for Young Scientists from Academia and Industry*, Technische Universität München, October 2007, München, Germany.

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Introduction

THIS THESIS IS CONCERNED WITH optimal material selection from a set of given materials with pre-defined properties so as to design the global layout of a multi-material composite structure under static loading conditions. This mechanical design problem comes up in a number of applications and in particular we consider optimal composite laminate design. Designing laminated composite structures optimally requires a material to be chosen in each layer of the laminate, including the question of orienting orthotropic materials in each of the layers.

Rational design methodologies for composite structures become more important with the increasing use of these materials in various industries ranging from military aerospace and marine applications to civil transportation, wind turbine blades, etc. Common for these applications is a desire for high structural performance and/or low weight (and cost) simultaneously, and often the raw material cost and thereby the total cost of these structures is relatively high. Thus, the potential savings are high if the materials can be utilized efficiently or even optimally. The increasing use of this class of materials seems to be continuing and with better analysis techniques and systematic design methodologies, the advantages of composite materials may be utilized even further, making composite materials an attractive alternative also for lower cost applications.

Regardless of the perspective taken - low cost or low weight - a key issue for a successful design is to select and employ the right material(s) in an intelligent¹ manner for the given application, i.e. to design the mechanical structure such that the potential candidate materials throughout the structure are utilized as efficiently as possible for the given application.

1.1 Materials, laminates and structures

The use of multiple materials fulfilling different purposes as parts of a *structure* is not new and is well-known from e.g. reinforced concrete, laminated plates/shells, and sandwich panels to name few. In this context the term *composite* may refer to

¹not as in “intelligent design”!

multiple scales at which the structure is composed of different elements. Sandwich panels for instance are characterized by a compliant core separating two stiff face sheets. At this level we talk about a composite *structure*, but at a smaller scale the skins are often composite *laminates* composed of layers of heterogeneous composite *materials* themselves made of reinforcing fibers held together by a weaker matrix. Similarly, composite laminates may be combined in other ways to form composite structures where the laminate consists of layers (plies) of homogeneous material or heterogeneous composite materials. In this thesis we are mainly interested in

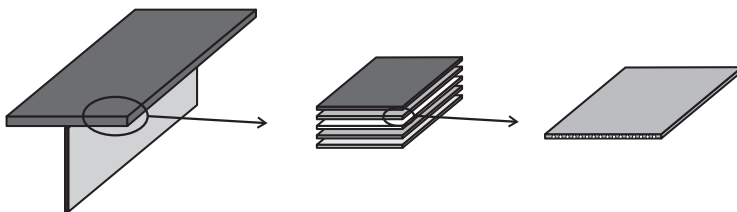


Figure 1.1: Length scales of composite *structure*, *laminate*, and *material*, respectively. The structure is composed of multiple laminates containing a number of layers which may be homogeneous or heterogenous composite materials.

designing composite *structures* and *laminates* and hence not necessarily *materials*. This distinction, however, is mainly a matter of length scale as shown in figure 1.1 and in principle the concepts and ideas presented in this thesis could also be applied at the level of material design. With the words of Bendsøe and Sigmund (2003); “*any material is a structure if you look at it through a sufficiently strong microscope*”.

We assume to have a set of existing (composite or homogeneous) materials at our disposal from which we want to select the best for each macroscopic design subdomain of consideration. Thus, we *a priori* fix the design discretization; the number of design subdomains as well as their spatial extension is fixed throughout the optimization process. This limitation may seem restrictive but as we will see, it may represent a quite comprehensive parametrization in terms of design freedom for distributing multiple phases so as to optimize an objective function within certain constraints.

In relation to laminate optimization this means that we fix the number of layers and then consider each layer as an individual subdomain for which we want to select the material in an optimal manner.

1.2 Design optimization

Compared to designing with a single isotropic material, the freedom and complexity of designing with multiple anisotropic materials is higher. On one hand

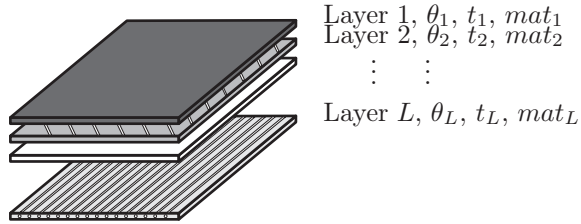


Figure 1.2: Laminate with layers consisting of different materials potentially oriented at different angles. The thickness of the layers may vary as well (not shown).

the design freedom in terms of number of design variables is much larger, on the other hand the number of restrictions and constraints for a (laminated) composite structure is larger as well. This situation potentially makes up a complex design problem and it may be difficult to exploit the full potential of the materials by intuition alone. Currently it is not possible to formulate and solve practical real-life composite design problems *completely* as mathematical optimization problems. Certainly, it is not impossible to a certain extent to do design optimization of composite structures, but to formulate and solve an optimization problem that allows for all imaginable design freedom and considers all imaginable constraints and restrictions that must be taken into account in practice, is still an ambitious endeavor for which there is no definitive framework yet. The question is whether it is possible or even desirable to include all possible information within a fully automated optimization based design process. Maybe rather optimization should be regarded as an aid to a human decision maker, typically the design engineer, who supervises the process, intervenes, modifies, and carries out the design decisions suggested by the optimizer.

The experienced designer intuitively knows when something is *good*. An other and more involved question is whether it is also *optimal*? And by what measure? These questions are explicitly addressed in design optimization and in this way the task of formulating optimization problems may be considered a creative challenge requiring imaginative capabilities at a high and abstract level. It requires the capability to “see through” the often vague and fuzzy statements of what is good and to put these into precise mathematical statements that allow the optimization problem to be solved in a hopefully efficient manner.

To outline some of the complexities involved with a fictitious full design optimization formulation for composite structures, we mention out of many; not yet resolved issues regarding prediction of the failure behavior of generally laminated composite structures under arbitrary loading (see e.g. Hinton et al. (2002) for a review of composite failure criteria), non-convexity of criteria functions, as well as the possible difficulties encountered in solving the large-scale optimization problems resulting from such a complete formulation. Nevertheless, if we could formulate

a design optimization problem with a large freedom in the parametrization, and still take into consideration important constraints, it should be possible to obtain a good design concept in terms of information about how to distribute a limited amount of expensive material so as to obtain the best structural performance possible.

The design problem we attempt to solve can be stated as; *given a number of pre-defined candidate materials with known properties, select in each point throughout the reference domain either no material or one of the candidates so as to minimize an objective (cost) function subject to physical constraints and resource constraints.* In its basic form, this material selection problem is discrete in nature. Physically, the material selection variables are binary; either a material is chosen throughout a domain or it is not. Such discrete problems are inherently hard to solve.

The work presented in this thesis is motivated by the increasing use of composite materials, in particular the simultaneous use of multiple different materials within a mechanical structure as it is seen in e.g. wind turbine blades where a number of quite different materials are employed simultaneously.

This thesis is a contribution to, what we believe is, a comprehensive parametrization of the optimization problem encountered when designing with multiple possibly anisotropic composite materials. The multi-material design problem is formulated very similar to topology optimization; a method which has become popular for conceptual layout design of systems whose physics are governed by partial differential equations, see e.g. Bendsøe and Sigmund (2003).

1.3 Composite laminate optimization

To fully exploit the potentials of laminated composites it is necessary to specify *material*, *thickness* and *orientation* for each layer of the laminate. Doing so, the directionality of the individual layers may be used beneficially so as to obtain the desired response of the laminated structure. From this it is clear that the number of *design variables* can be very large in laminate design problems.

The process of designing a laminated composite structure can be thought of as a matter of making decisions (regarding the design) so as to fulfill some purpose in the best way without violating constraints or requirements that must be met in order to have a feasible solution. The basic idea of such a design optimization is to formulate the mechanical design problem as a mathematical optimization problem and consequently obtain the design of the structure as a solution to this optimization problem. This requires the design problem statement to be parametrized and formulated unambiguously in terms of the design variables to be determined. The parametrization of the optimization problem has an impact on the number of design variables as well as on the difficulty of obtaining solutions in an efficient and reliable manner.

Typically laminate design is combined with optimization of the orientation of the anisotropic or orthotropic layers and materials. To start with, an overview of previous attempts in addressing the optimal orientation problem is given.

1.3.1 Optimization with anisotropic and orthotropic materials

Optimal structural design with composite materials has been studied extensively for more than forty years and it is not within the scope of this work to give an exhaustive account for the developments. For an overview and an introduction to laminate design optimization see the textbook by Gürdal et al. (1999) and the review paper by Abrate (1994) as well as two recent reviews by Ghiasi et al. (2009, 2010).

Inspired by Fang and Springer (1993) laminate optimization approaches may be categorized according to the following four categories: 1) analytical methods, 2) enumeration methods, 3) stochastic and heuristic search methods, 4) mathematical programming techniques. Furthermore, various combinations of these methods could be envisaged. Within this spectrum, the approaches taken in this thesis are placed in the two last categories with an emphasis on the mathematical programming oriented approaches. In the following we describe different composite design parametrizations.

Fiber angle and thickness optimization

Quite remarkably one of the first publications on optimization of composite structures, see Schmit and Farshi (1973), employed mathematical programming to minimize the mass under strength and stiffness constraints using layer thicknesses for pre-defined orientations as the design variables. Other early attempts primarily used analytical or optimality criteria approaches to optimize the response of plane problems involving orthotropic materials, e.g. Banichuk (1981) studied optimal orientation of orthotropic material in plane problems. Pedersen (1989) derived analytical expressions for optimal orientation of orthotropic material as functions of the strain field and later also optimized the thickness distribution in combination with the orientation in Pedersen (1991). Thomsen and Olhoff (1990); Thomsen (1991) studied optimal orientation and material density distribution for plane problems. Thomsen (1992) used a homogenization approach to design two-material structures in combination with orientation of the material.

Lamination parameters

An other parametrization of laminate design is the use of so-called lamination parameters originally proposed by Tsai and Pagano (1968). Lamination parameters provide a parametrization of the properties of laminates consisting of identical orthotropic material oriented differently in each layer. Using material invariants describing the elastic properties of orthotropic (and anisotropic) material, the laminate properties may be represented in terms of the lamination parameters. The lamination parameters are trigonometric functions of the layer thicknesses and

orientations. The laminate stiffness is linear in the lamination parameters. The lamination parameters are not mutually independent and for in-plane problems the relations between lamination parameters and their physical representation exist on closed form which was used for optimization purposes in a number of publications, see Miki (1982); Fukunaga and Vanderplaats (1991); Fukunaga and Sekine (1993). For more general problems involving combined in-plane and bending load these relations are not given on closed form and to return to a physical representation of the lay-up an inverse problem in the layer thicknesses and orientations must be solved subsequently, Hammer et al. (1997); Foldager et al. (1998).

Free Material Optimization

Free material optimization (FMO) was proposed by Ringertz (1993); Bendsøe et al. (1994) and has been studied since then by numerous researchers, for an overview and introduction to the method see Zowe et al. (1997); Ben-Tal et al. (2000); Kočvara and Zowe (2001); Kočvara et al. (2008) and for recent developments in terms of extensions to eigenvalue related criteria functions and stress constraints see Kočvara and Stingl (2007); Stingl et al. (2009*a,b*). The design parametrization in FMO varies the full elastic tensor with the only requirement that the material *behaviour* does not violate physical limits in the sense that the elastic tensor must be symmetric and positive semidefinite. The parametrization is not limited to existing manufacturable materials and hence the optimized FMO result needs to be interpreted under the technological restrictions for a given realization or manufacturing process. Such interpretations have been investigated by Hörnlein et al. (2001) and Bodnár et al. (2008).

Discrete Material Optimization

The developments within multi-phase topology optimization by Sigmund and Torquato (1997); Gibiansky and Sigmund (2000) lead to a generalization to any number of phases by the Discrete Material Optimization (DMO) approach proposed by Stegmann and Lund (2005); Lund and Stegmann (2005) where the discrete problem of choosing between multiple distinct materials is converted to a continuous problem enabling design sensitivity analysis and the use of gradient based optimizers to solve the problem. This parametrization uses weighting functions to parametrize the material properties as weighted sums of the chosen candidate materials. Within this parametrization discrete fiber angle optimization may be addressed by considering the different orientations as different materials, but also completely different materials may be mixed so as to choose between e.g. steel, fiber reinforced composites, foam materials etc. This allows for topological changes of the structure and in connection with design of laminates this allows for the occurrence of sandwich structures to emerge as an optimization result. This approach has been applied successfully to material selection problems involving global criteria functions such as maximization of structural stiffness, eigenfrequencies and buckling loads, see e.g. the references above and Lund (2009).

Alternative multi-phase parametrizations include level-set approaches Wang and Wang (2004); Wang et al. (2005), relative density parametrization Zhou and Li (2008) which similarly to the parametrization in Stegmann and Lund (2005) implicitly ensures unity summation of the weights. A recent idea for the parametrization of multi-material design optimization was presented by Bruyneel et al. (2010); Bruyneel (2011) who used finite element shape functions as weights to interpolate properties of candidate materials. Finally, we mention the peak-function approach Yin and Ananthasuresh (2001) that uses a single design variable to “slide” between a number of candidates which seems attractive in terms of the low number of design variables but according to our experience the numerical performance is highly dependent on parameter tuning.

1.4 Objectives

The present PhD project has been part of a larger project called “Multi-material design optimization of composite structures” running from June 2007 till August 2010 as a collaboration between the Department of Mechanical and Manufacturing Engineering, Aalborg University and the Department of Mathematics, Technical University of Denmark where Mathias Stolpe and Eduardo Muñoz have been project partners.

The aim of the present study is to develop continuous optimization formulations for discrete multi-material problems, that can be used in combination with methods for integer formulations developed at DTU. Furthermore it has been the aim to develop methods including strength/failure constraints on the individual phases. This challenging problem, however, has not been resolved within the present project and still remains open.

The objective of this project is to develop models based on a discrete material parametrization, and to develop continuous optimization formulations for optimal stiffness design of multi-material composite structures taking into account the global structural stiffness and the total mass of the structure. The objective is to *develop and implement methods that enable rational design of laminated composite structures using a discrete multi-material parametrization.*

In particular it has been the aim to develop continuous formulations that approximate the original *discrete problem* as closely as possible in order to be able to attack large-scale problems using gradient-based algorithms.

In the project the in-house research code MUST(MULTidisciplinary Synthesis Tool) has been used as a platform for research and experimentation. MUST is a finite element based analysis and design optimization tool developed by Professor Erik Lund and co-workers for more than ten years.

Outline of the Thesis

The thesis is organized as follows; the present chapter has given the background for the problems addressed in this thesis, Chapter 2 presents the theoretical background on multi-material optimization and discusses some of the problems involved in tackling these problems, Chapter 3 summarizes the contributions of the accompanying papers and concludes the thesis including directions for further research. Finally, the accompanying papers are appended.

Multi-material design optimization

This chapter describes the background of discrete multi-material design optimization problems; we review the formulation of the continuum minimum compliance multi-material problem, discretize it to obtain a mixed 0-1 design problem, and present approximations used in the solution process. Having described the parametrization and criteria functions we describe solution techniques and algorithms.

The minimum compliance problem has been studied extensively in the literature and in the following we present background material for the developments shown later in the thesis. For a further treatment of the minimum compliance problem please refer to the review paper by Eschenauer and Olhoff (2001) and the textbook by Bendsøe and Sigmund (2003).

2.1 Linear elasticity

This section reviews notation and basic assumptions regarding the governing physics and presents selected topics of relevance to the developments presented later.

We work within the framework of linear elasticity and assume quasi-static loading throughout this thesis. The governing equations on strong form are presented in matrix-vector notation to avoid confusion when introducing the design parametrization.

The kinematic relation between the strain field and the displacement field gives the components of the linearized symmetric strain tensor in vector form, $\boldsymbol{\varepsilon} \in \mathbb{R}^6$.

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \mathbf{L}\mathbf{u} = \frac{1}{2} (\nabla\mathbf{u} + \nabla\mathbf{u}^T) \quad (2.1)$$

where $\mathbf{u} \in \mathbb{R}^3$ is the displacement vector field and $\nabla\mathbf{u}$ denotes the gradient of the displacement field. We assume that the stresses $\boldsymbol{\sigma} \in \mathbb{R}^6$ are linked linearly to the strains $\boldsymbol{\varepsilon}$ through Hooke's law

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}) = \mathbf{E}\boldsymbol{\varepsilon} \Leftrightarrow \quad (2.2)$$

$$\boldsymbol{\varepsilon}(\boldsymbol{\sigma}) = \mathbf{E}^{-1}\boldsymbol{\sigma} = \mathbf{C}\boldsymbol{\sigma} \quad (2.3)$$

where $\mathbf{E} \in \mathbb{R}^{6 \times 6}$ is the symmetric material stiffness matrix containing the entries of a symmetric fourth-order tensor and \mathbf{C} is the corresponding compliance matrix. Finally three equilibrium equations are given by

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{f} = 0 \quad (2.4)$$

where $\nabla \cdot \boldsymbol{\sigma}$ is the divergence of the stress field, and $\mathbf{f} \in \mathbb{R}^3$ is the body force vector field (force per unit volume). Together with appropriate boundary conditions in terms of prescribed displacements and tractions applied to the surface of the body, Equations (2.1)-(2.4) define the boundary value problem of linear elasticity. In the following section we define strain and stress energy measures that are used later in the description of energy principles.

2.2 Energy principles

The equilibrium conditions may be given an alternative form using variational calculus and energy principles. Energy principles form the theoretical basis for the finite element method used for the actual calculations as described in Section 2.5 and are also used in the development of material interpolation schemes in Section 2.10.

2.2.1 Strain and stress energy

The strain energy density \bar{U} is defined as the energy required to deform a unit volume solid from a stress free reference state to deformed state. The strain energy density is given by

$$\bar{U} = \int_0^{\boldsymbol{\varepsilon}} \boldsymbol{\sigma}(\boldsymbol{\varepsilon}) \, d\boldsymbol{\varepsilon} \quad (2.5)$$

The total strain energy U is defined as the volume integral of the strain energy density (2.5):

$$U = \int_{\Omega} \bar{U} \, d\Omega \quad (2.6)$$

The complementary strain energy density or stress energy density U^C is given by

$$\bar{U}^C = \int_0^{\boldsymbol{\sigma}} \boldsymbol{\varepsilon}(\boldsymbol{\sigma}) \, d\boldsymbol{\sigma} \quad (2.7)$$

As for the strain energy the total stress energy U^C is defined as the volume integral of the stress energy density (2.7):

$$U^C = \int_{\Omega} \bar{U}^C \, d\Omega \quad (2.8)$$

Strain and stress energy with a linear constitutive law

If the relation between stress and strain is linear as defined in (2.2) and (2.3), the strain energy density and the stress energy density are identical

$$\bar{U} = \frac{1}{2} \boldsymbol{\varepsilon}^T \mathbf{E} \boldsymbol{\varepsilon} = \frac{1}{2} \boldsymbol{\sigma}^T \boldsymbol{\varepsilon} = \frac{1}{2} \boldsymbol{\sigma}^T \mathbf{C} \boldsymbol{\sigma} = \bar{U}^C \quad (2.9)$$

Thus the total energies are also identical: $U = U^C$.

If stresses and strains are related through an elastic constitutive relation as is the case for linear elasticity, the total strain energy U is also called the internal potential Π_i .

$$\Pi_i := U \quad (2.10)$$

2.2.2 External work

The work done by external forces W is given by

$$W = \int_{\Omega} \mathbf{f}^T \mathbf{u} \, d\Omega + \int_S \mathbf{p}^T \mathbf{u} \, dS = -\Pi_e \quad (2.11)$$

where \mathbf{f} are body forces per unit volume potentially acting throughout the body and \mathbf{p} are surface tractions applied on the surface of the body. The work done by the external forces also equals their lost potential to do work and therefore we call Π_e the external potential.

2.2.3 Principle of stationary total potential energy

If the strains are related to stresses through an elastic constitutive relation such as Hooke's law (2.2), an equivalent equilibrium condition to (2.4) may be expressed on weak form using the internal (2.10) and external potential energy (2.11). The total potential energy Π (TPE) is defined as:

$$\Pi = \Pi_e + \Pi_i = U - W \quad (2.12)$$

Equilibrium is formulated via the principle of stationary TPE; *among all kinematically admissible displacement fields, the one extremizing the total potential energy is the equilibrium displacement field.* The variational stationarity condition of the TPE is given by

$$\delta \Pi = \delta U - \delta W = 0 \quad (2.13)$$

where δ denotes kinematically admissible variations, i.e. variations of the displacement field satisfying kinematic boundary conditions, see e.g. Dym and Shames (1996). In the following we use the principle of stationary TPE as the equilibrium condition but other equilibrium conditions are equally valid.

2.3 Continuum problem formulation

The continuum infinite dimensional form of the optimization problem seeks to determine the optimal point-wise material distribution as follows: *given a number of*

distinct pre-defined candidate materials with known properties, select in each point throughout the reference domain either no material or one of the candidates so as to minimize the compliance under static loading subject to a resource constraint limiting the total mass of the structure. This constitutes a distributed 0-1 valued optimization problem. The admissible set \mathbf{E}_{ad} consists of a number of pre-defined materials with known properties that may vary pointwise throughout the reference domain. In some cases void is included as a choice to allow for the introduction of holes. Most often a resource constraint limits the mass of available material.

Maximizing the stiffness is equivalent to minimizing the compliance of the structure under a given load. The minimum compliance problem is stated in variational form in terms of the work done by the external forces to reach equilibrium.

$$\begin{array}{ll} \underset{\mathbf{u}, \mathbf{E}}{\text{minimize}} & W = \int_{\Omega} \mathbf{f}^T \mathbf{u} \, d\Omega + \int_S \mathbf{p}^T \mathbf{u} \, dS & \text{External work} \\ & & (2.14a) \end{array}$$

$$\begin{array}{ll} \text{subject to} & \delta U - \delta W = 0 & \text{Equilibrium} \\ & & (2.14b) \end{array}$$

$$\begin{array}{ll} \mathbf{E} \in \mathbf{E}_{ad} & \text{Parametrization constraints} \\ & (2.14c) \end{array}$$

Before describing the discretized formulation, we present an equivalent form of (2.14) in terms of the strain energy. This is used in Section 2.10.

If the external loads are independent of the displacements (dead loads) and if stresses are related linearly to strains, i.e. (2.2) and (2.9), then the external work equals twice the total strain energy (internal work), i.e. $W = 2U$, see e.g. Pedersen (1998). Thus (2.14) may be cast equivalently as

$$\begin{array}{ll} \underset{\mathbf{u}, \mathbf{E}}{\text{minimize}} & 2U = \int_{\Omega} \boldsymbol{\varepsilon}^T \mathbf{E} \boldsymbol{\varepsilon} \, d\Omega & \text{Total strain energy} \\ & & (2.15a) \end{array}$$

$$\begin{array}{ll} \text{subject to} & \delta U - \delta W = 0 & \text{Equilibrium} \\ & & (2.15b) \end{array}$$

$$\begin{array}{ll} \mathbf{E} \in \mathbf{E}_{ad} & \text{Parametrization constraints} \\ & (2.15c) \end{array}$$

Thereby minimizing the total strain energy stored in the structure at equilibrium is equivalent to minimizing the external work.

Note that the strain energy is related to the stress energy through the relations in (2.9) and hence the problem of minimizing the total strain energy U is equivalent to minimizing the total stress energy U^C .

To summarize, we may express the minimum compliance (maximum stiffness) problem either as minimizing the work done by the external forces, minimizing the total strain energy, or minimizing the total stress energy in the structure.

2.4 Design parametrization

The infinite dimensional continuous problem formulations presented above are hardly applicable in practice and we discretize the problem in terms of a spatial discretization of the *design field* as well as a spatial discretization of the *analysis field*. The analysis and the design field discretizations are not necessarily coincident though this is often the case. In this section we describe the set of admissible designs \mathbf{E}_{ad} for a spatially discretized design domain in terms of a parametrization of multi-material selection problems as well as simultaneous topology and multi-material selection problems. The discretization results in a finite dimensional approximation of the originally infinite dimensional admissible set. The parametrization presented is general and may be applied to a range of material distribution problems. However, the focus in this thesis is on plane problems and layered plate and shell structures. In particular the design problem of orienting orthotropic material optimally at distinct material directions is addressed.

Assume that a given fixed reference domain $\Omega \in \mathbb{R}^2$ or \mathbb{R}^3 is divided into a number of non-overlapping design subdomains (e.g. finite elements or layered finite elements) such that $\Omega = \Omega_1 \cup \Omega_2 \cup \dots \cup \Omega_{n^d}$, $\Omega_i \cap \Omega_j = \emptyset \forall i \neq j$. The definition of design subdomains may be chosen to coincide with the finite element analysis discretization as described in Section 2.5 but a design subdomain may also contain multiple finite elements in a so-called patch used for manufacturing reasons if it is not allowable to have material changes at the level of each finite element. A design subdomain may also be e.g. a single layer within a layered finite element, a layer covering multiple elements, a group of layers within a single element, a collection of elements for which the same material should be chosen etc.

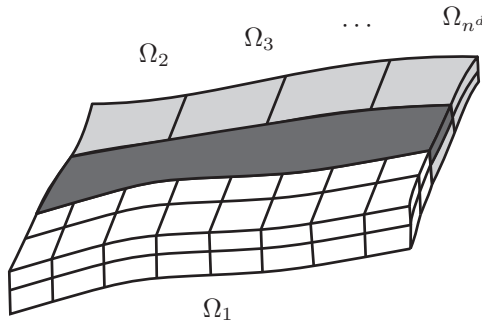


Figure 2.1: Example of discretization of the reference domain Ω into design subdomains Ω_j . Note that the subdomains may or may not coincide with the analysis discretization.

Within each design subdomain we want to select either no material or one from a set of possible candidates with known material properties. Inspired by solid-void topology optimization this design problem is parametrized using binary (0/1) design variables that determine the selection among the given candidates. Within each design subdomain a number of candidate materials is given and the selection among these is parametrized using a *binary* selection variable x_{ij} whose value determines the selection of a given material within the subdomain of interest

$$x_{ij} = \begin{cases} 1 & \text{if material } i \text{ is chosen in design subdomain } j \\ 0 & \text{if not} \end{cases} \quad (2.16)$$

To be physically meaningful this variable should only attain the values 0 or 1, i.e. $x_{ij} \in \{0, 1\}^n$ where the number of design variables n is described in the following.

The number of candidate materials may differ between the design subdomains, and thus the total number of design variables n is given as the sum of the number of candidate materials over all subdomains, $n = \sum_{j=1}^{n^d} n_j^c$. Typically, though, the number of candidate materials n^c is constant throughout the n^d subdomains and therefore the total number of design variables is simply given by $n = n^c \cdot n^d$.

2.4.1 Candidate materials

Any material with known material properties in terms of mass density ρ , elastic properties \mathbf{E} , etc. may serve as a candidate material. The elastic properties may be isotropic, orthotropic or arbitrarily anisotropic. In case of anisotropic or orthotropic candidate materials, discrete fiber angle optimization may be parametrized by candidate materials oriented along a number of distinct directions. Such parametrization of discrete fiber angle optimization is demonstrated in the papers.

Note that with the described parametrization, the design space is limited to physically available materials in contrast to e.g. Free Material Optimization (FMO) where the material tensor is varied freely over all imaginable material tensors without consideration of the physical existence of a material with these properties. Thus the design space of FMO is larger than that of DMO which is limited to existing or manufacturable materials. However, the two approaches complement each other in the sense that a DMO-like parametrization may be used to identify combinations of existing materials that approximate the optimal material tensor obtained from an FMO result as was demonstrated by Bodnár et al. (2008).

In the following sections we describe how the DMO parametrization may be applied to model different design problems. In Section 2.4.2 simultaneous topology and multi-material selection is presented as a generalization of the 0–1 solid-void topology optimization problem, and subsequently the multi-material design problem is presented in Section 2.4.3.

2.4.2 Simultaneous topology and multi-material optimization

The simultaneous topology and material selection problem considers the following question in every design subdomain: which material, if any, should be chosen given a number of possible candidates?

Previously, this problem has been parametrized by a number of variables that control the material selection and a separate topology variable scaling the contribution of all the other variables, see e.g. Sigmund and Torquato (1997); Gibiansky and Sigmund (2000). For instance with two candidate materials the effective material tensor would be parametrized as

$$\mathbf{E}(x) = x_{top} (\mathbf{E}_1 + x (\mathbf{E}_2 - \mathbf{E}_1)) \quad (2.17a)$$

$$= x_{top} ((1-x) \mathbf{E}_1 + x \mathbf{E}_2) \quad (2.17b)$$

$$0 < x_{min} \leq x_{top} \leq 1, \quad 0 \leq x \leq 1$$

where the variable x_{top} controls the topology and x controls the selection between the two materials. This parametrization implicitly ensures that there cannot be more than one material contributing fully at a time.

The generalization of the approach above to an arbitrary number of candidates is possible but cumbersome. Furthermore, in combination with intermediate density penalization the scheme is not invariant with respect to the ordering of the candidates, see Bendsøe and Sigmund (2003). Thus, with two equally good candidate materials, one is favored just by the (arbitrary) choice of the ordering. This is undesirable and calls for other approaches.

We propose to parametrize the simultaneous topology and material selection question as follows. Recall the parametrization (2.16). Naturally *at most one* material can be chosen in each design subdomain and thus within a subdomain we cannot allow two selection variables to be unity at the same time. Thus, in every subdomain we allow at most one material to be chosen, but we also allow *no material* to be chosen i.e. void. This condition is expressed for each design subdomain by the following linear *inequality* constraints

$$\sum_{i=1}^{n^e} x_{ij} \leq 1, \quad \forall j \quad (2.18)$$

Together with the parametrization (2.16) these constraints ensure at most one material to be chosen in each design subdomain. If any variable entering the sum attains one (i.e. the corresponding material is chosen) the remaining variables necessarily must be zero for the inequality to be satisfied. This constraint is also called a generalized upper bound constraint, analogously to the upper bound on the variables in solid-void topology optimization. Next, we change the inequality constraint to equality and study the consequences of doing so.

2.4.3 Multi-material optimization

Requiring *exactly* one material to be chosen in each subdomain (and hence not allowing holes) is imposed through a linear *equality* constraint

$$\sum_{i=1}^{n^c} x_{ij} = 1, \quad \forall j \quad (2.19)$$

Satisfying this constraint ensures that exactly one of the candidates $i = 1, 2, \dots, n^c$ is chosen and the remaining candidates are automatically not chosen within the subdomain in question.

2.4.4 Material parametrization

The effective material properties are parametrized using the binary material selection variables. The parametrization presented here is quite general in the sense that any material property of relevance for a given problem can be parametrized as we demonstrate for the mass density and the elasticity matrix.

The effective mass density for the j 'th subdomain, $\rho_j(x) \in \mathbb{R}$, is given by

$$\rho_j(x) = \rho_0 + \sum_{i=1}^{n^c} x_{ij} \Delta \rho_{ij}, \quad \forall j \quad (2.20)$$

where $\Delta \rho_{ij} = \rho_{ij} - \rho_0$. As explained above the 0'th phase typically is an ersatz material representing void. In case it is massless, the void mass density is of course zero and consequently $\Delta \rho_{ij} = \rho_{ij}$. The properties of the n^c materials with an associated selection variable are those of the candidate materials among which we want to choose.

If one variable attains 1 and Eqn. (2.18) or (2.19) is fulfilled, the effective mass density is that of the corresponding material. If all variables are 0 the effective properties are those of the 0'th phase, void. The effective mass density is used later in the constraint limiting the total mass of the structure.

The effective elasticity tensor from (2.2) is represented by a symmetric matrix $\mathbf{E}_j(x) \in \mathbb{R}^{6 \times 6}$

$$\mathbf{E}_j(x) = \mathbf{E}_0 + \sum_{i=1}^{n^c} x_{ij} \Delta \mathbf{E}_{ij}, \quad \forall j \quad (2.21)$$

where $\Delta \mathbf{E}_{ij} = \mathbf{E}_{ij} - \mathbf{E}_0 \in \mathbb{R}^{6 \times 6}$. Again phase 0 typically is given properties approximating those of void, and the properties of the remaining phases are those of the physical candidate materials.

With the proposed parametrization, multi-material selection problems, or simultaneous multi-material and topology problems may be formulated within the same parametrization with the only difference being if the sparse linear constraints are inequality constraints (2.18) or equality constraints (2.19).

2.5 Discretized problem formulation

The finite element method is used to discretize the analysis field and in this case the finite elements naturally also form a discretization of the design field where the material properties are element-wise constant.

In the following, “tilde” denotes approximated quantities. We use the finite element method to determine an approximate displacement field $\tilde{\mathbf{u}}$ as a function of the nodal degrees of freedom \mathbf{d} . The relation between $\tilde{\mathbf{u}}$ and \mathbf{d} is established through the chosen finite element interpolations also called the shape functions \mathbf{N} . Within each element these functions determine the interpolation of displacements from the nodes within each element, $\tilde{\mathbf{u}}_e = \mathbf{N}_e \mathbf{d}_e$, see e.g. Hughes (2000); Cook et al. (2001). The finite element form of the TPE (2.12) looks as follows

$$\tilde{\Pi} = \tilde{U} - \tilde{W} = \frac{1}{2} \mathbf{d}^T \mathbf{K} \mathbf{d} - \mathbf{r}^T \mathbf{d} \quad (2.22)$$

where $\mathbf{K} = \sum_{e=1}^{n^e} \int_{\Omega_e} \mathbf{B}_e^T \mathbf{E}_e \mathbf{B}_e d\Omega_e$ is the global stiffness matrix obtained as a summation over all n^e element stiffness matrices that depend on the element-wise constant constitutive properties \mathbf{E}_e and the strain-displacement relations $\mathbf{B}_e = \mathbf{L} \mathbf{N}_e$. \mathbf{r} is the vector of work-equivalent nodal forces, for details consult any standard textbook on the finite element method. In case of layered structures the material properties are not necessarily constant throughout the element but rather within each layer of the element. In this work this has been handled with layered shell elements using numerical or explicit integration of the material properties through the thickness. For multi-layered structures with many layers (say, more than four), explicit integration is faster compared to numerical integration through the thickness. These elements were developed and implemented in the Master’s thesis project Hansen and Hvejsel (2007).

The stationarity condition for the TPE applied to (2.22) yields a system of linear equations governing equilibrium for the finite element discretized continuum.

$$\delta \tilde{\Pi} = \frac{\partial \tilde{\Pi}}{\partial \mathbf{d}} = \mathbf{0} \Leftrightarrow \mathbf{K} \mathbf{d} - \mathbf{r} = \mathbf{0} \quad (2.23)$$

The variation and hence the partial differentiation is taken with respect to each non-prescribed degree of freedom in \mathbf{d} , i.e. the kinematically admissible variations.

With the reference domain discretized by finite elements it is natural to employ this discretization for the design field as well. Thus material properties are constant within each element and thereby the distributed infinite dimensional 0-1 problem is reduced to a finite dimensional 0-1 problem where the material properties $\mathbf{E}(\mathbf{x})$ and hence the stiffness matrix $\mathbf{K}(\mathbf{x})$ are parametrized in terms of the design

variables $\mathbf{x} \in \{0, 1\}^n$. Thereby the discretized form of (2.14) is

$$\begin{aligned} & \underset{\mathbf{x} \in \{0, 1\}^n, \mathbf{d} \in \mathbb{R}^d}{\text{minimize}} && \tilde{W} = \mathbf{r}^T \mathbf{d}(\mathbf{x}) && \text{External work} && (2.24a) \end{aligned}$$

$$\text{subject to } \mathbf{K}(\mathbf{x})\mathbf{d} - \mathbf{r} = \mathbf{0} \quad \text{Equilibrium} \quad (2.24b)$$

The equivalent problem formulation in terms of the strain energy given by (2.15) finite element form looks as

$$\begin{aligned} & \underset{\mathbf{x} \in \{0, 1\}^n, \mathbf{d} \in \mathbb{R}^d}{\text{minimize}} && 2\tilde{U} = \mathbf{d}(\mathbf{x})^T \mathbf{K}(\mathbf{x})\mathbf{d}(\mathbf{x}) && \text{Total strain energy} && (2.25a) \end{aligned}$$

$$\text{subject to } \mathbf{K}(\mathbf{x})\mathbf{d} - \mathbf{r} = \mathbf{0} \quad \text{Equilibrium} \quad (2.25b)$$

Recall, from (2.9) that with a linear constitutive law the strain energy is identical to the stress energy, $U = U^C$, and hence the problem of minimizing the total strain energy U is equivalent to minimizing the total stress energy U^C . These relations between the different energy measures are used later in the study of material interpolation schemes, Section 2.10.

2.6 Discretized binary design problem

In the following we formulate the binary design problem and present continuous relaxations used in the solution approaches proposed in this thesis.

The original problem is a non-convex mixed 0-1 (binary) problem; the design variables can physically only attain binary values as discussed in Section 2.4. The unknown optimal nodal displacements $\mathbf{d} \in \mathbb{R}^d$ are continuous and d is the number of free finite element degrees of freedom. Thus with the description of the admissible designs the design problem in (2.24) is the following.

$$\begin{aligned} & \underset{\mathbf{x} \in \{0, 1\}^n, \mathbf{d} \in \mathbb{R}^d}{\text{minimize}} && c(\mathbf{x}) = \mathbf{r}^T \mathbf{d} && (2.26a) \end{aligned}$$

$$\text{(P-SAND) subject to } \mathbf{K}(\mathbf{x})\mathbf{d} - \mathbf{r} = \mathbf{0} \quad (2.26b)$$

$$\sum_j \rho_j(\mathbf{x})\Omega_j \leq \overline{M} \quad (2.26c)$$

$$\sum_{i=1}^{n^c} x_{ij} = 1 \text{ or } \sum_{i=1}^{n^c} x_{ij} \leq 1, \quad \forall j \quad (2.26d)$$

$$x_{ij} \in \{0, 1\}, \quad \forall (i, j) \quad (2.26e)$$

Ω_j is the volume of the j 'th design subdomain and \overline{M} is a resource constraint limiting the total mass of the structure. $\mathbf{K}(\mathbf{x}) \in \mathbb{R}^{d \times d}$ is the design dependent global stiffness matrix which is affine in the design variables in the following manner

$$\mathbf{K}(\mathbf{x}) = \int_{\Omega} \mathbf{B}^T \mathbf{E}(\mathbf{x})\mathbf{B} \, d\Omega = \sum_{j=1}^{n^d} \int_{\Omega_j} \mathbf{B}_j^T \mathbf{E}_j(\mathbf{x})\mathbf{B}_j \, d\Omega_j \quad (2.27)$$

where $\mathbf{E}_j(\mathbf{x}) \in \mathbb{R}^{6 \times 6}$ is the effective constitutive matrix for domain j from (2.21) and $\mathbf{B} \in \mathbb{R}^{6 \times d}$ is the strain-displacement matrix. (P-SAND) is not convex (due to the bi-linear term in the equilibrium equations) and is on the form of a mixed 0-1 program which in general is hard to solve. One way to attack (P-SAND) is to use decomposition techniques such as Generalized Benders' Decomposition (GBD) as shown in Muñoz (2010) and applied in Paper B. Another possibility is to use nonlinear Branch-and-Bound methods as in Stolpe and Stegmann (2008).

The mass constraint is only relevant for multi-material problems where the candidate materials have different mass density i.e. in the case of pure fiber angle optimization the mass constraint is redundant.

A feasible solution satisfies all linear constraints and thus in every design sub-domain a material with non-vanishing stiffness is chosen and if the structure is sufficiently constrained against rigid body motion, the stiffness matrix is non-singular. If $\mathbf{K}(\mathbf{x})$ is non-singular, the nodal displacements can be eliminated by use of the equilibrium equations $\mathbf{d}(\mathbf{x}) = \mathbf{K}(\mathbf{x})^{-1}\mathbf{r}$ to obtain an equivalent optimization problem in the design variables \mathbf{x} only. Thus, the original non-convex 0-1 program is reformulated as a 0-1 program with a convex objective function in so-called nested form.

$$\underset{\mathbf{x} \in \{0,1\}^n}{\text{minimize}} \quad c(\mathbf{x}) = \mathbf{r}^T \mathbf{K}(\mathbf{x})^{-1} \mathbf{r} \quad (2.28a)$$

$$(P) \quad \text{subject to} \quad \sum_j \rho_j(\mathbf{x}) \Omega_j \leq \overline{M} \quad (2.28b)$$

$$\sum_{i=1}^{n^c} x_{ij} = 1 \text{ or } \sum_{i=1}^{n^c} x_{ij} \leq 1, \quad \forall j \quad (2.28c)$$

$$x_{ij} \in \{0, 1\}, \quad \forall (i, j) \quad (2.28d)$$

This binary problem is in general hard to solve but its continuous relaxation may be solved using standard continuous nonlinear programming algorithms. The solution to (P) is denoted by \mathbf{x}_P^* .

2.6.1 Continuous relaxation

If the binary constraints on the variables are relaxed, we obtain the continuous relaxation (R) whose feasible set is a superset of (P)'s feasible set.

$$\underset{\mathbf{x} \in \mathbb{R}^n}{\text{minimize}} \quad c(\mathbf{x}) = \mathbf{r}^T \mathbf{K}(\mathbf{x})^{-1} \mathbf{r} \quad (2.29a)$$

$$(R) \quad \text{subject to} \quad \sum_j \rho_j(\mathbf{x}) V_j \leq \overline{M} \quad (2.29b)$$

$$\sum_{i=1}^{n^c} x_{ij} = 1 \text{ or } \sum_{i=1}^{n^c} x_{ij} \leq 1, \quad \forall j \quad (2.29c)$$

$$0 \leq x_{ij}, \quad \forall (i, j) \quad (2.29d)$$

Note that the constraints (2.29c) in combination with (2.29d) ensure that the variables fulfill $x_{ij} \leq 1$ and hence there is no need for an upper bound on the variables.

Provided that the stiffness matrix is parametrized by (2.27) using (2.21) for the material interpolation, the compliance function in (R) is convex as shown by e.g. Svanberg (1994); Stolpe and Stegmann (2008), and with the feasible set given by linear constraints this constitutes a convex optimization problem, see e.g. Boyd and Vandenberg (2004), and thereby a local optimum \mathbf{x}_R^* is also a global optimum of (R). Furthermore the feasible set of (R) is a superset of the feasible set of (P). Thus the following properties hold:

1. The solution to (R) is better than or as good as the solution to (P), i.e. $c(\mathbf{x}_R^*) \leq c(\mathbf{x}_P^*)$.
2. If the solution to (R) happens to be binary then it is also a solution to (P).
3. If there is no feasible solution to (R) then there is no feasible solution to (P) either.

The first property is of interest since it gives a bound on the attainable performance and thereby makes it possible to assess the quality of any given binary design. This property is used in global optimization, see Muñoz (2010) and Paper B. Since all constraints are linear, feasibility of (R) is relatively easily detected by the algorithm.

In the continuous relaxation the design variables may be interpreted as volume fractions of each candidate material in the given domain. Thus the constraints originally formulated in binary form in (2.18) and (2.19) may be interpreted as constraints on the total volume fraction of material in each domain. Allowing intermediate volume fractions implies non-distinct material choices (i.e. mixtures) which are not feasible with respect to the originally binary problem. However, if the solution to the relaxed problem formulation attains discrete values after optimization, the result is meaningful and manufacturable.

In the following we discuss techniques for obtaining binary solutions by use of continuous problem formulations related to (R). All of the approaches studied here solve the convex continuous relaxation (R) as the first sub-problem within a sequence of sub-problems.

2.7 Solution techniques

Having formulated the optimization problem (P) and its continuous relaxation (R) we now turn our attention to solution techniques and algorithms to solve these problems.

As described in Section 2.6.1 the solution to (R) gives information that is used in the solution procedures applied to determine a binary solution. Hence we start by describing how (R) is solved followed by descriptions of the techniques for attacking (P).

2.7.1 Solving (R)

The continuous relaxation (R) is convex and hence it may be solved to optimality using any large-scale non-linear programming algorithm capable of handling a large number of variables and (sparse) linear constraints. In this study we use the sparse sequential quadratic programming (SQP) algorithm SNOPT Gill et al. (2005, 2008). This SQP implementation is considered to be mature and stable. It takes a general problem formulation where the nonlinear parts of constraints are distinguished from linear parts which are taken care of separately, and sparsity is exploited throughout.

The solution to (R) typically contains subdomains with a mixture of two or more candidate materials, in particular if the mass constraint is active. Thus, further steps are needed to obtain designs with no or only small amounts of intermediate-valued variables. Despite of the need for a discrete design, the continuous solution to (R) contains valuable information that can be used in the search for a discrete design. This is used in the heuristic procedure presented in Section 2.9.2.

2.8 Non-convex penalty constraint (Paper A)

One way to obtain a binary design using a continuous solution approach is to suppress intermediate designs through a constraint that explicitly addresses the “discreteness” of the variables. Based on the continuous relaxation (R), a related problem is formulated by adding a constraint that explicitly ensures binary feasibility. This approach is studied in Paper A where a non-convex quadratic constraint is used to gradually reduce the continuous design space to the binary feasible set of (P). Explicit constraints to suppress intermediate densities were also studied by Borrvall and Petersson (2001*a,b*) who used explicit constraints of regularized (filtered) intermediate densities to obtain distinct designs to solid-void topology optimization problems. We use a similar approach to suppress intermediate densities but we do not use any regularization. The following concave quadratic constraint suppresses intermediate valued variables

$$g(x) = \sum_{i,j} x_{ij} (1 - x_{ij}) \leq \varepsilon, \quad 0 \leq \varepsilon \ll 1 \quad (2.30)$$

A sequence of problems is solved starting out by solving the convex problem (R) and then use the solution to this problem as a starting guess for a sequence of non-convex problems. The non-convex problems are obtained by augmenting (R) with the quadratic constraint (2.30). The parameter ε is a small number used to relax/tighten the constraint gradually. The constraint can be made inactive by

selecting ε sufficiently large at the initial design. By reducing ε to zero the design is constrained to be integer feasible. Different continuation strategies for ε are studied and the influence on the results is examined through numerical examples as shown in Paper A. As for the convex relaxation (R), SNOPT is used to solve the non-convex relaxations. The method does not guarantee convergence to the global optimal solution but it implicitly provides a lower bound from the solution to (R) and therefore it is possible to assess the worst case gap between the obtained design and the global optimum.

2.9 Global optimization (Paper B)

Global optimization techniques are concerned with determining the best solution(s) to an optimization problem and certifying it's quality. Compared to finding designs fulfilling only local optimality conditions, global optimization is considerably harder and consequently, everything else being equal, the problems that can be solved to global optimality are often significantly smaller.

In the following it is shown how the solution to the continuous relaxation can guide and accelerate the search process for a global optimum of the integer problem using the Generalized Benders' Decomposition technique, see Geoffrion (1972). GBD applied to structural optimization problems was studied in detail by Muñoz (2010) where the theoretical background for this technique is given.

The results summarized in this section (and presented fully in Paper B) are a joint effort between Eduardo Muñoz and the author of this thesis.

2.9.1 Generalized Benders' Decomposition

The problem (P-SAND) is a non-convex mixed 0-1 nonlinear program with continuous variables for the displacements and 0-1 valued design variables. Generalized Benders' Decomposition (GBD) is a technique to attack hard optimization problems having special structure in the variables. Under certain assumptions the method guarantees convergence to a global optimum and hence it is a deterministic exact global optimization method as opposed to indeterministic and heuristic approaches.

With the GBD method the solution to the original problem is approached iteratively through solution of a sequence of simpler problems; the so-called (relaxed) master problems and sub problems, respectively. The sub problems are linear programs in the displacements \mathbf{d} and the relaxed master problems are integer linear programs in the 0-1 valued design variables \mathbf{x} .

The main effort in the GBD algorithm lies in solving the relaxed master problems. The solutions to the master problems are binary designs fulfilling the condition that they are better than or at least as good as the previously obtained designs. With each new solution obtained a new constraint is added to the following master

problems. The constraints are also called cuts; they cut away regions of the feasible set within which the optimal solution is to be located. With good cuts the region to search for the optimal solution is limited and hence the solution is likely to be obtained sooner. The quality of the cuts may be assessed based on the notion of Pareto dominance. According to this concept cuts coming from designs with a lower objective function value are better than cuts coming from designs with a higher objective function. Even cuts coming from continuous relaxations can be used and hence the cut generated from the optimal solution to the continuous relaxation is *the best* cut that can be included. The inclusion of this special cut was shown to have a significant impact on the solution process for truss topology optimization problems, Muñoz (2010), and was also used with success for multi-material optimization in Paper B.

2.9.2 Heuristics

Heuristics employ experience-based knowledge to solve hard problems in a reasonable amount of time. They can be considered as educated guesswork in the sense that they do not provide guarantees of the quality of the obtained design but typically the designs are reasonably good. Used in combination with exact global optimization procedures, heuristics can assist the exact procedure in converging faster to a proven global optimum. In this section we describe one such heuristic that combines a relaxation based neighborhood search heuristic that can speed up the convergence of the GBD algorithm without sacrificing the guarantee for global optimality of GBB. Actually, the procedures studied in Paper A and C are also heuristic solution procedures in the sense that they do not guarantee to locate global optima. However, they may also be used as heuristic techniques speeding up an exact procedure. Popularly speaking the quality of a heuristic lies in its ability to generate good solutions, since this typically will improve the exact solver the most. However, to assess whether a given solution is in fact a global optimum, an exact procedure is needed. This is one of the motivations for employing exact solvers.

In Muñoz (2010) it was found that the convergence rate of the GBD algorithm may be improved if a “good” 0-1 design and/or a tight lower bound estimate is obtained early in the iterative process. By “good” we mean a design that has an objective function close to that of the optimal solution. Whether the good design is obtained within the sequence of relaxed GBD master problems or by some external procedure does not matter since the GBD algorithm converges to a global optimum. Thus it is of interest to have heuristic procedures that generate good but not necessarily optimal designs at relatively low or at least controlled computational cost.

The GBD-RENS heuristic studied in Paper B is inspired by the so-called Relaxation Enforced Neighborhood Search (RENS) proposed for mixed-integer linear programs by Berthold (2007). The idea is to generate a good integer design by rounding the solution to the continuous relaxation. The rounding problem is for-

mulated as a binary problem in the non-integral valued variables of the continuous solution. Furthermore, the solution to the relaxation provides a lower bound that may be used as a valid lower bound within the GBD procedure as described in the previous section.

If a continuous solution contains a number of subdomains within which a distinct selection could be made, these domains are also *likely* to have the same value in the optimal discrete solution. This statement contains no guarantees and it only manifests a hope. To motivate it recall that if the continuous solution happens to be completely binary-valued (i.e. no domain containing mixture) it is in fact the global binary solution.

This reasoning is the motivation for a heuristic procedure that may be formulated as follows: *take the continuous solution to (R) , fix the variables that are binary-valued and solve a sub-problem in the remaining variables to obtain a binary design for them.* This idea is the basis of the heuristic procedure proposed in Paper B where the heuristic procedure is described in detail and shown to accelerate the convergence behavior of the GBD procedure.

2.10 Material interpolation schemes (Paper C)

Approximating the 0-1 topology problem using material interpolation schemes is probably the most popular technique to solve large-scale topology optimization problems. For practical problems the number of design variables easily exceeds hundreds of thousands and this prohibits the use of exhaustive search or combinatorial techniques applied directly to the original 0-1 problem. This is one of the main reasons for the use of gradient-based algorithms in the search for local optima.

Having introduced the parametrization of the stiffness and the mass, one can attack the continuous relaxation directly and obtain useful knowledge from it's solution as described in Section 2.6.1 and 2.9. However, the solution to the convex relaxed problem is rarely binary feasible and hence it is not a feasible solution to the original optimization problem.

Material interpolation schemes allow intermediate material choices during the solution process and through penalization of intermediate choices the solution is "encouraged" to converge towards distinct choices honoring the original binary requirement on the selection variables (2.16). It is often argued that the popular material interpolation schemes violate rigorous bounds on the attainable properties of material mixtures for certain parameter intervals, see the discussion in Bendsøe and Sigmund (1999). In the present work the use of interpolations is regarded as a method that is viable as long as the final solution honors the binary condition (for which there is no ambiguity regarding the effective properties). The existence of intermediate solutions should be considered as a computational tech-

nique that allows for the use of gradient-based optimizers enabling the solution of large-scale problems not tractable by combinatorial or exact methods. The choice of interpolation scheme is not unique and in the following a number of schemes with different properties are described.

2.10.1 Voigt interpolation

The so-called Voigt interpolation is the simplest possible interpolation scheme given by the volume fraction weighted arithmetic average of the constituent stiffnesses

$$\mathbf{E}_j(x) = \mathbf{E}_0 + \sum_{i=1}^{n^c} x_{ij} \Delta \mathbf{E}_{ij}, \quad \forall j \quad (2.31)$$

This stiffness is obtained for a heterogeneous medium if all phases are subjected to the same uniform strain Voigt (1910). It is not physically possible in a heterogeneous composite material to expose all phases to exactly the same strain state since the stresses at phase boundaries would not be in equilibrium, Hill (1963). Thus, the stiffness given by the Voigt estimate/interpolation is an upper bound on the attainable stiffness of a heterogeneous composite .

2.10.2 Multiphase ‘‘SIMP’’

SIMP is an abbreviation for ‘‘Solid Isotropic Material with Penalization’’. We use quotation marks here since the effective material properties in our approach are not necessarily isotropic, for instance when interpolating between anisotropic materials. The scheme is a direct generalization of the original scheme proposed for interpolation between void and solid. We take the discrete parametrization from (2.21) and raise the, now relaxed, design variable to a power $p \geq 1$. We keep the generalized upper bound constraints and obtain the following interpolation scheme for the full constitutive matrix

$$\mathbf{E}_j^S(x) = \mathbf{E}_0 + \sum_{i=1}^{n^c} \underbrace{x_{ij}^p}_{w_{ij}} \Delta \mathbf{E}_{ij}, \quad p \geq 1, \quad \forall j \quad (2.32)$$

For $p = 1$ the sum of the weights controlling the contribution from each stiffness phase add to unity if the design variables do. For $p > 1$ intermediate material selections are unfavorable since the total stiffness contribution is reduced in the sense that the weights do not sum to unity for intermediate choices, even if the design variables do. Thus intermediate choices intrinsically are penalized, see also the discussion below in Section 2.10.4.

Note that for $n^c = 1$, the generalized scheme (2.32) reduces to the well-known two-phase SIMP scheme. For this particular case, however, only the generalized upper bound inequality (2.18) is relevant while requiring (2.19) would lead to a trivial problem.

2.10.3 Multiphase RAMP

In Stolpe and Svanberg (2001) the so-called RAMP scheme was proposed as an alternative interpolation scheme for two-phase topology optimization. RAMP stands for “Rational Artificial Material with Penalization” and the idea of the scheme is that for isotropic two-phase interpolation a certain value of the penalization parameter yields a *concave* objective function increasing the probability of locating an optimum at the boundary of the feasible domain meaning a distinct design. We propose a generalization to multiple materials similar to the SIMP generalization (2.32).

The interpolation scheme for the constitutive matrix is given by

$$\mathbf{E}_j^R(x) = \mathbf{E}_0 + \sum_{i=1}^{n^c} \frac{x_{ij}}{1 + q(1 - x_{ij})} \Delta \mathbf{E}_{ij}, \quad q \geq 0, \quad \forall j \quad (2.33)$$

The effect of the penalization parameter q is analogous to that of p in the SIMP scheme; it makes intermediate selections unfavorable by reducing the net material contribution in the stiffness interpolation.

2.10.4 Penalizing effect

For both schemes presented above the penalizing effect of intermediate densities fulfilling Equation (2.18) or (2.19) comes from the fact that the sum of the penalized weights is less than unity. In Figure 2.2 we show the sum of the penalized weights for $n^c = 2$ for a range of penalization parameters for both schemes. We use $x_1 + x_2 = 1$ to eliminate x_2 and plot the sum of the penalized stiffness weights, e.g. for the SIMP weights we have $w_1 + w_2 = x_1^p + x_2^p = x_1^p + (1 - x_1)^p$.

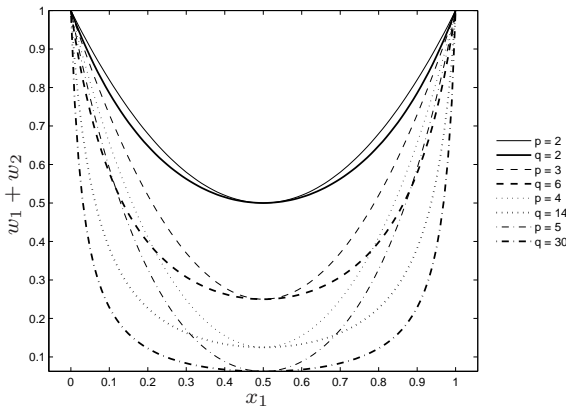


Figure 2.2: Sum of penalized stiffness weights for $n^c = 2$ for the SIMP and the RAMP interpolation scheme for different penalization parameters.

2.10.5 Illustrative example

The following example demonstrates properties of the material interpolation schemes proposed in this work and illustrates the effect of penalization. We investigate the influence of the penalization in combination with the applied loading and candidate materials on the likelihood of obtaining a distinct material selection.

Usually for solid-void topology optimization the ability of the SIMP (and RAMP) scheme to obtain 0/1 solutions is attributed to its reduced stiffness relative to the full contribution in the mass/volume constraint at intermediate densities. However, the situation is quite different if we are to select between candidate materials with the same mass density but different directional properties, i.e. anisotropic or orthotropic materials.

The following example is constructed so as to remove the influence of the mass constraint; both materials have the same mass density and thus the mass constraint plays no role. The two candidate materials are instances of the same orthotropic material but are oriented differently. The idea is to study the optimal material selection for different stress states for which we a priori know the solution in terms of an optimal distinct material choice and observe which solution the proposed interpolation schemes would lead to.

Consider a bi-axial plane stress state as shown in Figure 2.3. Different characteristic stress states are obtained by varying the principal stress ratio; $-1 \leq \frac{\sigma_{II}}{\sigma_I} \leq 1$. The design problem that we address is that of choosing between two distinct orientations of an orthotropic material. This problem we regard as a material selection problem with two candidate materials where each material orientation represents a distinct candidate material. The first candidate material that we consider is an orthotropic material with its principal material direction coincident with the first principal stress direction (i.e. $\theta = 0^\circ$) and the second candidate material has the principal material direction coincident with the second principal stress direction ($\theta = 90^\circ$). As described in Section 2.2.1 the compliance of the structure is directly

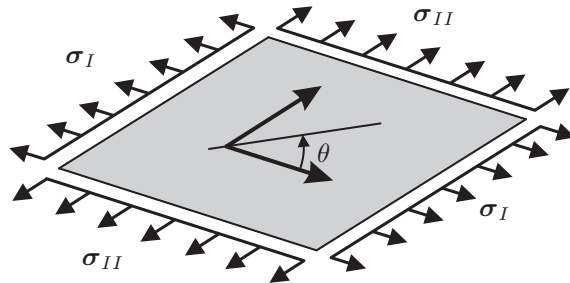


Figure 2.3: Bi-axial stress states with coordinate system.

linked to the pointwise stress energy density. Recall the stress energy density from

$$(2.7) \quad \bar{U}^C = \frac{1}{2} \boldsymbol{\sigma}^T C(x) \boldsymbol{\sigma} = \frac{1}{2} \boldsymbol{\sigma}^T E^{-1}(x) \boldsymbol{\sigma} \quad (2.34)$$

Multi-material parametrizations

Now, for a given stress state $\boldsymbol{\sigma}$ and two candidate materials we explore the design space for different interpolations. We want to investigate the interpolation scheme in terms of its behaviour when selecting between two materials and thus we eliminate the topology question by requiring Equation (2.19) to hold. This makes it possible to eliminate one variable whereby the problem is parametrized in x_1 only. Thus, $x_1 = 1$ means that the orthotropic material oriented at $\theta = 0^\circ$ is chosen and for $x_1 = 0$ the same material at $\theta = 90^\circ$ is chosen.

Using the simplifications described above the generalized SIMP scheme in Equation (2.32) reduces to

$$\mathbf{E}(x) = x_1^p \mathbf{E}_{0^\circ} + (1 - x_1)^p \mathbf{E}_{90^\circ} \quad (2.35)$$

For $p > 1$ the sum of the weighting of the individual phases is less than or equal to one, $w_1 + w_2 \leq 1$ for $0 < x_1 < 1$. Thereby mixtures are penalized in the sense that the amount of stiffness contributing material effectively is reduced. In Figure 2.4 the resulting stress energy density is shown for different principal stress ratios and different values of the penalization parameter p . From the figure we observe a number of properties for this scheme

- For a distinct material selection, i.e. $x_1 = 0.0$ or $x_1 = 1.0$ the scheme yields the same objective function value, regardless of the value of p .
- For $p = 1.0$ the compliance is *convex* in x_1 . For all loads except the uni-directional load ($\frac{\sigma_{II}}{\sigma_I} = 0.0$), the optimum is a mixture.
- For large p the compliance level generally is higher for mixtures. This is due to the fact that the weights on the phases do not sum to unity meaning that intermediate choices also encompass choosing less material in total.
- For $p > 1$ the compliance is non-convex with several local minima and hence a non-binary point may be a local optimum.
- The scheme is indifferent with respect to ordering of the phases, i.e. the ordering does not bias the tendency to select any of the phases over the other.

Similarly for the RAMP scheme (2.33) using the equality selection constraint (2.19) the interpolation reduces to

$$\mathbf{E}(x) = \frac{x_1}{1 + q(1 - x_1)} \mathbf{E}_{0^\circ} + \frac{1 - x_1}{1 + qx_1} \mathbf{E}_{90^\circ} \quad (2.36)$$

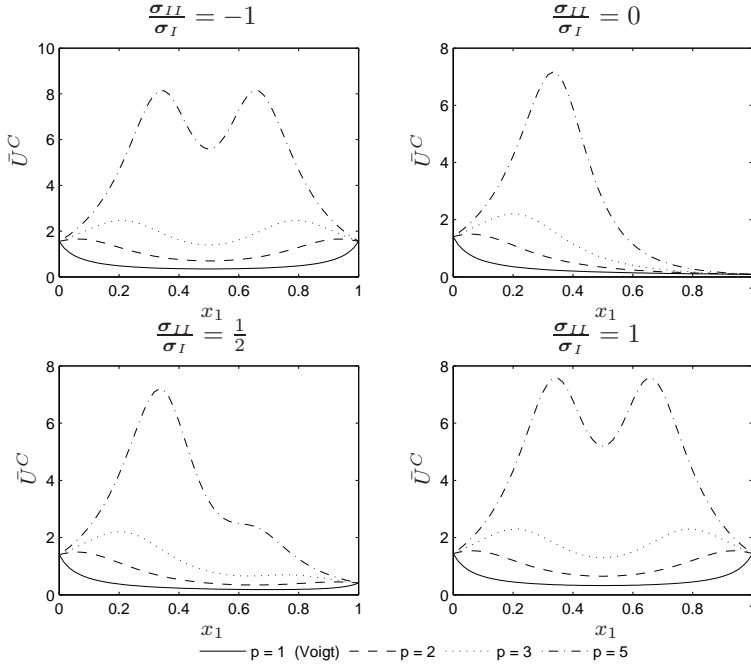


Figure 2.4: Stress energy density for different fixed bi-axial stress states obtained using the SIMP interpolation (2.35).

where $q \geq 0$ is the penalization parameter used to make intermediate choices unfavorable. The observations made for the SIMP scheme carry over to the RAMP scheme. Actually, for $q = 0$ the RAMP scheme is identical to the SIMP scheme for $p = 1$. The overall shapes of the curves are similar except for some minor differences in slope and curvature near 0 and 1 where the RAMP scheme in general is steeper. Note that the curves shown take into account the sum to unity constraint eliminating x_2 , and thereby the slope of the curves rather represent the reduced gradient than the pure derivative wrt. x_1 . Therefore the expected vanishing slope of the SIMP scheme is not observed at $x_1 = 0$.

2.10.6 Other ideas

In the previous section it was demonstrated how the penalization discourages intermediate density solutions by reducing the net amount of material for intermediate choices. An other material interpolation scheme which works in a different manner is the so-called the Voigt-Reuss scheme, see Swan and Arora (1997); Swan and Kosaka (1997*a,b*). This scheme is a hybrid of the Voigt and the Reuss mixture schemes, respectively. The Voigt scheme presented previously in Section 2.10.1 obtains the effective material properties for a mixture of phases exposed

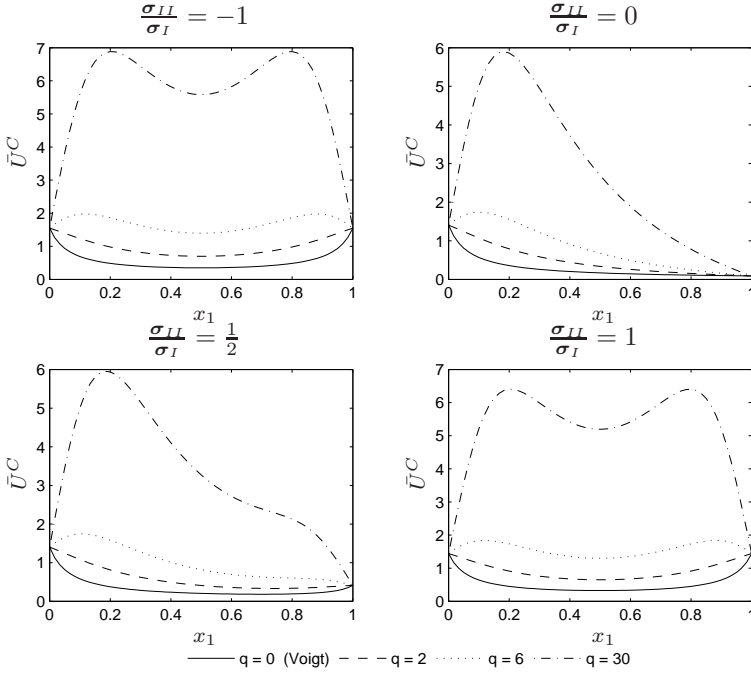


Figure 2.5: Stress energy density for different fixed bi-axial stress states obtained using the RAMP interpolation (2.36).

to the same state of strain whereas its counterpart, the Reuss scheme, obtains the effective properties for a mixture of phases exposed to the same state of stress. One could also envision these two mixture rules embodied as springs coupled in series (Voigt) versus springs coupled in parallel (Reuss). This idea was proposed in the above mentioned publications where gradual penalization was introduced through continuation shifting the interpolation from the Voigt scheme to the Reuss scheme. Looking at Figure 2.4 and 2.5, respectively, the Reuss interpolation would generate a straight line connecting the value of the stress energy density at $x_1 = 0$ to the corresponding value at $x_1 = 1$. This indicates that the Reuss interpolation forms a *concave* stress energy density function. Doing some algebraic manipulations, one can show that the two-phase RAMP scheme, see Stolpe and Svanberg (2001), is identical to the Reuss interpolation scheme exactly for the parameter setting for which the RAMP scheme becomes concave. This fact combined with the statement in Bendsøe and Sigmund (2003, p.63) to look for concave interpolations, gave hope to the Voigt-Reuss approach. However, despite of numerous attempts to get this procedure to work, it was abandoned at some point due to numerical difficulties. The approach was tested in combination with SNOPT which is an implementation of the Sequential Quadratic Programming algorithm with a limited memory quasi-Newton approximation to the Hessian of the Lagrangian. In the Hessian

approximation procedure a check for positive curvature is implemented to ensure a positive-definite approximate Hessian. However, a positive Hessian approximation for a concave function is impossible per se. In other words, the algorithm intrinsically “fights against” the nature of the problem and this combination of algorithm and problem formulation did not match. Experience with the algorithm showed that with the Reuss interpolation, the convergence of the SQP algorithm slowed down to make almost no progress. It may be that a Sequential Linear Programming algorithm as used in the original papers is better suited for the Voigt-Reuss interpolation scheme though this was never tested within the present work.

2.11 Existence of solutions

Similar to solid-void topology optimization, the continuum form of the multi-material optimization problem shown in (2.15) is ill-posed and lacks existence of solutions. The discretized finite-dimensional problem *has* existence of solutions. However, the solution to the discretized problems is mesh-dependent.

To obtain a well-posed problem regularization is needed. It is beyond the scope of this work to give a complete description of techniques available to reduce mesh dependency of topology optimization problems, but a few comments and thoughts are worthwhile. We give a brief description of these problems in the setting of topology optimization and extend some of the ideas and concepts to multi-material optimization problems.

It is well-known from topology optimization that the infinite dimensional 0-1 (void-solid) minimum compliance problem lacks existence of solutions, see e.g. Lurie (1993); Strang and Kohn (1986); Kohn and Strang (1986*a,b,c*). Mathematically the problem is ill-posed and lacks existence of solutions. The mechanical explanation is that the introduction of more holes leading to microstructure gives a better structural efficiency (higher stiffness) without affecting the resource constraint. Macroscopically such fine scale regions appear as “grey” with macroscopically anisotropic properties which to some extent explains why grey solutions and composites are good from an optimal point of view. The study of such optimal micro structure is done extensively in the so-called “microstructure” or “homogenization” approach, see Eschenauer and Olhoff (2001); Bendsøe and Sigmund (2003) for references to this branch of optimal design. Allowing grey in the solution space amounts to accepting infinitesimally small features in the solution which is typically not wanted from a practical point of view. The finite-dimensional discretized problem with element-wise constant density *has* existence of solutions itself. However, refining the mesh by increasing the number of elements and thereby the number of design domains leads to qualitatively different structures with finer structural details which was first observed and addressed in optimal plate design, see Cheng and Olhoff (1981, 1982). This is unwanted since the solution thereby inherently depends on the (more or less arbitrarily chosen) mesh and furthermore

the occurrence of fine scale features is often unwanted for manufacturing reasons. The point of refining the mesh was to improve the analysis field but not necessarily to change the design field. From an engineering point of view we are interested in having a minimum length scale of variation in the solution, i.e. to prevent small scale features and variations in the solution. To counter these issues the problem needs to be regularized and a number of techniques exist for this, for further explanations see Sigmund and Petersson (1998), and Sigmund (2007) for a recent review.

A mesh-independent length scale may be obtained using filtering techniques such as the so-called sensitivity filter proposed by Sigmund (1994). Here the original sensitivity field is smoothed heuristically. As pointed out by Sigmund (2007) this heuristic technique does not work with line-search based optimizers such as SNOPT that require consistent sensitivities, see Gill et al. (2008). Thus, this type of filter is currently not applicable for multi-material optimization using the solution approaches described in this thesis. An other possibility that gives consistent sensitivities would be to filter the material densities as shown by Bourdin (2001); Bruns and Tortorelli (2001). An immediate question that comes up for filtering techniques used with multiple phases is how to filter the densities. One idea could be to evaluate each material density as an average of the surrounding corresponding material densities. In combination with penalization this should control the minimum size features of each phase.

The issues touched upon in this section are relevant and important theoretically as well as practically but have not been addressed in this thesis. The challenge is to generalize the concepts developed for two-phase topology optimization to multi-material problems. It is our belief that the solution to some of these problems will be an important step towards making multi-material optimization a mature technology.

Summary and concluding remarks

This chapter summarizes the main results of the three papers accompanying this thesis, the relationship among them and gives an assessment of the significance and impact of the results and points to future directions of research.

3.1 Summary of results

The papers address the minimum compliance discrete material selection problem as formulated in (2.28) using continuous relaxations in the solution process enabling the use of gradient-based optimization algorithms in the search for binary solutions. The results presented in this thesis have shown how the multi-material optimization problem can be formulated and solved very similar to traditional void-solid topology optimization using continuous variables that eventually obtain binary values approximating the originally binary problem. This is obtained using material interpolation schemes and explicit constraints that address the tendency towards intermediate-valued designs if not penalized or constrained. Furthermore it is shown how continuous solutions obtained using a gradient based optimizer can assist and accelerate a Generalized Benders' Decomposition algorithm in obtaining solutions to problems not tractable otherwise.

Paper A: Discrete Multi-material Stiffness Optimization for Multiple Load Cases

In this paper we attacked the discrete material selection problem by solving a sequence of non-convex continuous relaxations with a quadratic constraint that explicitly prevents intermediate density solutions. A lower bound on the attainable performance is obtained by solving a continuous convex relaxation and this solution is used as a starting guess for the non-convex problems. It is found that the best binary solutions are found if all intermediate non-convex problems are solved to (local) optimality with a tight tolerance. An alternative strategy with looser convergence tolerances in the intermediate problems is found to be a good compromise between computational cost and the quality of the obtained solutions. Problems with a small amount of mixture in the relaxed solution are found to be

easier to get to converge to a distinct solution compared to problems with many domains with mixture.

Paper B: Discrete Multi-material Optimization: Combining Discrete and Continuous Approaches for Global Optimization

This paper presents a heuristic approach to improve the numerical performance of the Generalized Benders' Decomposition algorithm for global optimal design of laminated composite structures. The main idea of the paper is to use the solution of a continuous relaxation to formulate a reduced size sub-problem corresponding to the original full MINLP with a large number of variables fixed at the value obtained in the continuous solution. The solution to the reduced sub-problem is often close to the global optimal solution and thereby it may be used to improve the convergence rate of the overall GBD algorithm. The approach is tested on a set of numerical examples, and problems with up to 23.000 variables are solved to global optimality. It is found that the heuristic improves the convergence rate of overall GBD algorithm significantly.

Paper C: Material Interpolation Schemes for Unified Topology and Multi-material Optimization

In this paper we propose material interpolation schemes as direct generalizations of the well-known two-phase SIMP and RAMP scheme, respectively. The schemes provide generally applicable interpolation schemes between an arbitrary number of pre-defined materials with given (anisotropic) properties and favors distinct choices by implicitly penalizing intermediate choices. The method relies on a large number of sparse linear constraints to enforce the selection of at most one material in each design subdomain. The proposed schemes can parametrize multi-material optimization as well as simultaneous topology and multi-material optimization within a unified parametrization. The penalizing effect of the interpolation schemes is analyzed and attributed to the fact that the penalized weights controlling the stiffness contribution do not sum to unity for intermediate selections. Thereby the net stiffness of a mixture of two equally good materials is worse than that of either phase alone and thus the mixture is unfavorable compared to a distinct choice.

3.2 Contributions and impact

The number of design variables in multi-material optimization problems of practical interest is very high and often it is beyond the size of what global optimization techniques can handle. Therefore continuous relaxations that can be solved using gradient-based algorithms are important. For the minimum compliance problem addressed in this work, the continuous relaxation is convex and therefore its solution forms a rigorous lower bound on the attainable performance of any binary

solution. Thus, given any binary feasible solution we are able to assess its quality which was done for the solutions presented in Paper A. This property was further used in Paper B where the convex relaxation solution was used to obtain a rigorous lower bound, and as the basis for a large neighborhood search heuristic in the non-binary valued variables. This heuristic turned out to improve the capabilities of the Generalized Benders' Decomposition technique significantly for optimal design of laminated composite structures. To the authors' knowledge, the use of the RENS heuristic for MINLP's is novel, the idea is generally applicable and may very well be useful for other mixed-binary problems where a continuous relaxation can be solved at relatively low cost. The improvement of GBD obtained using this single heuristic indicates that other heuristic techniques may also improve the convergence rate of the algorithm.

Paper C proposes generalizations of the SIMP and RAMP material interpolation schemes to any number of phases, including topology optimization, within a unified parametrization which is novel. The idea is demonstrated on the minimum compliance problem, but the material parametrization is completely general and enables multi-material optimization for all types of problems where two-phase topology optimization has proven successful.

3.3 Future research

The examples addressed in this thesis mainly focus on laminated plate-like structures though the design parametrization is completely general and may as well be applied to solid domains as well. This could be of interest with other physics as seen in two-phase topology optimization.

The generalization to multiple phases also opens up for adapting filtering techniques originally developed for topology optimization, to multi-material optimization. The use of filters could also be a way to include manufacturing constraints in multi-material optimization, see e.g. Guest (2009). A recent idea for a manufacturing aware parametrization of the topology design problem was put forward by Gersborg and Andreasen (2011). Such approaches might be adapted to multi-material and laminate design as well. Combining unified topology and multi-material design with manufacturing constraints allowing only outer layers to be removed opens for the possibility to design also the number of layers in the laminate.

Another issue with the multi-material optimization approach is the large number of design variables which is not a problem as long as the number of criteria functions in the optimization problem is low. With an increasing number of criteria functions e.g. with stress constraints, the resulting problem quickly grows beyond what can be solved with currently available optimization algorithms. It is clear that this challenge requires alternative parametrizations or techniques such as constraint aggregation proposed by e.g. Yang and Chen (1996); Duysinx and Sigmund (1998);

Poon and Martins (2007); París et al. (2010) or penalty approaches as shown by Kočvara and Stingl (2009) for the stress constrained FMO problem.

The heuristics based improvements of the Generalized Benders' Algorithm may be developed even further. In this work we only investigated a relaxation based search heuristic whose computational cost may be high in itself. Other heuristic techniques with a lower or controlled computational could be employed as well.

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Paper A

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Optimization strategies for discrete multi-material stiffness optimization

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Abstract Design of composite laminated lay-ups are formulated as discrete multi-material selection problems. The design problem can be modeled as a non-convex mixed-integer optimization problem. Such problems are in general only solvable to global optimality for small to moderate sized problems. To attack larger problem instances we formulate convex and non-convex continuous relaxations which can be solved using gradient based optimization algorithms. The convex relaxation yields a lower bound on the attainable performance. The optimal solution to the convex relaxation is used as a starting guess in a continuation approach where the convex relaxation is changed to a non-convex relaxation by introduction of a quadratic penalty constraint whereby intermediate-valued designs are prevented. The minimum compliance, mass constrained multiple load case problem is formulated and solved for a number of examples which numerically confirm the sought properties of the new scheme in terms of convergence to a discrete solution.

Keywords laminated composite materials · optimal design · sensitivity analysis · solution strategies · integer optimization

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1 Introduction

Optimal design of high performance and cost-effective laminated composite structures is a complex design problem due to the large number of different materials employed along with conflicting requirements such as low weight and cost while maintaining sufficient stiffness and strength. For these requirements composite materials are advantageous compared to isotropic metals because of their superior specific properties (strength- and stiffness-to-weight ratio) and the possibility to tailor the structural response by utilizing the directional properties. Optimal orientation of orthotropic material has been dealt with by e.g. Sun and Hansen (1988); Pedersen (1989, 1991); Thomsen and Olhoff (1990); Mateus et al (1991); Fukunaga and Vanderplaats (1991); Setoodeh et al (2004), and for further references see also the review paper by Abrate (1994) and the textbook by Gürdal et al (1999).

To design a laminated composite structure it is necessary to specify material, thickness and orientation in each layer of the laminate. Doing so, the directionality of the individual layers may be used beneficially so as to obtain the desired response of the laminated structure. Thus, the number of design variables tends to be large in laminate design problems. In this paper we address the laminate layup design problem of choosing among multiple non-vanishing materials (CFRP¹, GFRP², polymeric foam, balsa wood, etc.) potentially oriented in different predefined discrete directions. We assume that the layer thicknesses as well as the total laminate thickness are given and fixed a priori. Thus we solve a material distribution problem on a fixed spatial domain and discretization. The authors acknowledge the importance of including stress constraints in the design problem as in e.g. Schmit and Farshi (1973); Duysinx and Bendsøe (1998);

¹ Carbon fiber reinforced polymer

² Glass fiber reinforced polymer

Bruyneel and Duysinx (2006) but in this work such constraints have not been included for a number of reasons. The inclusion of strength constraints poses several theoretical as well as computational challenges that have to be overcome before such constraints can be included in practical multi-material optimization problems with many design variables. One step on the way is to have a continuous method that yields integer solutions eventually which is one of the contributions of the present paper. The design problem is stated as; *given a fixed domain in space and number of pre-defined candidate materials, select the distinct material in each design subdomain that minimizes an objective function subject to physical and resource constraints*. This statement we regard as a discrete material distribution problem; either a material is selected or not in a given point in the design domain. The problem we address is a generalization of the 0-1 (void-solid) topology optimization problem and thus encompasses this problem as a special case with void being one of the “materials”. As such, the multi-material design problem also lacks existence of solution in its continuum infinite dimensional form, as known for the solid-void topology optimization problem, Lurie (1980); Kohn and Strang (1982, 1986); Cherkaev (1994). The implication of this is that in a finite element discretized problem, the solution is mesh dependent in the sense that finer meshes lead to finer details in the solution, and potentially also to qualitatively different structures. This is unwanted and to counter this issue, a number of different techniques exist. To obtain a well-posed problem one can introduce microstructure (or composites) to the solution space or restrict fine scale features from occurring in the design. The present work does not introduce microstructure nor composites to the design space but rather we give the possibility of selecting a pre-defined existing composite material throughout pre-defined fixed spatial design subdomains. Thus, the present work does not introduce composites as a means for relaxing the design problem or interpreting “grey” intermediate valued design variables. In the present work we have not taken any measures against the issues regarding existence of solutions or mesh dependency. Note that in theory the problem exists for the approach taken here but as it is seen from the results, it does not seem to pose too severe problems.

The multi-material design problem can be modeled using integer material selection variables leading to a mixed-integer problem. Such discrete modeling leads to combinatorial problems that are hard to solve. In topology optimization a similar situation exists in the basic problem (solid or void) and a well-known approach is to relax the integer requirement on the selection variables to allow intermediate values - grey - during the optimization, see e.g. Bendsøe and Kikuchi (1988); Bendsøe (1989). These ideas were extended to multi-phase problems by Sigmund and Torquato (1997); Gibiansky and Sigmund (2000) for two non-vanishing phases

and void. Stegmann and Lund (2005) and Lund and Stegmann (2005) proposed the so-called Discrete Material Optimization (DMO) approach where the discrete optimization problem described above is converted to a continuous problem enabling design sensitivity analysis and the use of gradient based optimizers. DMO may be regarded as a ground structure approach for optimal material selection amongst multiple (anisotropic) materials. The idea is to relax the integer constraint on the selection variables so as to allow intermediate selection variable values between 0 and 1 during the optimization, representing mixed-material properties obtained as weighted averages of the constituent properties. This approach has been applied successfully to material distribution problems with criterion functions such as maximization of structural stiffness, eigenfrequencies and buckling loads, see e.g. the references above and Lund (2009). Stolpe and Stegmann (2008) formulated convex minimum compliance mass constrained problems and solved fiber angle problems (without a mass constraint) to global optimality by solving relaxations within a branch-and-bound framework using a special purpose Newton method. The problems solved in that paper did not include a constraint on the mass as the examples only included problems with one orthotropic material to be oriented at different discrete directions. For these problems it was reported that most of the design variables at the optimal solution to the continuous relaxation attained their lower or upper bounds, i.e. satisfied the original integer requirement. However, in general this is not guaranteed and particularly when an active mass constraint is present, the solutions tend to contain mixtures if no penalization of intermediate selections is applied. In this paper we model the problem similar to Stolpe and Stegmann (2008) and furthermore we impose a quadratic constraint that can be activated to prevent intermediate solutions. The quadratic constraint (or any other intermediate penalty constraint) has the advantage of giving a direct control of the amount of intermediate-valued variables in contrast to material interpolation schemes that typically encourage, but do not ensure, integer feasibility. The constraint allows us to solve (multiple load case) minimum compliance multi-material problems with a constraint on the mass. The idea is to solve a convex problem to optimality, and then use this solution as a starting guess for a non-convex problem where the quadratic constraint is imposed to obtain an integer feasible solution. Without proof we claim that the current approach of using the intermediate penalty constraint to control integer feasibility may also be used in other optimal design problem formulations including discrete variables, be it minimizing the maximum compliance for multiple load cases or minimum weight problems with a constraint on the compliance.

A key issue in DMO is that the continuous design variables eventually are pushed to their limit values, thus fulfilling the integer constraints and allowing for a physical interpreta-

tion of the final design. To obtain a distinct solution to a continuous problem one may 'encourage' distinct choices through penalization of intermediate selections either as a penalty to the objective function or through a constraint preventing intermediate design variables. For either approach, continuation on the degree of non-convexity may be applied to avoid local minima while gradually improving the possibility of obtaining a discrete solution with a good objective function value. In general, continuous relaxations combined with implicit and explicit penalization methods are heuristic approaches often used in the topology optimization community to address otherwise hard integer design problems. Either approach introduces some degree of non-convexity to the design problem in order to converge towards an integer solution (0-1). Thus any of these approaches cannot be guaranteed to converge to the global optimal solution since points fulfilling the KKT conditions may just be local minimizers.

Penalizing the objective function may be done either through a constitutive interpolation scheme that implicitly penalizes mixtures or by adding an explicit penalty term to the objective function. The interpolation scheme approach has gained large acceptance in the topology optimization community since the seminal paper by Bendsøe (1989). It is also known as the SIMP-approach (Solid Isotropic Material with Penalization), see e.g. Rozvany et al (1992); Bendsøe and Sigmund (1999, 2003). Other interpolation schemes have been proposed and in particular the so-called RAMP (Rational Approximation of Material Properties) scheme seems to have gained acceptance as well, Stolpe and Svanberg (2001). As an alternative to the material interpolation approaches, explicit penalization of intermediate densities has been applied as well. This is typically done by adding a penalty term to the objective function preventing intermediate solutions from being optimal solutions. Quadratic penalty functions have been proposed as such penalty terms, see e.g. Borrvall and Petersson (2001b).

The paper is organized as follows; in Section 2 we state and model the problem, develop reformulations and formulate the method used to solve the problem. Section 3 contains descriptions of a set of test problems that we solve, and present the results of in Section refsec:Results. A discussion of the method and the results obtained is given in Section 5 and finally we conclude the paper with a view towards future research in Section 6.

2 Problem Formulation

Given n^c predefined materials with known constitutive properties and mass density, we want to select the material in each of the n^d design subdomains such that a given objective function is minimized.

A discrete-valued material selection variable $x_{ij} \in \{0, 1\}$ is introduced to represent the selection of a given candidate material, i , in each design domain, j .

$$x_{ij} = \begin{cases} 1 & \text{if material } i \text{ is chosen in design subdomain } j \\ 0 & \text{if not} \end{cases} \quad (1)$$

A design subdomain may be a single layer in a finite element, a layer covering multiple elements, multiple layers within a single element etc. The definition of design subdomains may be chosen to coincide with the finite element discretization but a design subdomain may also contain multiple elements in a so-called patch. Patches may be used due to manufacturing reasons if it is not allowable to have changes in material or fiber orientations at the level of the finite element discretization. Furthermore, the number of candidate materials may differ for the various design subdomains. Thus, the total number of design variables n is given as the sum of the number of candidate materials for all design domains, $n = \sum_{j=1}^{n^d} n_j^c$, where n_j^c is the number of candidate materials in each of the n^d design subdomains. Typically, and throughout this paper, we have the same number of candidate materials in all subdomains, i.e. $n_j^c = n^c \forall j$, and therefore the total number of design variables is simply given by $n = n^c n^d$.

In each design subdomain exactly one material should be chosen. This is enforced by the following equality constraints called the generalized upper bound constraints.

$$\sum_{i=1}^{n^c} x_{ij} = 1 \quad \forall j \quad (2)$$

This constraint, together with the constraints (1), ensures that exactly one material is chosen. If any variable entering the sum attains 1 the remaining variables necessarily must be 0 in order for the equality to hold.

2.1 Original problem

We want to solve discrete multi-material (multi-load case) minimum compliance problems subject to a mass constraint by means of solving a sequence of continuous relaxations. In the following we formulate the original problem and then formulate continuous relaxations. We treat the multiple independent load cases by forming a weighted sum of the compliance for the individual load cases. The relative importance of each load case is given by a weighting factor $w_l > 0$ normalized such that $\sum_{l=1}^L w_l = 1$.

The original problem is a non-convex mixed-integer problem; the design variables can physically only attain integer values, i.e. $x_{ij} \in \{0, 1\}$. The unknown optimal nodal displacements $u_l \in \mathbb{R}^d$ are continuous and d is the number

of free finite element degrees of freedom. We consider the problem

$$\underset{x \in \mathbb{R}^n, u_1, \dots, u_L \in \mathbb{R}^d}{\text{minimize}} \quad c(x) = \sum_{l=1}^L w_l p_l^T u_l \quad (3a)$$

$$\text{(P-SAND)} \quad \text{subject to} \quad K(x)u_l = p_l \quad l = 1, 2, \dots, L \quad (3b)$$

$$\sum_{i,j} x_{ij} \rho_i V_j \leq \bar{M} \quad (3c)$$

$$\sum_i x_{ij} = 1 \quad \forall j \quad (3d)$$

$$x_{ij} \in \{0, 1\} \quad \forall (i, j) \quad (3e)$$

where ρ_i is the mass density of material i , V_j is the volume of the j 'th design subdomain and \bar{M} is a resource constraint limiting the total mass of the structure. $K(x) \in \mathbb{R}^{d \times d}$ is the design dependent global stiffness matrix. Equivalent Single Layer (ESL) shell finite elements based on First-order Shear Deformation Theory (FSDT) are used for the analysis, and the stiffness matrix is linear in the design variables in the following manner

$$K(x) = \sum_{i,j} x_{ij} K_{ij} = \sum_{i,j} x_{ij} \int_{\Omega_j} B_j^T E_i B_j d\Omega_j = \sum_j \int_{\Omega_j} B_j^T \left(\sum_i x_{ij} E_i \right) B_j d\Omega_j \quad (4)$$

where $E_i \in \mathbb{R}^{6 \times 6}$ is the constitutive matrix for material i and $B_j \in \mathbb{R}^{6 \times d}$ is the global level strain displacement matrix for domain j .

(P-SAND) is not convex (due to the bi-linear term in the equilibrium equations) and is on the form of a mixed-integer program which in general is hard to solve.

The mass constraint is only relevant for multi-material problems where the candidate materials have different mass density. In the case of pure fiber angle optimization the mass constraint is redundant.

A feasible solution satisfies all linear constraints and thus in every design domain a material with non-vanishing stiffness is chosen. If we furthermore assume that the structure is sufficiently constrained (i.e. constrained against rigid body displacements) then the stiffness matrix is non-singular. If $K(x)$ is non-singular, the original non-convex 0-1 program may be reformulated as a 0-1 program with a convex objective function in so-called nested form where the nodal displacements are eliminated by use of the equilibrium equations for each load case, i.e. $u_l(x) = K(x)^{-1} p_l$ to obtain an equivalent optimization problem in the design variables

x only.

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad c(x) = \sum_{l=1}^L w_l p_l^T K(x)^{-1} p_l \quad (5a)$$

$$\text{(P)} \quad \text{subject to} \quad \sum_{i,j} x_{ij} \rho_i V_j \leq \bar{M} \quad (5b)$$

$$\sum_i x_{ij} = 1 \quad \forall j \quad (5c)$$

$$x_{ij} \in \{0, 1\} \quad \forall (i, j) \quad (5d)$$

This discrete problem is in general hard to solve. In the following we formulate a relaxation to (P) which may be solved using standard continuous nonlinear programming algorithms. The optimal solution to (P) we denote x_P^* .

2.2 Convex continuous relaxation

If the integer constraints on the variables are relaxed, we obtain a continuous relaxation (R) whose feasible set is a superset of (P)'s feasible set.

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad c(x) = \sum_{l=1}^L w_l p_l^T K(x)^{-1} p_l \quad (6a)$$

$$\text{(R)} \quad \text{subject to} \quad \sum_{i,j} x_{ij} \rho_i V_j \leq \bar{M} \quad (6b)$$

$$\sum_i x_{ij} = 1 \quad \forall j \quad (6c)$$

$$0 \leq x_{ij} \quad \forall (i, j) \quad (6d)$$

Note that the generalized upper bound constraints from (2) ensure that the variables fulfill $x_{ij} \leq 1$. Thus there is no need for an upper bound on the variables and it is enough to ensure non-negative design variables.

The optimization problem given by (R) is convex as shown by Svanberg (1994); Stolpe and Stegmann (2008). Thus a locally optimal solution x_R^* is also a global optimum to (R). Furthermore (R) is the continuous relaxation of (P) and therefore less constrained than (P). In other words the feasible set of (P) is a subset of the feasible set of (R). Thus

- If the optimal solution to (R) happens to be an integer solution then it is also an optimal solution to (P).
- The optimal solution to (R) is better than or as good as the solution to (P), i.e. $c(x_R^*) \leq c(x_P^*)$.
- If there is no feasible solution to (R) then there is no feasible solution to (P) either.

For a single load case problem, the formulation in (R) is the same optimization problem that Stolpe and Stegmann (2008) investigated and developed a dedicated Newton method for.

In the continuous relaxation the design variables may be interpreted as volume fractions of each candidate material

in the given domain. The equality constraints formulated in Eq. (2) represent physical constraints on the volume of available material in each domain. Allowing intermediate volume fractions implies non-distinct material choices (i.e. mixtures) which is not physical in a DMO parametrization. However, if the solution to the relaxation attains discrete values after optimization, the result is meaningful and manufacturable. If the result is non-integer it needs to be made integer for a meaningful physical interpretation. One approach is to apply simple rounding to nearest integer feasible solution. However, this approach may lead to designs violating the mass constraint. An other solution is to apply penalization through a material interpolation scheme to make intermediate selections uneconomical in the objective function and thereby encourage discrete solutions. Finally, there is the possibility to impose a constraint preventing intermediate solutions. In the following we describe a quadratic constraint that is added to (R) to prevent non-integer solutions.

2.3 Non-convex continuous relaxation

The optimal solution to the convex continuous relaxation (R) does in general not obey the integer requirement of the original problem (P). Our interest is to obtain a good (but not necessarily globally optimal) solution to (P) meaning that the solution should satisfy the integer requirement. To obtain integer solutions we need to either penalize intermediate values of the design variables, constrain them from occurring, or round non-integer solutions to e.g. nearest integer solution. Rounding to nearest integer solution may give designs that are not feasible with respect to the mass constraint. If we instead impose a constraint that prevents intermediate solutions, the integer feasible designs obtained should also respect the mass constraint. Thus we extend (R) by imposing an intermediate penalty constraint $g(x)$ that controls integer feasibility.

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad c(x) = \sum_{l=1}^L w_l p_l^T K(x)^{-1} p_l \quad (7a)$$

$$\text{(R-Penal)} \quad \text{subject to} \quad \sum_{i,j} x_{ij} \rho_i V_j \leq \bar{M} \quad (7b)$$

$$\sum_i x_{ij} = 1 \quad \forall j \quad (7c)$$

$$g(x) \leq \varepsilon \quad , \quad \varepsilon \in [0; \infty[\quad (7d)$$

$$0 \leq x_{ij} \quad \forall (i, j) \quad (7e)$$

The function $g(x)$ is a concave penalty function that is violated for mixtures. For each design domain with non-discrete design variables it should contribute to violating the inequality and give no contribution if a distinct (0/1) selection has

been made in that domain. By including the concave constraint in the optimization problem, (R-Penal) becomes non-convex.

The feasible set described by $g(x) = 0$ is identical to the original discrete set of points given by Equation (3e). Since the optimization problem given by (R-Penal) is non-convex, points satisfying usual first-order optimality conditions for (R-Penal) can not be guaranteed to be more than locally optimal solutions. If $\varepsilon = 0$ the feasible set of (R-Penal) is reduced to that of (P), and any of these integer feasible points ($x_{R-Penal}$) will have a worse (or as good) objective function value as the global optimal solution to (P), i.e. $c(x_P^*) \leq c(x_{R-Penal})$. Thus, the global optimal solution to (P) is bounded from below by the solution to (R) and above by any feasible point of (R) and hence (R-Penal) if $\varepsilon = 0$.

$$c(x_R^*) \leq c(x_P^*) \leq c(x_{R-Penal}) \quad \text{if } \varepsilon = 0. \quad (8)$$

Attacking the non-convex relaxation is a heuristic used to obtain a discrete solution and it may or may not work well depending on the given problem. For certain problems the upper bound obtained as the solution to (R-Penal) is close to the lower bound indicating that the solution has a performance close to that of the global optimal solution. In the present paper we do not devise further means for improving the lower or upper bound, but the bounds obtained may still be used to give a worst case estimate of the closeness of the current solution to the global optimal solution.

2.3.1 Intermediate penalty constraint

The intermediate penalty function is satisfied only if the design is integer feasible, given that the user-controlled parameter ε is zero. Borrvall and Petersson (2001a,b) used a regularized (filtered densities) version of this penalty function for topology optimization. We use the following concave quadratic constraint

$$g(x) = \sum_{i,j} x_{ij} (1 - x_{ij}) \leq \varepsilon \quad (9)$$

The idea is to solve a sequence of problems starting out by solving the convex problem (R) and then use the solution to this problem as a starting guess for the non-convex problem (R-Penal). The parameter ε is a user-controlled parameter used to relax/tighten the constraint. The constraint can be made inactive by selecting ε sufficiently large at the initial design. By gradually reducing ε to zero the solution is constrained to be integer feasible. Different continuation strategies for ε and the influence on the results are examined through numerical examples.

2.3.2 Design sensitivity analysis

For the solution of (R) and (R-Penal) by use of a gradient based algorithm efficient calculation of design sensitivity analysis for the non-linear criterion functions is needed. In the current problems the weighted compliance is the only implicit non-linear function which we calculate analytical design sensitivities for. The remaining constraints are linear and quadratic functions for which the sensitivities are straightforward. The non-linear function for which we need sensitivities is the weighted compliance function, Equation (6a). Recall that the weighted compliance is given by

$$c(x) = \sum_{l=1}^L w_l p_l^T K(x)^{-1} p_l \quad (10)$$

If the applied loads are design independent and the stiffness matrix is given by Equation (4), the sensitivity of the (weighted) compliance with respect to a design variable x_{ij} is given by

$$\begin{aligned} \frac{\partial c(x)}{\partial x_{ij}} &= \sum_{l=1}^L w_l p_l^T \frac{\partial (K^{-1}(x))}{\partial x_{ij}} p_l = \\ &= - \sum_{l=1}^L w_l p_l^T K^{-1}(x) \frac{\partial K(x)}{\partial x_{ij}} K^{-1}(x) p_l \\ &= - \sum_{l=1}^L w_l u_l^T \frac{\partial K(x)}{\partial x_{ij}} u_l = - \sum_{l=1}^L w_l u_l^T K_{ij} u_l \quad (11) \end{aligned}$$

see e.g. Svanberg (1994).

2.3.3 Obtaining an initial design

In principle the initial guess for (R) is immaterial since the problem is convex and hence the optimizer will find the same optimal solution (if a feasible solution exists) regardless of the initial guess. However, in general the number of iterations taken to determine an optimal point is lower if the algorithm is started from a feasible initial point. Thus we need a procedure to determine a feasible point to (R) in a fast manner.

Stolpe and Stegmann (2008) proposed to solve a linear program to obtain a feasible initial point. We take the same approach and briefly outline the procedure. First, we distribute all candidate materials uniformly within each element, $\bar{x}_{ij} = \frac{1}{n_j^c} \forall j$ (i.e. $\sum_{i=1}^{n_j^c} \bar{x}_{ij} = 1 \forall j$). At this point we make a first-order approximation of the objective function $c(d) \approx c(\bar{x}) + d^T \nabla c(\bar{x})$ and solve the following linear

program in d .

$$\begin{aligned} \text{minimize} \quad & c(\bar{x}) + d^T \nabla c(\bar{x}) \quad (12a) \\ \text{(LP-feas)} \quad \text{subject to} \quad & \sum_{i,j} (\bar{x}_{ij} + d_{ij}) \rho_i V_j \leq \bar{M} \quad (12b) \\ & \sum_i (\bar{x}_{ij} + d_{ij}) = 1 \forall j \quad (12c) \\ & 0 \leq \bar{x}_{ij} + d_{ij} \forall (i,j) \quad (12d) \end{aligned}$$

The optimal solution \bar{d} to (LP-feas) is used to update the uniform distribution to a feasible initial point as follows

$$x_0 = \bar{x} + \bar{d} \quad (13)$$

The cost of this procedure is the cost of a design sensitivity analysis to construct the first-order approximation plus the cost of solving the linear program, which is relatively low even for large problems.

2.4 Algorithm and implementation

The major optimality tolerance h^{opt} determines the requested accuracy for the fulfillment of the stationarity and complementarity conditions in the first-order optimality conditions (the KKT-conditions). This tolerance is used in the procedure(s) summarized in the following steps:

1. Distribute all candidate materials uniformly, \bar{x} .
 2. Solve (LP-Feas) to obtain a mass feasible starting guess x_0 .
 3. Use x_0 as a starting guess and solve (R) to optimality x_R^* .
 4. Use x_R^* as a starting guess and solve (R-Penal) using one of the following strategies for setting the value of ε in Equation (7d):
 - A. Set $\varepsilon = 10^{-3}$ directly and solve (R-Penal) to optimality with a major optimality tolerance $h^{opt} = 2 \cdot 10^{-4}$.
 - B. Solve a sequence of (R-Penal) problems where ε is tightened sequentially. Continuation: $\varepsilon_{k+1} = \max\{10^{-3}, r\varepsilon_k\}$ where $r = 0.2$ and $\varepsilon_0 = g(x_R^*)$. All intermediate problems in the continuation sequence are solved to optimality with a major optimality tolerance $h^{opt} = 2 \cdot 10^{-4}$.
 - C. As B, but in this strategy the subproblems solved in the beginning of the continuation are solved with a looser optimality tolerance which is tightened sequentially towards the end of the continuation. The major optimality tolerance is set as: $h_{k+1}^{opt} = \max\{2 \cdot 10^{-4}, r h_k^{opt}\}$, where $r = 0.2$ and $h_0^{opt} = 1.0$.
- All strategies are stopped when $\varepsilon \leq 10^{-3}$. Furthermore each sub-problem in the continuation is stopped after at most 200 major iterations.

5. Finally, a heuristic rounding to 0/1 is applied and all criterion functions are re-evaluated with this integer design, $x_{0/1}$. This procedure rounds the largest design variable in a given domain to 1 and the remaining to 0, whereby the generalized upper bound constraints (see e.g. Equation (2)) are still satisfied. The final rounding is only a *minor* modification since the design obtained after step 4 is already almost integer, except for the small tolerance allowed, $g(x) \leq \varepsilon = 10^{-3}$.

The procedure proposed in this paper is implemented in our in-house research code MUST (MULTidisciplinary Synthesis Tool) mainly written in Fortran 90. MUST takes a finite element discretization as input from e.g. ANSYS and together with a few additional lines of information defining the optimization problem, the problem is set up and ready to be analyzed and optimized in MUST.

All examples are discretized using 9-node degenerated shell elements with 5 degrees of freedom per node (3 translational and 2 rotational), see e.g. Ahmad et al (1970); Panda and Natarajan (1981). For purely plane problems such elements are unnecessarily complicated and computationally expensive, but these examples illustrate that the proposed approach is able to solve the material distribution problem within the plane of the structure as well as through the thickness in layered structures. Note that the method may be used with any kind of displacement based finite elements.

(R-Penal) is solved by use of the sequential quadratic programming (SQP) algorithm SNOPT 7.2-8, see Gill et al (2005, 2008). Linear mass and material selection constraints are treated as such which is utilized within SNOPT in the sense that linear constraints are always satisfied before calling the non-linear functions. In SNOPT default parameter settings are used except for the so-called “New Superbasics Limit” which is set to 100.000, the “Major iterations limit” to 200, and the “Minor iterations limit” to 1000. The major optimality tolerance is set as described previously and the “Function precision” is set accordingly, see Gill et al (2008). (LP-Feas) is solved using the sparse implementation of the primal simplex method available in SNOPT. For the LP’s default parameters are used.

All results presented in this paper were obtained using a standard desktop PC running Windows XP equipped with an Intel Core2 Quad CPU at 2.4 GHz and 3.2 GB RAM. The source code is compiled using Intels Visual Fortran compiler and makes use of Intels Math Kernel Library (MKL).

3 Examples

In this section we describe a set of problems for which we test the proposed method for solving discrete multi-material problems. Computational results for the presented examples are reported in Section 4.

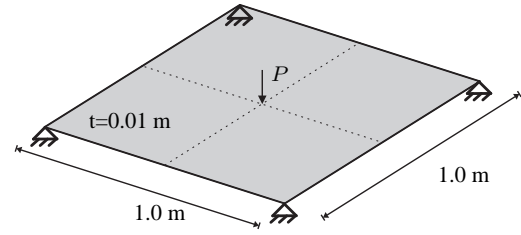


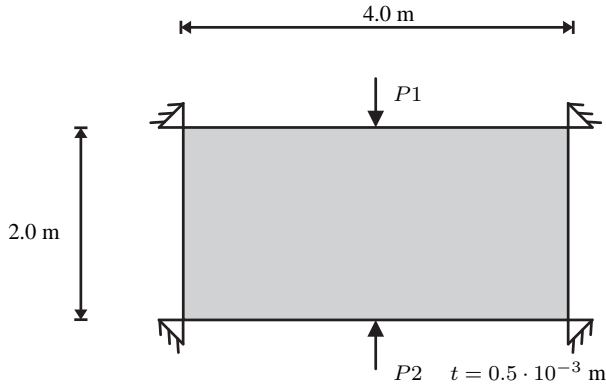
Fig. 2 Example 4-8. Multi-layered (4 or 8) corner-hinged plate with point load applied at the center. See Figure 3.1 for material properties.

3.1 Examples 1–3

In these examples we solve plane problems with two independent load cases of equal importance ($w_1 = w_2 = 0.5$) and loads with equal magnitude ($|P1| = |P2|$). In both load cases the plate is hinged at all corners ($u_i = 0$), see Figure 3.1. The physical domain within which the material is distributed is a rectangular plate of dimension $4.0m \times 2.0m \times 0.5 \cdot 10^{-3}m$. The domain is discretized by three different meshes, (40×20) , (60×30) and (120×60) respectively and in each element five candidate materials are possible. The first candidate material is a light and soft material representing e.g. isotropic foam and the remaining four candidate materials represent a heavier and stiffer orthotropic material oriented at four distinct directions, -45° , 0° , 45° or 90° . We set the mass constraint such that the heavy orthotropic materials can be chosen in 35% of the domain. In principal material coordinate system the constitutive properties of the foam material and the stiff orthotropic material are given in Figure 3.1.

3.2 Examples 4–8

This example is concerned with the design of a multi-layered plate structure. The physical domain within which the material is distributed is a quadratic plate of dimension $1.0m \times 1.0m \times 1.0 \cdot 10^{-2}m$. The plate is loaded at the center by a point load P and each corner is hinged ($u_i = 0$). A sketch of the problem is shown in Figure 2. Examples 4-6 employ a (24×24) in-plane discretization. Example 4 is discretized through the thickness with 8 layers whereas example 5 and 6 have 4 layers. Examples 7-8 have a coarser (12×12) in-plane discretization. Example 7 is discretized through the thickness with 8 layers, whereas Example 8 has 4 layers through the thickness. The candidate materials are identical to those in Example 1–3, i.e. a light and soft isotropic foam material and a heavy and stiff orthotropic material oriented at four distinct directions.



	Foam	Orthotropic
E_x [Pa]	$65.0 \cdot 10^6$	$34.0 \cdot 10^9$
E_y [Pa]	—	$8.2 \cdot 10^9$
E_z [Pa]	—	$8.2 \cdot 10^9$
G_{xy} [Pa]	—	$4.5 \cdot 10^9$
G_{yz} [Pa]	—	$4.0 \cdot 10^9$
G_{xz} [Pa]	—	$4.5 \cdot 10^9$
ν_{xy}	0.47	0.29
ρ [kg/m ³]	200.0	1910.0

Fig. 1 Example 1-3. Left: Domain geometry and boundary conditions. Loads act independently. Right: Material properties in principal material coordinate system for the candidate materials.

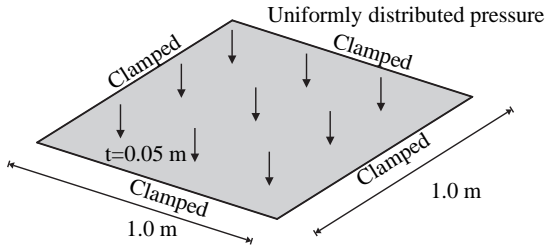


Fig. 3 Examples 9–10. Single-layered clamped plate with uniform pressure applied over the top surface.

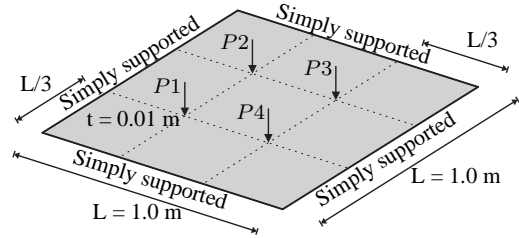


Fig. 4 Example 11. Eight-layer plate. Domain geometry and boundary conditions. Each load acts independently. See Figure 3.1 for material properties.

3.3 Examples 9–10

These examples were proposed and solved by Lund and Stegmann (2005) using the original DMO approach, and they illustrate a discrete fiber angle orientation problem formulated as a multi-material selection problem.

A single-layer clamped plate subjected to uniform pressure is solved for minimum compliance. The plate has dimension $1.0m \times 1.0m \times 0.05m$ and is discretized by a 20×20 mesh of isoparametric 9-node degenerated shell elements. The material is orthotropic with $E_x = 54GPa$, $E_y = E_z = 18GPa$, $\nu = 0.25$, $G_{xy} = G_{yz} = G_{xz} = 9GPa$. First the problem is parametrized by 4 DMO design variables per element such that the orthotropic material can be oriented in 4 directions (0° , -45° , 45° and 90°). A sketch of the problem is shown in Figure 3.

With 400 elements this amounts to 1600 design variables in total. Then we increase the resolution in the orientations to 12 candidate directions (-75° , -60° , \dots , 0° , 15° , \dots , 75° , 90°) leading to 4800 design variables.

3.4 Example 11

In this example we solve a multi-layered plate problem with four independent load cases of equal importance ($w_1 = w_2 = w_3 = w_4 = 0.25$) and loads with equal magnitude ($|P1| =$

$|P2| = |P3| = |P4|$). In each load case the plate is simply supported along the edges, that is all translational degrees of freedom are fixed, see Figure 4. The physical domain within which the material is distributed is a quadratic plate of dimension $1.0m \times 1.0m \times 0.01m$. The domain is discretized by (24×24) elements in-plane and 8 layers through the thickness and in each domain five candidate materials are possible. The first candidate material is a light and soft material representing e.g. isotropic foam and the remaining four candidate materials represent a heavier and stiffer orthotropic material oriented at four distinct directions, -45° , 0° , 45° or 90° . The material properties are identical to those in Example 1-3.

4 Results

In the following we report results and computational statistics for the solution of the previously presented problems summarized in Table 1. Each example is solved with all three continuation strategies proposed in Section 2.4. The three strategies we denote by A, B and C, respectively. Recall that each strategy involves the solution of the initial feasibility problem (LP-Feas) as well as the solution of the continuous convex relaxation (R), these results are identical and common to all three continuation strategies and are summa-

Problem	# Materials	Discretization	Variables	DOF	LC's	\bar{M} (kg)
1	5	800 (40x20x1)	4000	12585	2	3.0
2	5	1800 (60x30x1)	9000	27885	2	3.0
3	5	7200 (120x60x1)	36000	109785	2	3.0
4	5	4608 (24x24x8)	23040	9113	1	6.8
5	5	2304 (24x24x4)	11520	9113	1	6.8
6	5	2304 (24x24x4)	11520	9113	1	10.6
7	5	1152 (12x12x8)	5760	2393	1	6.8
8	5	576 (12x12x4)	2880	2393	1	10.6
9	4	400 (20x20x1)	1600	5600	1	n/a
10	12	400 (20x20x1)	4800	5600	1	n/a
11	5	4608 (24x24x8)	23040	8849	4	6.8

Table 1 Problem characteristics for the numerical examples.

rized in Table 2. The results obtained for each continuation strategy are given in Table 3, 4 and 5, respectively. We report the following quantities.

$c(x_0)$ Compliance of the optimal solution to (LP-Feas).

Itn Number of major iterations (for (R) and (R-Penal), respectively)

nFun Total number of function calls during the major iterations. For each function call the stiffness matrix is assembled and factorized using LDL^T factorization and the displacements are calculated by forward and backward substitution.

nGrad Total number of sensitivity analyses (gradient evaluations) performed during the major iterations. Each gradient evaluation entails n vector-matrix-vector products at the element level as shown in Equation (11).

Time Wall clock time to perform optimization.

$c(x_R^*)$ Compliance of the optimal solution to the relaxation (R), lower bound.

$g(x_R^*)$ Value of the penalty constraint function for the optimal solution to the convex relaxation (R).

$g_{max} = g(\bar{x})$ Maximum value of the quadratic penalty constraint function. Obtained for a uniform mixture of candidate materials, \bar{x} .

$c(x_{R-Penal}^*)$ Compliance of the (almost discrete) optimal solution to the non-convex relaxation (R-Penal), upper bound. We also report the number of iterations taken to obtain this solution.

Obj. gap Relative gap between upper and lower bound,
 $\frac{c(x_{0/1}) - c(x_R^*)}{c(x_R^*)} 100\%$.

5 Discussion

In the following paragraphs we discuss the results presented above. We discuss the influence of the continuation strategy on the results obtained as well as implications of the discrete nature of the original problem for a continuous solution approach. We study examples (Examples 4-6) where the parametrization in combination with the mass constraint

and discretization plays a role in terms of how hard the problem is to solve.

5.1 Examples 1–3

The three examples solved here represent different discretizations of the same physical design problem. From the solution to (R) it is seen that the degree of mixture ($g(x_R^*)/g_{max}$) is around 0.32 – 0.35 for all three problems. This value indicates a fairly mixed optimal solution to the convex continuous relaxation and thus the lower bound obtained through this relaxation is not very strong in the sense that any integer solution must be quite different from the solution to (R). The objective gaps obtained by use of each of the different continuation strategies are reported in Table 3, 4 and 5, and it is seen that strategy B obtains the best design for all three discretizations. Strategy C obtains as good or slightly worse designs compared to B and strategy A obtains the worst designs. The differences in the objective gaps are minor but it is noteworthy that the computational cost of strategy B is significantly higher than the other strategies, and the results obtained with strategy C are almost as good as with B. The magnitude of the gap is considered to be acceptable, given the amount of mixture in the lower bound solution. The results obtained using strategy B for Examples 1 and 2 are visualized in Figure 5 and 6. Comparing Example 1 with Example 2 it is observed that the topologies obtained with the two different meshes are very similar. The results for Example 3 are not visualized, but the topology is very similar to that for Example 1 and 2. The obtained topology looks as expected and is similar to that obtained for isotropic topology optimization under the same loading conditions. Here, we furthermore obtain information about how the orthotropic material should be oriented for structural efficiency. A similar example was addressed by Bendsøe et al (1995); Hörnlein et al (2001); Bodnár (2009), where the design problem was investigated using Free Material Optimization (FMO). The results obtained using FMO are not directly comparable to those obtained in this paper due to the

Problem	(LP-Feas)				(R)		
	$c(x_0)$	Itn.	nFun	nGrad	Time (s)	$c(x_R^*)$	$g(x_R^*)/g_{max}$
1	789.3	95	99	97	411	22.72	226.7/640.0=0.354
2	200.1	104	112	110	1108	5.834	468.8/1440.0=0.3256
3	50.31	79	85	83	5468	1.544	1904.2/5760.0=0.331
4	167.3	23	26	24	526	28.77	339.8/3686.4=0.0921
5	771.3	45	48	46	437	34.83	486.5/1843.2=0.264
6	22.05	56	65	63	426	20.53	168.7/1843.2=0.0915
7	208.8	24	33	31	118	28.61	81.36/921.6=0.0883
8	85.35	88	105	103	162	81.69	39.10/460.8=0.085
9	9.043	9	12	10	11	8.895	68.25/300.0=0.2275
10	8.832	24	29	27	66	8.707	85.09/366.66=0.232
11	38.39	44	52	50	3278	17.94	471.6/3686.4=0.12

Table 2 Computational statistics for solution of linear feasibility problem (LP-Feas) and the continuous convex relaxation (R). Common part for all three continuation strategies.

Problem	(R-Penal)					Total	
	Itn.	nFun	nGrad	Time (s)	$c(x_{R-Penal}^*)$	Obj. gap (%)	Time (s)
1	5	10	8	30	26.81	18.01	450
2	5	11	9	78	7.001	19.37	1186
3	4	7	5	214	1.793	16.16	5762
4	6	12	10	137	29.78	3.51	911
5	28	45	43	270	353.8	918.01	768
6	3	6	4	30	20.76	1.13	474
7	4	10	8	27	29.76	4.03	163
8	4	17	15	22	82.44	0.927	193
9	5	8	6	7	9.007	1.25	22
10	3	6	4	10	8.814	1.23	81
11	7	12	10	430	19.56	9.02	3794

Table 3 Computational statistics for continuation strategy A.

Problem	(R-Penal)					Total	
	Itn.	nFun	nGrad	Time (s)	$c(x_{R-Penal}^*)$	Obj. gap (%)	Time (s)
1	237	296	280	1055	25.84	13.72	1470
2	434	1052	1034	8168	6.683	14.55	9433
3	273	1081	1063	50120	1.771	14.72	60100
4	140	580	564	7211	29.11	1.19	7797
5	394	577	559	3958	60.65	74.156	4463
6	132	494	478	3094	20.72	0.93	3586
7	127	477	461	1424	28.92	1.01	1554
8	88	248	234	361	82.41	0.863	531
9	45	102	88	97	9.007	1.25	111
10	53	151	135	305	8.814	1.23	380
11	279	848	830	36550	18.85	5.091	39840

Table 4 Computational statistics for continuation strategy B.

full freedom of design of the material tensor in FMO compared to the setting of DMO where the design is restricted to a set of physically available materials. Nevertheless, the results obtained here have similarities to those obtained by FMO in the sense that the stiff material is chosen in the same areas where the FMO results indicate a need for stiffness and the fiber orientations obtained here resemble those shown by Bodnár (2009).

5.2 Examples 4–6

These examples illustrate features of the parametrization and discretization of the design problem. First we examine Example 4 and 5 and highlight similarities and differences in the obtained results.

Examples 4 and 5 are instances of the same design problem except that Example 5 has a coarser discretization through the thickness. In Example 4 there are 8 layers through the

Problem	(R-Penal)					Total	
	Itn.	nFun	nGrad	Time (s)	$c(x_{R-Penal}^*)$	Obj. gap (%)	Time (s)
1	46	116	100	363	25.84	13.72	780
2	16	43	25	266	6.750	15.74	1386
3	22	59	41	1701	1.793	16.16	7282
4	19	53	37	545	29.78	3.51	1135
5	138	302	284	2067	67.18	92.91	2573
6	9	27	11	113	20.76	1.13	601
7	9	215	199	615	29.76	4.03	744
8	9	31	17	34	82.44	0.927	205
9	9	32	18	26	9.007	1.25	42
10	9	34	18	49	8.814	1.23	122
11	58	119	101	4009	19.56	9.02	7232

Table 5 Computational statistics for continuation strategy C.

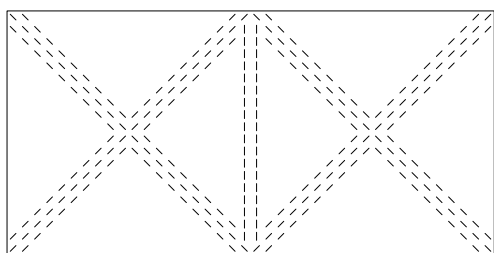


Fig. 5 Example 1 strategy B, elements with orientation shown indicate the optimal fiber angle for the element. Elements without any orientation indicate that the compliant material has been chosen. Design for strategy C is identical.

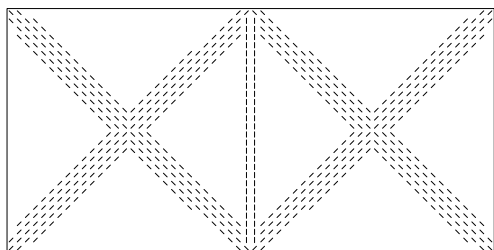


Fig. 6 Example 2 strategy B, elements with orientation shown indicate the optimal fiber angle for the element. Elements without any orientation indicate that the compliant material has been chosen.

thickness whereas Example 5 has 4 double thickness layers through the thickness. The mass constraint for both examples is set such that the heavy and stiff orthotropic material can be chosen in at most 28.07% of the design domain. For Example 4 this corresponds to 1293 domains (out of 4608) and for Example 5 to 646 domains (out of 2304). Note that the design problem is symmetric around the mid-plane of the plate and therefore the design is expected to have a corresponding symmetry. Mechanically, the optimal structure should resemble a sandwich structure due to bending in the plate; the best material utilization is obtained by moving stiff (and heavy) material from the inner layers of the plate to the outer layers. It is seen from the optimal solution to (R), Table 2, that the amount of mixture for Example 4 is somewhat lower than that for Example 5, 0.085 against 0.264. Looking

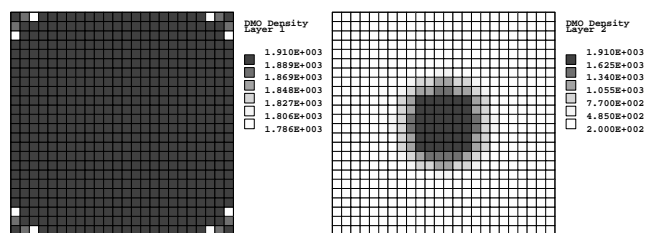


Fig. 7 Example 4, interpolated mass density for solutions to the continuous relaxation (R). Left: Layer 1 and 8. Right: Layer 2 and 7. In the four inner layers the soft and light material has been chosen throughout. Note the different gray scales.

at the final objective gap for both examples it is seen that for Example 4 it is below 3.6% for all three strategies whereas for Example 5 it ranges from 74% to 918%! The results obtained for Example 4 are considered to be satisfactory. The results for Example 5 require some more explanation.

For Example 4 the mass constraint allows for stiff material in 1293 domains, and the number of domains per layer is $24^2 = 576$. Thus, the mass constraint allows for a bit more than two layers (one on each side) completely filled with stiff material. Thereby, Example 4 has the possibility to obtain a sandwich design within the mass constraint. The solution to (R) demonstrates how heavy (and stiff) material is placed almost throughout the outer layers and some stiff material in the next layer, Figure 7. For Example 5 the physical size of each domain has doubled and now the mass constraint allows for stiff material in 646 domains. The number of domains per layer is still $24^2 = 576$ and thereby there is not “enough” material to fill the two outer layers with stiff material to obtain a sandwich-type structure. Thus in Example 5 soft material appears in the outer layers in order to fulfill the mass constraint, see Figure 8.

From Figure 8 the interpolated density from the solution to the continuous relaxation is seen. It is seen that the interpolated mass density ranges from 477.4 kg/m^3 to 1910.0 kg/m^3 . The lower value shows that there is no region in this layer where pure light material has been chosen. The upper value

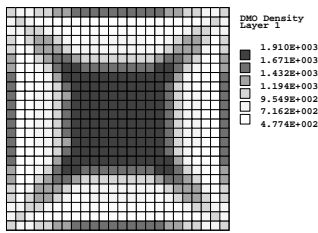


Fig. 8 Example 5, interpolated mass density for solution to the continuous relaxation (R). Layer 1 and 4 (outer layers). In the two inner layers the soft and light material has been chosen throughout.

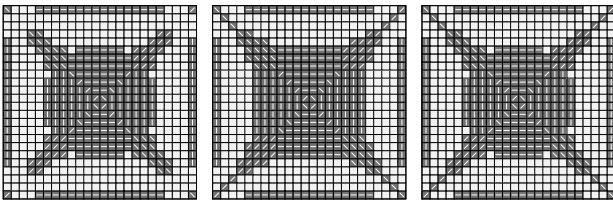


Fig. 9 Example 5, layer 1 and 4: integer solutions obtained by the three different continuation strategies A, B and C from left to right. Dark grey indicates heavy orthotropic material, orientation is indicated in white. In the two inner layers the soft and light material has been chosen throughout.

indicates an interpolated density reaching the maximum value. Please note that it does not show how this density was achieved, e.g. if it is a mixture of the four heavy orthotropic materials or stems from one distinct material. Nevertheless, the plot of the material density gives an indication of where the heavy and stiff material is needed. It is seen that a region in the middle of the plate attracts material and reaches towards the corners where the plate is supported. From the plot it is seen that large regions contain intermediate value densities compared to Figure 7. The final integer solutions for layer layer 1 and 4 obtained by use of the three different continuation strategies are shown in Figure 9. The large objective gap obtained for Example 5 may be explained from these figures. The large gap reported in Table 3 corresponds well with the leftmost figure in Figure 9. Here it is seen that the central part of the plate where the stiff material has been chosen is disconnected from the corner supports and therefore this isolated island of stiff material is pushed through the plate under loading. The designs obtained with continuation strategy B and C have a narrow connection of stiff material to the corner supports and perform much better than the left design. The objective gap for these designs is still considered to be high, though. Finally, we show Example 6 which is similar to Example 5, but with a higher mass constraint allowing for heavy material to be chosen in 50.3% of the design domain or approximately 2 layers. It is seen from Table 2 that the solution to (R) is more distinct than that of Example 5 ($g(x_R^*)/g_{max} = 0.0915$) and the integer solutions obtained from the different continuation strategies all

have an objective gap below 1.5%. These gaps are considered to be satisfactory from an engineering point of view. The designs obtained after the relaxation as well as the continuation all place the heavy material in the outer layers as expected.

The difference in the designs obtained for Examples 4 and 5 illustrates how changes in parametrization and design freedom may lead to completely different results in terms of convergence to a discrete solution as well as ability to close to objective gap. This may seem obvious but in practice it can be hard to identify whether an intermediate density result is due to the parametrization/design employed, or if it is due to the nature of the design problem. That being said, it should be noted that Example 5 is a badly formulated design problem since the parametrization prevents an efficient sandwich structure from occurring. One layer makes up a quarter of the total thickness and thus the resulting sandwich structure has thick face sheets relative to the core thickness. For sandwich structures to be structurally efficient, the core to face sheet thickness ratio should be at least 5.77, Zenkert (1997).

5.3 Examples 7–8

Examples 7 and 8 are analogous to Examples 4 and 6, except for a coarser in-plane discretization, now 12×12 . The observations regarding the influence of the discretization through the thickness for Examples 4 and 6 carry over to these examples without significant differences. Qualitatively, the material distribution in the plane of the plate is similar to that obtained for the previous examples except for a coarser resolution obtained here.

5.4 Examples 9–10

The solutions obtained for these examples are shown in Figure 10. All three continuation approaches obtained identical results for each of the examples. The fiber orientations resemble those obtained previously using the original DMO approach as well as the orientations obtained using a classical continuous fiber angle parametrization, see Lund and Stegmann (2005). From Table 2 it is seen that the solutions after the initial LP have an objective function value quite close to the corresponding final solution obtained after solving (R-Penal). This fortuitous behavior is not representative for all design problems though. The reason for this behavior may be attributed to the load carrying mechanism of the initial design which is quite similar to the load carrying behavior of the optimal design. Therefore a first order approximation of the compliance at the initial design (uniform mixture of all candidate directions) is reasonably good

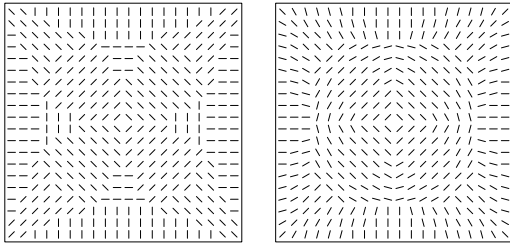


Fig. 10 Examples 9–10. Discrete optimal fiber directions. Left: Example 9, four candidate orientations per element. Right: Example 10, twelve candidate orientations per element.

and consequently the optimal design obtained from this approximation is also good. In the other examples shown, the initial uniform mixture of materials has a quite different load carrying behavior compared to the optimal design. In such situations, the first-order approximation of the compliance is not as accurate as in this example and the design obtained from the first-order approximation may be quite poor.

5.5 Example 11

The last example is a layered plate subjected to four independent load cases. Strategy A and C obtain an integer solution with an objective gap of 9.02% and strategy B obtains a better integer solution with an objective gap of 5.1%. Compared to the other 8-layer examples (Example 4 and 7) the lower bound solution (R) is more mixed and correspondingly the objective gap is a bit higher. It is interesting to note that the solution obtained by strategy B (which is better than the other solutions obtained) does not look as “nice” as the other solutions in terms of symmetry. The problem has symmetry around the mid-plane as well as vertical and horizontal symmetry, and the optimal solution obtained by a gradient based optimizer is expected to have these symmetries as well. However, the optimal solution obtained by strategy B has a few elements that do not fit with these symmetries, but they do yield an improvement in the objective function. Whether the globally optimal solution is symmetric or not remains open, it may be determined using global optimization techniques such as branch-and-bound/cut or other techniques.

6 Conclusion and Future Research

The paper demonstrates a method for solving optimal stiffness design problems of discrete (laminated) multi-material structures subjected to multiple independent load cases. We have shown the use of a quadratic penalty constraint to obtain integer solutions for continuous relaxations of the original discrete multi-material design problems. The solutions

are obtained using a standard nonlinear programming optimizer. As a part of the solution procedure a rigorous lower bound is calculated. From the continuous solution a discrete solution is obtained through the quadratic penalty constraint that is imposed gradually through a sequence of related problems. It turns out that the best designs are obtained by solving all intermediate problems in this sequence to optimality (strategy B) but the computational cost of this approach may be quite high. As an alternative, the intermediate problems can be solved to optimality with a larger convergence tolerance and this approach has shown to be a good compromise of computational cost and quality of the obtained solutions.

The results obtained by use of the procedure described in this paper possess features not previously obtained for the considered class of problems. An important feature is the possibility of giving a worst-case estimate of closeness to global optimality. Any feasible integer solution, no matter how it is obtained, may be compared to the lower bound obtained as the solution to the convex continuous relaxation. Thus with a small gap, the given integer solution is known to be good in the sense that its performance *must* be close to that of the global optimal solution. However, a large gap does not necessarily mean that the current integer solution is far away from the global optimal solution, it rather means that we can not certify/guarantee that it is close to it. Thus, the value of the solution to the convex continuous relaxation (R) is twofold. First, it gives a good starting point for obtaining an integer solution by means of solving a (sequence of) related non-convex problems. Second, it gives valuable information in terms of a lower bound on the attainable performance. For most examples solved in this paper a reasonably small gap is obtained, but for certain examples the gap is large and therefore only a weak assessment of the closeness to the global optimal solution can be given. To improve this gap in order to obtain a guaranteed globally optimal solution, global optimization techniques such as branch-and-bound/cut or other techniques using decomposition are necessary. These techniques in combination with the approach shown here are currently investigated.

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Paper B

E. Munoz and C.G. Hvejsel: Discrete Multi-Material Optimization (2010): Combining Discrete and Continuous Approaches for Global Optimization, to be submitted.

Discrete Multi-Material Optimization: Combining Discrete and Continuous Approaches for Global Optimization

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Christian Gram Hvejsel†

1st June 2010, 17:15

Abstract

Composite laminate lay-up design problems may be formulated as discrete material selection problems. Using this modeling, we state standard minimum compliance problems in their original Mixed-Integer Problem (MIP) formulation, which we aim to solve to global optimality. We use different techniques for continuous and discrete optimization, and a Generalized Benders' Decomposition algorithm for obtaining globally optimal solutions. By solving the continuous relaxation of the mixed integer problem, a considerable amount of information is passed to the mixed-integer problem. This is mainly due to a convexity property of the continuous relaxation of the original problem. In particular, we use an efficient heuristic technique, which is very likely to find close-to optimal solutions. This technique consists in solving a related sub-MINLP problem, based on the solution to the continuous relaxation of the original MINLP optimization problem. This sub-MINLP problem corresponds to the original mixed integer problem, where a large number of variables are fixed (up to 90%). Solving the resulting problem is much easier and requires significantly less computational effort. The selection of the variables to be fixed depends strongly in the solution of the continuous relaxation. This heuristic can be also used to improve the performance of other optimization techniques in the field of mixed-integer optimization. A number of numerical examples in design of composite laminated structures is presented. Several of them are solved to global optimality, and in extension the strengths of the method are discussed. Numerical examples of medium size of up to 23.000 design variables are solved and gives promising results in solving large design problems to optimality, considering a small tolerance. At the same time, the independence of the design discretization with respect to the finite element discretization allows the method to be used in real life design problems and still obtain globally optimal solutions.

Keywords: structural design optimization, global optimization, heuristics, laminated composite materials.

1 Introduction/Literature review

Almost every structural or mechanical design problem can be formulated as an optimization problem with either continuous or integer decision/design variables. Despite of the fact that most practical design problems are discrete in nature, the vast majority of works on structural optimization focus on design problems with continuous variables. The reasons for this are many; continuous problems are (much) easier to solve, the size of manageable continuous problems is significantly larger compared to equivalent integer problems, off-the-shelf continuous large-scale optimization algorithms exist, and in addition many integer problems may be attacked heuristically using continuous approaches. Typically, the integer nature of the decision variables comes from the fact that it is not desirable or possible to allow

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for e.g. every imaginable bar or plate thickness, material property etc., for the design of a mechanical structure. Often the designer is restricted to choose from a set of predefined properties for the entity in question; be it a cross section from a table of available standard cross sections, or a material from a set of predefined suitable candidate materials. Problems of truly discrete nature are not necessarily suitable for continuous approaches and furthermore most continuous approaches give no guarantee or assessment about the quality of the solutions obtained, except that they yield some design improvement compared to the initial design. To perform true optimization, that is to obtain the best solution(s) (the set of global optimal solutions), more rigorous approaches are needed, and this is the topic of global optimization (with integer variables), which we consider in this paper. The application addressed in this paper is that of having a design domain, which is subdivided into a finite number of regions. Each of these regions will be called throughout this paper, a design sub-domain. In every design sub-domain, the selection of a material from a set of given candidate materials is to be done. This formulation covers multi-material topology optimization problems such as optimal composite laminate lay-up design with different candidate material as well as discrete fiber orientation problems. We propose to use a combination of exact global optimization algorithms, continuous relaxations and heuristics to obtain guaranteed globally optimal solutions to these discrete design problems, which would not be possible to solve by either approach independently. In this paper heuristic procedures only have the purpose of assisting in finding globally optimal solutions, while global optimization methods are used to both finding globally optimal solutions, and also to prove the optimality of these solutions. In this article we intend to use two heuristics procedures. First, the resolution of sub-MINLP formulations (mixed 0/1 formulations, identical to the original mixed 0/1 formulation, where most of the variables are fixed, in order to ease the process of finding a solution). Global optimality of a solution is often done by generating valid lower bounds for the optimal objective functions. In this article, we intend to use the Generalized Benders' Decomposition (GBD) method, as a global optimization method. The difficulty of proving global optimality depends strongly in the nature of each problem. In particular, convexity properties of the continuous relaxation of an optimization model gives a superlative help in accomplishment of this task. As a matter of fact, the optimal solution to the convex continuous relaxation gives a meaningful lower bound for a global optimum of the 0/1 problem.

Structural design of laminated composite structures entails decisions about the number of layers, selection of material in each layer (CFRP¹, GFRP², polymeric foam, balsa wood, etc.), orientation of orthotropic materials ($0^\circ, 45^\circ, \dots, 90^\circ$), individual layer thicknesses. In the current work we fix the number of layers as well as the layer thicknesses a priori and thus we only consider the problem of selecting the optimal material among multiple candidates hereunder the problem of orienting orthotropic materials at predefined discrete angles. Thus we continue along the lines of (discrete) topology optimization meaning that we work on a given fixed domain within which we want to select in each design sub-domain the optimal material from a number of given candidate materials. These were first presented by Sigmund and Torquato (1997); Gibiansky and Sigmund (2000) in the setting of three-phase topology optimization (void and two materials). Since then Stegmann and Lund (2005); Lund and Stegmann (2005) generalized the problem to include multiple (orthotropic) materials to be selected among in the setting of optimal composite laminate design. In this paper the modeling of the continuous relaxation closely follows that of Stolpe and Stegmann (2008).

In contrast (sic!) to two-phase topology optimization, the design question is extended to include multiple distinct phases whereby the problem is enlarged. This design problem is a generalization of the void-solid (or two-phase) topology optimization problem and includes this problem as a special case where void is one of the "materials". Thus, the multi-material minimum compliance problem also lacks existence of solutions in its continuum infinite dimensional form, as it is well-known for the two-phase topology optimization problem, see Lurie (1980); Kohn and Strang (1982, 1986); Cherkaev (1994). For a finite element discretized design domain, this means that the optimal solution is mesh dependent in the sense that finer meshes may produce finer resolution and qualitatively different solutions which is of course unwanted. Preferably, the optimal design should not depend on the analysis discretization. To make the solution mesh independent, different techniques exist and have been used for topology optimization. One way to obtain a well-posed problem is to introduce micro structures (i.e. composites) to the design space, or to exclude unwanted small scale features from the feasible set (see Bendsøe and Sigmund (2003)). In this work we do not ensure existence of solutions through e.g. minimum length

¹Carbon fiber reinforced polymer

²Glass fiber reinforced polymer

scale or composites. We introduce the possibility of selecting pre-defined (composite) materials from a set of candidate materials, throughout the also pre-defined spatial design sub-domain. Since the problem of mesh dependency exists for two-phase topology design, it also exists for the multi-material problem since the former is just a special case of the latter. In practice, however, it is our experience that mesh dependency does not pose too severe problems. Nevertheless, it still exists and should be taken care of in future research. Here we just briefly mention the issues related to defining meaningful length scales when multiple phases are involved. These issues are, to our knowledge, not resolved yet and require further research.

As a general fact, the original formulation of discretized structural design problems falls into the category of nonlinear non-convex mixed-integer problems, where the state variables are continuous variables and the decision/design variables are integer variables. This corresponds to a so-called SAND (Simultaneous ANalysis and Design) formulation (see Fox and Schmit (1966); Haftka (1985); Haftka and Kamat (1989)). To handle this class of problems, several techniques are found in the literature. We briefly mention the branch-and-bound method (Land and Doig (1960), Gupta and Ravindran (1985)), the branch-and-cut method (Stubbs and Mehrotra (2002)), the Outer Approximation Duran and Grossmann (1986), and the Generalized Benders' Decomposition (GBD, Benders (1962), Geoffrion (1972)). In this work we apply the GBD method to treat directly the mixed 0/1 structural design problem in the sense described by Munoz (2010a,b). This technique was first introduced by Benders (Benders' Decomposition, (BD), Benders (1962)), and aimed to solve linear mixed-integer problems. The method was generalized to a particular class of nonlinear mixed-integer problems in Geoffrion (1972), where the name Generalized Benders' Decomposition (GBD) was introduced. Furthermore, a new generalization to a larger class of nonlinear problems was introduced by Lazimy (1986). In the last two decades, a large number of publications about variations and improvements of the method (specially in the BD method, as Rei et al. (2008), Magnanti and Wong (1981)) and applications in industry have been published (Noonan and Giglio (1977), Habibollahzadeh and Bubenko (1986)). It seems that this tendency will continue in the coming years. With respect to structural optimization, Munoz (2010a,b) applied GBD for the design of simple 2-D truss structures. That article and the present are up now to our knowledge, the only existing applications of GBD to structural optimization. Munoz (2010a,b) pointed out the limitation of the method to solve large-scale topology optimization problems (i.e. many sub-domains and design variables) in terms of convergence within a reasonable amount of time and memory. Therefore, in the case of large-scale problems, the capacity of this and other methods of integer optimization is still limited. A way to treat large-scale problems is to reformulate the SAND form in a nested formulation, where the state variables are eliminated by use of the state equations. This leads to an optimization problem in the discrete variables only. A relaxation of this problem is obtained if the integer variables are allowed to take on continuous variables. The continuous variable approach typically uses penalization of intermediate variable values to obtain integer feasible solutions eventually. (see e.g. Bendsøe and Sigmund (1999) for a review of interpolation schemes in topology optimization). In topology optimization, the SIMP scheme (Solid Isotropic Material with Penalization) seems to be the scheme of choice for most applications involving two phases (solid/void or solid1/solid2). However, the scheme is not easily generalized to an arbitrary number of phases. Apart from this, the penalization introduces local minima in the design space meaning that for some situations, intermediate densities do appear no matter how high the penalization becomes, Stolpe and Svanberg (2001b). An alternative interpolation scheme is the so-called RAMP (Rational Material with Penalization) proposed by Stolpe and Svanberg (2001a). For a certain penalization parameter value this scheme yields a concave compliance function, meaning that optimal solutions are located at the boundary of the feasible set, i.e. 0/1 solutions. The size (which is not necessarily related to the difficulty) of the problems that we want to attack is roughly characterized by two quantities. The first is the size of the analysis problem, i.e. the number of continuous state variables (the free degrees of freedom) in the finite element discretized analysis problem. The number of degrees of freedom ranges from a few hundred up to millions. In this paper, we stay below 10^6 . The second quantity is the size of the design problem, namely the number of integer design variables which is related to the design domain discretization and the number of candidate materials. The coarsest design domain discretization may be if the same material (out of a set) is to be chosen throughout the structure. A more realistic and interesting design problem is if we are to choose the optimal material in a larger number of design sub-domains. These could be given as a layered configuration covering large areas of the structure or even layered configurations changing from element to element. For the considered applications the number of design sub-domains is typically up to about 10^4 . FIXME.

The number of candidate materials is typically between four and up to about fifteen. These numbers could be obtained for instance in optimal laminate design where where the layerwise design question is to choose among an orthotropic material oriented at four or twelve predefined distinct directions as well as other physically viable candidate materials such as polymeric foam, balsa wood or other materials. (A small paragraph stating why such candidate materials are relevant in a DMO problem).

Apart from the above mentioned approaches for discrete optimization problems a number of heuristic approaches such as genetic and evolutionary algorithms exist. However, these approaches give no guarantees in terms of convergence to a global optimum and furthermore they typically require many function evaluations which may be prohibitive.

Organization of the Paper

In Section 2 we present the formulation of the discrete mass constrained minimum compliance problem. In Section 3 follows a description of a method to solve the discrete problem by use of Benders' decomposition. It turns out that this method may take advantage of solutions with lower objective function value which help tightening the gap between the lower and upper bound of the global optimum objective function value. Therefore, all solutions with this property (discrete or even continuous solutions) are expected to improve the convergence of the method. This leads to a description of one such method in Section 4, namely a continuous relaxation, that may be used for this purpose. The continuous relaxation is also used as part of a rounding heuristic described in Section 5. In Section 6 we present a method combining the previously described procedures and point out in what way this improves its practical and numerical performance. Following the presentation of the methods developed in this work, in Section 8 we demonstrate numerical examples solved by each of the methods independently as well as examples where both methods are used in combination to demonstrate the improvement gained through the combination of the methods. Finally, we round off with a discussion in Section 10, point to future use of the methods and conclude in Section 11.

2 Problem Formulation

Consider a (layered shell) structure $\Omega \in \mathbb{R}^3$. We aim to construct an optimization model to design a multi-material composite laminated structure. Ω is considered as a fixed design domain, where the distribution of material has to be assigned. A set of candidate materials with different mechanical and mass properties is provided, and our goal is to find, if a suitable objective function is given, the optimal distribution of the materials satisfying the imposed constraints. We assume linear elasticity for the mechanical model, which we discretize by finite elements, reducing the continuum problem to a finite-dimensional problem with degrees of freedom, $u \in \mathbb{R}^d$. Considering appropriate support/boundary conditions and a given load condition, $f \in \mathbb{R}^d$, the finite element equilibrium equations take the following form

$$K(x)u = f \quad (1)$$

where the stiffness matrix $K(x) \in \mathbb{R}^{d \times d}$ depends on the material constitutive properties as well as the (fixed domain) finite element strain-displacement relation as defined in (7). The constitutive properties are assumed to be given by Hooke's law

$$\sigma = E\varepsilon \quad (2)$$

where E is the constitutive matrix.

Given a number of predefined materials, n^c , with known constitutive properties E_i and mass density ρ_i , we want to minimize the compliance under static loading. In order to build the optimization model, a second discretization of the design domain Ω is made. This discretization is for the design problem, and it is independent of the finite element discretization. More precisely, the second discretization of Ω introduces a set of n^d design subdomains, and a material selection variable $x_{ij} \in \{0, 1\}$ is introduced to represent the selection of a given candidate material, $i \in \{1, \dots, n^c\}$, in every design domain, $j = 1, \dots, n^d$.

$$x_{ij} = \begin{cases} 1 & \text{if material } i \text{ is chosen in design domain } j \\ 0 & \text{if not} \end{cases} \quad (3)$$

A (design) subdomain may be a single layer in an element, a layer covering multiple elements, multiple layers within a single element etc. We remark that the discretization of the design domain may, or may not coincide with the finite element discretization. The total number of design variables n is given as the sum of the number of candidates defined within each design sub-domain, i.e. in general $n = \sum_{j=1}^{n^d} n_j^c$. However, if the number of candidate materials in all sub-domain is identical the number of variables is simply $n = n^d \cdot n^c$.

In each subdomain, it is required that only one material is chosen. This is enforced by the following linear equality constraints also called generalized upper bound constraints.

$$\sum_{i=1}^{n_j^c} x_{ij} = 1 \quad \forall j \quad (4)$$

In each subdomain, the design-dependent mass density is given by $\rho_j(x) = \sum_{i=1}^{n_j^c} x_{ij} \rho_i$ and consequently the total mass of the structure is

$$M(x) = \sum_{j=1}^{n^d} \rho_j(x) V_j = \sum_{j=1}^{n^d} \sum_{i=1}^{n_j^c} x_{ij} \rho_i V_j, \quad (5)$$

where V_j is the (fixed) volume of subdomain j . We consider the discrete minimum compliance, mass constrained problem given by

$$\underset{x \in \mathbb{R}^n, u \in \mathbb{R}^d}{\text{minimize}} \quad c(x) = f^T u(x) \quad (6a)$$

$$\text{(OP)} \quad \text{subject to} \quad K(x)u = f, \quad (6b)$$

$$(M(x) \leq \overline{M}) \quad (6c)$$

$$\sum_{i=1}^{n_j^c} x_{ij} = 1, \quad \forall j, \quad (6d)$$

$$x_{ij} \in \{0, 1\}, \quad \forall i, j \quad (6e)$$

where f are design independent nodal loads, $u(x)$ are the nodal displacements obtained as the solution to Equation (1) and $M(x)$ is the total mass of the structure, Equation (5), which is limited by \overline{M} . The only assumption we make with respect to \overline{M} , is that it must satisfy

$$0 < \overline{M} < \sum_{j=1}^{n^d} \max_i \{\rho_i\},$$

So the problem is not infeasible, neither has a trivial solution. The mass constraint is only relevant for multi-material problems where the candidate materials have different mass density. In the case of pure fiber angle selection problems (i.e. same physical material at different orientations), the mass constraint is redundant since all candidate materials in these problems have the same mass density.

3 Generalized Benders' Decomposition Applied to 0-1 Design Optimization Problems

In this section, we introduce the resolution of the problem (6) by means of Generalized Benders' Decomposition (GBD); we give a brief description of the method, and introduce an important theoretical result with respect to the convergence of the algorithm to a global optimum. Then, we characterize the conditions and modes to improve and accelerate the practical convergence of the method.

3.1 Description of the Method

In this section, we present the resolution of the problem (6) by means of the Generalized Benders' Decomposition (GBD, see Geoffrion (1972)). GBD is a known optimization algorithm for nonlinear

mixed-integer problems. It is based on separating the optimization model into two sequences of simpler optimization programs. The first sequence of problems only considers the integer variables of the problems, plus a single scalar continuous variable, making a sequence of linear mixed integer problems. The other sequence deals only with the set of continuous variables, and it is given by a special reformulation of the equilibrium equations.

In Munoz (2010a), a standard topology optimization in its mixed-integer formulation was studied. We consider the stiffness matrix $K(x)$ as linear in the design variables

$$K(x) = \sum_{ij} x_{ij} B_j^T E_i B_j = \sum_{ij} x_{ij} K_{ij} \quad (7)$$

where $B_j \in \mathbb{R}^{6 \times d}$ is the finite element strain-displacement matrix for subdomain j , $E_i \in \mathbb{R}^{6 \times 6}$ is the constitutive matrix for the i 'th candidate material, and $K_{ij} = B_j^T E_i B_j$ is the resulting positive semidefinite local stiffness matrix related to the design element j for the candidate material i . Under this assumption, the GBD method applied to the minimum compliance problem given by

$$\begin{aligned} & \underset{x \in \mathbb{R}^n, u \in \mathbb{R}^d}{\text{minimize}} && c = f^T u && (8a) \\ \text{(OP-GBD)} & \text{subject to} && K(x)u = f, && (8b) \\ & && \rho^T x \leq \overline{M}, && (8c) \\ & && Ax \leq b, && (8d) \\ & && x \in \{0, 1\}^n, && (8e) \end{aligned}$$

converges in a finite number of iterations to a global optimal design. Problem (8) corresponds to the problem (6), where a general set of linear constraints $Ax \leq b$ is replaced by the particular case of the selection material constraints $\sum_{i=1}^{n^c} x_{ij} = 1, \forall j$.

The GBD algorithm applied to the the problem (6) supposes the inclusion of two sequences of simpler optimization problems. The first is the sequence of the so called subproblems (SP), considering the displacement field u (a continuous variable). The second is the sequence of master problems (MP), considering the design variable x (a 0-1 variable).

The subproblem corresponds to the problem (6) with the variable x is fixed to a given design $x := x^k \in \{0, 1\}^n$, so the optimization problems only takes into consideration the displacement field u

$$\begin{aligned} & \underset{u \in \mathbb{R}^d}{\text{minimize}} && c(x^k) = f^T u && (9) \\ & \text{subject to} && K(x^k)u = f. \end{aligned}$$

Problem (9) simply corresponds to solve the analysis problem $u^k = K(x^k)^{-1}f$ and evaluate the compliance related to the design x^k , by $c(x^k) = f^T u^k$. Notice that we are implicitly pointing out that the analysis problem possesses a unique solution. This is due to the fact that the global stiffness matrix $K(x^k)$ is positive definite, since the optimization problem (6) is not a strict topology problem, but a multi-material selection problem, which means that all candidate materials included have non-vanishing stiffness.

The master problem, is defined almost exactly as it was defined in Munoz (2010b), and we repeat its description and notation used, adapted to the problem (6). The master problem for iteration N corresponds to the following linear mixed 0-1 problem.

$$\begin{aligned} & \underset{x \in \mathbb{R}^n, y \in \mathbb{R}}{\text{minimize}} && y && \\ & \text{subject to} && l_c^*(x, u^k, \nu^k) \leq y, \quad \forall k = 1, \dots, N, && \\ & && \rho^T x \leq \overline{M}, && \\ & && \sum_{i=1}^{n^c} x_{ij} = 1, \quad \forall j && \\ & && x \in \{0, 1\}^n, && \end{aligned} \quad (10)$$

where l_c^* is a function defined as

$$\begin{aligned} l_c^*(x, u^k, \nu^k) &= f^T u^k + \nu^{kT} [x^k - x], \\ \nu^k &= \left(u^{kT} K_{11} u^k \quad u^{kT} K_{12} u^k \quad \dots \quad u^{kT} K_{n^c n^d} u^k \right)^T, \end{aligned} \quad (11)$$

where u^k is given by the subproblem (9), and x^k is the solution of the k -th relaxed master problem.

The following explanation rule is equivalent to the ones stated in Munoz (2010a). We repeat it almost exactly, since they define the notation used through the article.

Remark 1. *The notation used here is slightly different from the one used in Munoz (2010a,b), where the expression ν^k was defined differently. It is important to have this in mind before comparing the equations and algorithms presented here with those in the mentioned articles.*

3.2 GBD by Level Sets

In Munoz (2010c), a variation of the GBD technique, named *GBD by level set cuts*, was introduced, showing a significant improvement with respect to the classical GBD algorithm. The principle of this algorithm is essentially the same, but instead of including GBD cuts related to the solutions of the master problems, a bisection procedure allows to find a non integer points at the level set of the incumbent solution. The bisection procedure requires to have previously computed the solution of the continuous relaxation of the problem. In Munoz (2010c), all details about this technique are explained extensively. Along this article, we will only use this technique for all experiments. Since we do not use the classical GBD algorithm at any moment, will use the name GBD algorithm to refer to this improved variation of the GBD technique.

3.3 Convergence of the Algorithm

The convergence of the GBD algorithm to a global optimum was proven in Munoz (2010a), and it is based on the convexity of the relaxation to $[0, 1]^n$, of the projection of the compliance function $c(x, u) = f^T u(x)$ on the design variable space $c(x) = f^T K(x)^{-1} f$. The proof is rather technical and not given here.

3.4 Description of the Algorithm

The GBD algorithm is briefly described in this subsection. A flowchart with the algorithm description is shown in figure 1. A complete and detailed statement of the algorithm is presented in Munoz (2010a).

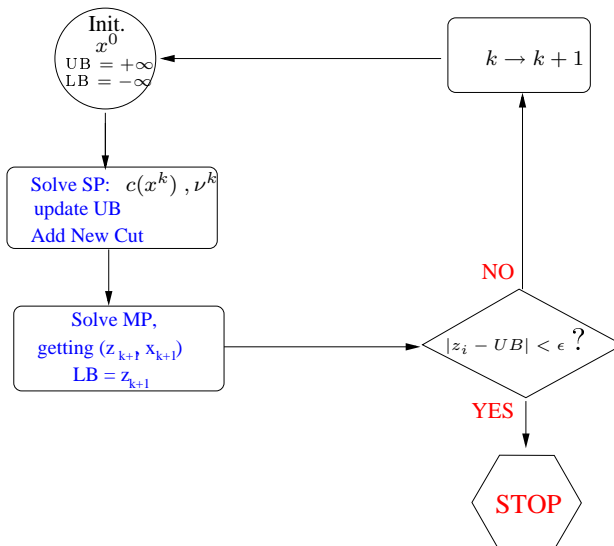


Figure 1: Flowchart of the GBD Algorithm

The main idea of the GBD algorithm is to approximate the projection of the nonlinear mixed-integer problem on the integer design variable. This approximation produces a linear mixed-integer problem, where all the continuous variables of the original problem have been removed by the projection operation, and only one scalar continuous variable is considered. At each iteration the algorithm adds a linear constraint which is a linear approximation of the projected compliance function at a given design x^k . You can see how these linear constraints approximate the compliance on Figure 2.

Algorithm 1 Generalized Benders' Decomposition

```
UB ← ∞
LB ← -∞
k ← 0
x0 ∈ [0, 1]n such that it is mass feasible
ε > 0
while |zk+1 - UB| > ε do
  uk, νk ← solve (SP) using xk
  lc*(x, uk, νk), see (11)
  (xk+1, zk+1) ← solve (MP) including lc*(x, uk, νk) ≤ y, see (10).
  LB = zk+1
  if c(xk+1) ≤ UB then
    UB ← c(xk+1)
  end if
  k ← k + 1
end while
```

It is important to remark that even if there is a theoretical convergence of the method in a finite number of iterations, there is no guarantee that this convergence is going to be reached within reasonable CPU resources (time and memory). This is due to the fact that a master problem, which is a linear mixed 0 – 1 problem, takes longer and longer to be solved and consumes more memory, as more linear constraints are added. As a consequence, the size of the problem must be selected in a way that the convergence of the method is observed in numerical experiments. There are also other parameters that need to be taken into account in order to have practical convergence. For example, the ratio between the stiffness among the different candidate materials influences the ability of the algorithm to converge. This will be shown on the numerical experiments section. CGH: do we actually show this in the numerics?

4 Convex Continuous Relaxation

The original non-convex mixed-integer program, (OP), can be reformulated in so-called nested form as an integer program with a convex objective function if the displacements u are eliminated by use of the equilibrium condition (given that the stiffness matrix $K(x)$ is non-singular, i.e. $u(x) = K(x)^{-1}p$). Thereby we obtain an equivalent integer program with a convex objective function in the design variables x only. Furthermore if the integer requirement on the design variables is relaxed, a convex continuous optimization problem is obtained

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad c(x) = p^T K(x)^{-1} p \quad (12a)$$

$$(R) \quad \text{subject to} \quad \sum_{i,j} x_{ij} \rho_i V_j \leq \overline{M} \quad (12b)$$

$$\sum_i x_{ij} = 1 \quad \forall j \quad (12c)$$

$$0 \leq x_{ij} \quad \forall (i, j) \quad (12d)$$

Note that the generalized upper bound constraints from (4) ensure that the variables fulfill $x_{ij} \leq 1$. Thus there is no need for an upper bound on the variables and it is sufficient to ensure non-negative design variables.

The optimization problem given by (R) is convex as shown by Svanberg (1994); Stolpe and Stegmann (2008), and thus a locally optimal solution x_R^* is also a global optimum of (R), and such solution may be obtained using any suitable nonlinear optimization algorithm such as SNOPT (Gill et al., 2005) or Ipopt (Wächter and Biegler, 2006). Furthermore, (R) is a (nested form) continuous relaxation of (P) and it has a larger feasible set than (P). In other words the feasible set of (P) is a subset of the feasible set of (R). Thus,

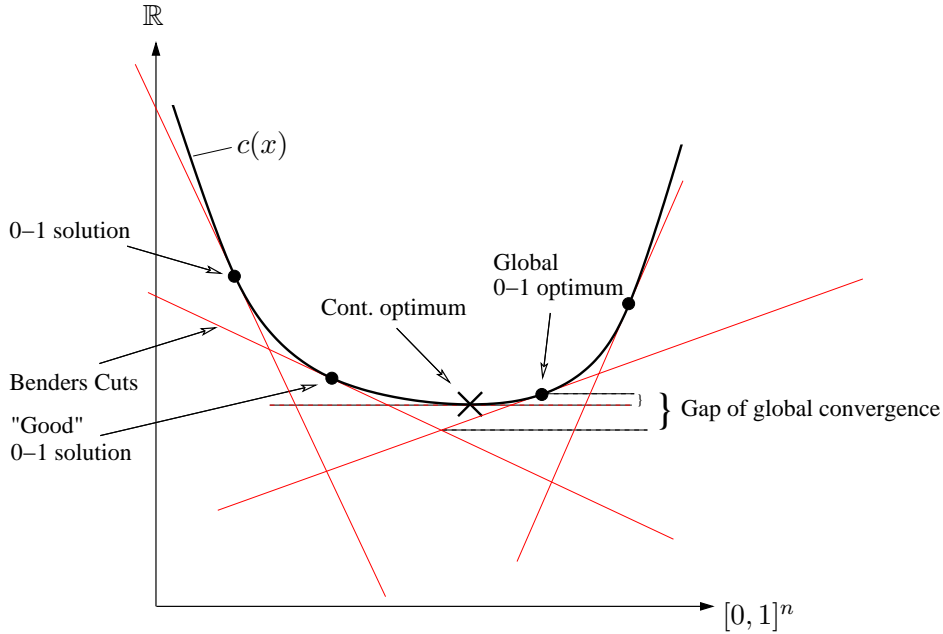


Figure 2: Conceptual illustration of the GBD algorithm on an unconstrained problem. The projection of the compliance $c(x)$ is approximated by linear functions (in red). In case of a constrained problem the continuous optimum will in general not generate a horizontal cut.

- If the optimal solution to (R) happens to be an integer solution then it is also an optimal solution to (P).
- The optimal solution to (R) is better than or as good as the solution to (P), i.e. $c(x_R^*) \leq c(x_P^*)$. Thus, it may be used as a lower bound estimator for the original 0/1-problem.
- If there is no feasible solution to (R) then there is no feasible solution to (P) either.

The motivation for solving a convex continuous relaxation in the process of attacking the integer optimization problem is that it can be solved to global optimality with reasonable resources, and thereby it may be used as a relatively fast way of obtaining a good lower bound assessment of the attainable performance of the original integer optimization problem. This lower bound can be used as a valid lower bound within GBD if it is better than the best valid lower bound obtained from the master problems (MP). Recall that the goal within GBD is to improve iteratively the lower and upper bound so as to close the gap between them. If a good valid lower bound can be obtained early in the solution process of GBD, the sequence of sub- and master problems the method is more likely to converge within reasonable CPU resources. Depending on the specific problem, the continuous optimum may give valuable information about the integer solution. As stated above, if the continuous solution is integer-valued it is in fact the integer optimal solution. This situation, however, is very unlikely and virtually never seen in the considered types of problems. Nevertheless, it is not unusual to see that a fraction, typically 50 – 90%, of the continuous variables attain integer values in the continuous optimum, and furthermore most domains at least have some of their variables at the lower bound, i.e. in many domains the continuous optimum has "discarded" some of the candidate materials. Note that this situation, does not mean that those materials are not part of the optimal integer solution, but it still gives information about a provenly good design, though continuous. The (reasonable) hope though is, that the solution to the integer problem is close in some sense to the continuous optimal solution. If many of the continuous variables take integer values in the optimal continuous solution, this hope is most certainly reasonable. The larger the number of continuous valued variables in the optimal continuous solution, the less reasonable this assertion is. These observations motivate the use of a heuristic procedure that can obtain a good upper bound (incumbent solution) in terms of an integer and feasible solution with a good objective function.

5 Use of Heuristics

As described in the section on GBD a (possibly long) sequence of MILPs are solved in the Master Problems (MP). MILPs are typically solved by implicit enumeration strategies such as branch-and-bound/cut algorithms. These algorithms rely on the solution of relaxations at each node visited in the enumeration tree and on basis of this solution, branching in the tree is done. The efficiency of these algorithms relies heavily on the use of heuristics to obtain feasible solutions as well as heuristics for improving feasible solutions. State-of-the-art MILP solvers such as the commercial codes CPLEX and Gurobi as well as the academic code SCIP (Achterberg, 2007) employ a number of heuristics to speed up the convergence rate.

5.1 GBD-RENS

The use of heuristics within branch-and-bound/cut algorithms is well-known and standard nowadays. In this paper we propose to also use heuristics to enhance the rate of convergence of the GBD algorithm itself. Thus we use heuristics to obtain a good (but not necessarily optimal) integer solution early in the solution process as a sort of "warm start" of the GBD algorithm. The motivation for doing so was pointed out by Munoz (2010a,b) where it was shown that the GBD algorithm may take advantage of a good initial solution (upper bound) as well as a lower bound as obtained from a relaxation. As already described, we solve the continuous relaxation of a nonlinear integer program. This solution yields a lower bound on the attainable performance of any integer feasible solution and furthermore it is also used in a Large Neighborhood Search heuristic. The heuristic is inspired by the so-called Relaxation Enforced Neighborhood Search (RENS) proposed for MILPs by Berthold (2007). The idea of this heuristic is to solve a continuous relaxation to optimality and observe which variables that attain integer values in this solution. Integer-valued variables are then fixed at their obtained value and a Large Neighborhood Search in the remaining intermediate-valued variables is performed through a sub-MINLP where only the intermediate-valued variables from the relaxation are considered (now as integer variables). Thus, we formulate the rounding heuristic as a sub-MINLP. The resulting sub-MINLP is solved using GBD on the reduced problem. The size and thereby the cost of solving the sub-problem naturally depends on the integrality of the continuous solution. Note that by solving the sub-problem to optimality we obtain *the* best rounding possible for a given continuous relaxation solution. Also, if the feasible set of the sub-MINLP turns out to be empty, no feasible rounding of the continuous solution exists, see Berthold (2007). The solution obtained for the sub-MINLP is passed back to the global problem and used as a good initial solution in the complete GBD. Also note that the continuous relaxation of the complete MINLP minimum compliance and the corresponding sub-MINLP problems have exactly the same solutions. Therefore, the continuous relaxation of the sub-MINLP problem does not give any additional information. For some examples the resulting sub-MINLP problem is not easy to solve either. This could happen if the fraction of fixed variables is not big enough, and thus there is no real advantage in attacking the sub-MINLP problem. An alternative to overcome this complication, is to introduce a variation of the GBD-RENS heuristics, which is to do a selected rounding of the solution of the continuous relaxation before fixing variables with integer values. This means that we set a threshold $\lambda_s \in [0, 0.5]$, such that each design variable with a value outside the interval $[0.5 - \lambda_s, 0.5 + \lambda_s]$ in the solution of the continuous relaxation is rounded. In exchange, it is also expected that if a variable attains a non-integer value, it is less likely that this variable will have an integer value in the solution of the original integer problem. So it is clear that the larger the number of fixed variables, the less likely it is to be able to find an optimal solution when treating the sub-MINLP problem. In addition, it is even possible that, if too many variables are fixed, the resulting sub-MINLP may not be a feasible problem. As a consequence, to make the heuristic more robust with respect to the type of problem, a second variation of the heuristic is introduced, by running the heuristic procedure iteratively, in such a way that the number of fixed variables decreases each time the GBD-RENS heuristic is executed. This iterative procedure is controlled by the parameter α_s , which is updated each time before starting it. Another aspect to take into account is the fact that this heuristic may be used to control the size of the resulting sub-MINLP we are willing to solve. This would be helpful if we want to attack a design problem of maybe 50.000 variables. Suppose that in this hypothetical example, the continuous relaxation solution obtained has for instance 35.000 $0 - 1$ values. In this case, the remaining sub-MINLP problems has 15.000 variables, which is still too big. In this case, we are able to control the size of the sub-MINLP problem by setting a value of the threshold parameter $\lambda_s < 0.5$. We could also set the minimum percentage of variables to

be fixed in the sub-MINLP problem. In this way, the use of the modified GBD-RENS heuristic may lead to fix maybe 48.000 variables. Then we have a sub-MINLP of 2.000 variables, which is more likely to be succesfully attacked by the GBD-RENS heuristic.

5.2 Modified Compliance Function (Quadratic Interpolation Heuristic?)

The performance of the GBD algorithm can be improved by use of a different law for assembling the stiffness matrix, as it was done in Munoz (2010a,b). This means that the stiffness matrix given by (7), is replaced by

$$K(x) = \sum_{ij} [\alpha x_{ij} + (1 - \alpha)x_{ij}^2] B_j^T E_i B_j \quad (13)$$

where $\alpha \in [0, 1]$ is a parameter controlling the mixture of two interpolations schemes. It is important to note that for any value of $\alpha < 1$, the continuous relaxation is not convex, and therefore the GBD method can not longer guarrantly convergence to global optimality. For that reason, for these values of α , the GBD method is no more than a heuristic to find good solutions. In addition, numerical experiences show that for a low value of the mixture parameter α , the GBD algorithm converges quickly, but less chances of finding good solutions exists. Therefore, again, the use of an iterative procedure, calling this heuristic several times, updating each time the value of α , from $\alpha_0 \in (0, 1)$ to $\alpha = 1$ seems to be a robust procedure to find designs with low objective value in short time.

Remark 1. *Note that all heuristics described here produce one or several candidate designs. These solutions not only helps in the improvement of the upper bound of the optimal value, but also produce one compliance GBD cut per each of these solutions. This remark is important in order to notice that if a problem is large in terms of design variables, probably a large cpu-time is used in finding good solution candidates.*

6 Combining Methods

In this section we present a way of improving the performance of the optimization algorithm by combining the Benders algorithm, with solutions to continuous relaxations of the original problem (6). We describe the implementation of these combined methods, and indicate possible variations of them. A comparison of the performance of the different combinations is given in Section 8 on numerical examples.

As it was indicated in (reference to MunozStolpe), the Benders decomposition method applied to the minimum compliance problem 6 converges to an optimal solution in a finite number of iterations. However, in practice, this number is unknown and could potentially be very large. Furthermore, the size of the master problem grows with the number of iterations (one or more cuts added at each iteration), leading to a longer solution time for each master problem, which may prevent the algorithm to converge in a reasonable amount of time. On the other hand, at any stage of the algorithm, it is possible to asses the closeness of the current solution to the global optimum. This information might be useful, depending on the order of magnitude of the gap between the best bounds obtained. If this is not the case, one could use any method that gives a better estimate of a lower bound for the global optimum. As shown by (MunozPaper on Pareto Optimal Cuts) the quality of any cut is defined according to their Pareto dominance value, which depends on the objective function value of the solution generating the cut. Thus, better objective feasible solutions may in the case of the problem given by 6 be used to generate good cuts in the sense that they have a positive influence on the convergence rate compared to dominating (less good) cuts.

To sum up, the convergence rate of Benders decomposition may be improved by

1. using the solution to a convex continuous relaxation to improve the estimate of a lower bound for the global optimum. This continuous solution also generates a good cut that can be included.
2. including cuts generated from good 0/1-solutions.

Ad 1) Recall that the Voigt interpolation scheme is simply the natural continuous relaxation of the originally 0/1-valued feasible design space. The model induced by this relaxation is convex, satisfying constraint qualifications, and therefore a global optimum exists, its unique, and it corresponds to any point satisfying the KKT conditions. This solution may be found by use of any suitable NLP optimization

algorithm, such as SNOPT (ref. to SNOPT), Filter-SQP (ref. ...), etc. In fact this solution generates the only non-dominated cut, that is, the best cut in the sense of Pareto dominance.

Ad 2) A way to generate good 0/1-solutions is to use a continuation approach to make the solutions to the continuous relaxations converge to 0/1-solutions within a tolerance, and finally round these solutions to 0/1. One such approach has been described in detail in Section 4 but any other method producing good 0/1-designs may be used as well. One important thing to note is that the design should stay feasible after rounding the solution. This is not ensured automatically by the rounding heuristic which only rounds without consideration of feasibility of the constraints or the optimality of the rounded solution. Thus, for some problems it may be necessary to improve the heuristic such that the rounded design is indeed feasible.

TODO

- Presentation of basic idea/concept - statement of method, refer to flow chart in Benders section. Present rounding heuristic idea: solving tighter constrained continuous relaxations if previous rounded solution was infeasible after rounding.
- Give overview of different possibilities of combining the methods - mainly Benders' alone, Benders' including Voigt solution cut, and Benders' + Voigt solution cut + 0/1 solution cut. A table comparing these results for one example.

7 Implementation

In this section, we describe briefly, the implementation of the algorithms described in the article in numerical experiments. The GBD algorithm was implemented for the design of multimaterial composite laminated structures. The code was written in the platform for analysis and optimization of shell structural models MUST (reference??) The resolution of the Master Problem was attacked the mixed-integer optimization solver GUROBI (Gurobi Optimization (2009)). The continuous relaxation to the minimum compliance problem was attacked with the NLP solver SNOPT (ref). All numerical examples were run on the Fyrkat cluster (Description of Fyrkat).

8 Numerical Examples

In this section, we present a set of numerical examples to be solved with the proposed algorithms applied to optimal design of multimaterial (laminated) composite structures. This type of structure is often modeled as shells, and therefore, a shell finite element (FE) discretization is used to perform the static equilibrium analysis. The design discretization does not necessarily match the FE discretization, as it will be the case in many of the examples. For some examples we make use of so-called patches, which are groups of elements having the same design variable associated with them. This serves as a way of reducing the number of design variables as well as a means of providing for more manufacturing near designs in the sense that the laminates are typically produced using mats covering larger areas (i.e. multiple elements) of the structure.

Table 1 shows the general description of the set of examples included in the article. It includes the number (*Prob*) and Name (*Description*) of the problem, the number of candidate materials considered in the problem (*# Mat.*), the design discretization of the problem (*Design Discr.*) in the format $PaxbxcL$, where a, b represents the in-plane design discretization, and c represents the number of layer of the structure considered in the design problem. The field *Variables* states the total number of design variables introduced in the optimization problem. *FE Discr.* specifies the FE discretization of the problem, in the format $Edxe$, where d, e represents the finite element analysis discretization in each direction in the plane. *# LC's* stands for the number of load cases considered in the problem. Finally, \overline{M} represents the mass limit for the mass constraint of the design problem.

8.1 Examples 1-3

These first three examples illustrate the application of the proposed method to a doubly curved parabolic shell structure. All three instances are solved using an FE discretization of 32 by 32 shell elements in the plane of the structure. In all three examples the design discretization through the thickness comprises eight layers of equal and fixed thickness ($8 \cdot 0.01m$). In the plane, Example 1 has 2 by 2 design domains

in each layer, Example 2 has 4 by 4 design domains per layer and Example 3 8 by 8. In all three examples the structure is subjected to one load case: a central point load acting in the vertical direction. The design task is to select the optimal material out of five possible in each domain. Four of the materials are instances of a relatively stiff orthotropic material oriented at four pre-defined directions ($-45^\circ, 0^\circ, 45^\circ, 90^\circ$) defined relative to the global x-axis. The fifth candidate material is a polymeric sandwich foam of low weight and stiffness.

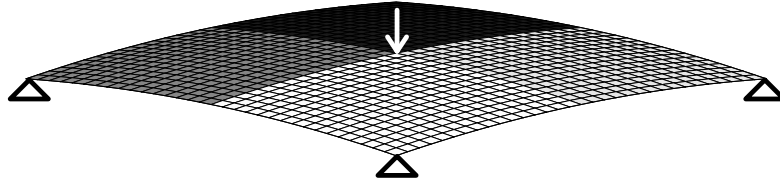


Figure 3: Example 1: sketch of parabolic shell. Geometry: base lengths $1.0 \cdot 1.0 \text{ m}^2$, height 0.1 m , shell thickness 0.08 m ($= 8 \cdot 0.01 \text{ m}$), design discretization in greyscale (2×2 patches), analysis discretization (32×32 elements), vertical point load in the center and hinged support at each corner. Short notation: P2x2x8L, E32x32.

!!!!!!! Table with material properties !!!!!

8.2 Examples 4-7

These four examples illustrate optimal discrete fiber angle orientation on a plane disc problem. All four instances are solved using an FE discretization of 32 by 32 shell elements in the plane of the structure. The disc is clamped along the left edge and subjected to a vertical downward acting point load in the lower right corner. The design discretization for the three examples is of increasing resolution in the plane of the disc, Example 4 has 4 by 4 design domains in the plane, Example 5 has 8 by 8 , Example 6 has 16 by 16 and Example 7 32 by 32 . The design problem is a pure fiber orientation problem, i.e. all candidate represent the same orthotropic material oriented at four ($-45^\circ, 0^\circ, 45^\circ, 90^\circ$) or twelve ($-75^\circ, -60^\circ, \dots, 0^\circ, 15^\circ, \dots, 90^\circ$) distinct directions. Thus, the example has no mass constraint (of relevance). The material properties are identical to those of the orthotropic material in Example 8-9 (!!!!!!!!!!!!!!TODO: check that this is correct!!!!!!!!!!!!).

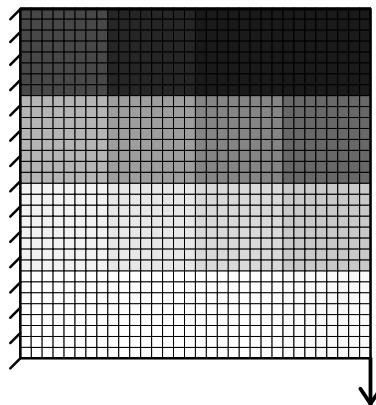


Figure 4: Example 4: sketch of clamped membrane disc. Geometry: side lengths $1.0 \cdot 1.0 \text{ m}^2$, thickness $0.5 \cdot 10^{-3} \text{ m}$, design discretization in greyscale (4×4 patches), analysis discretization (32×32 elements), vertical downward acting point load at lower right corner. Clamped (all DOFs fixed) along left edge. Short notation: P4x4x1L, E32x32.

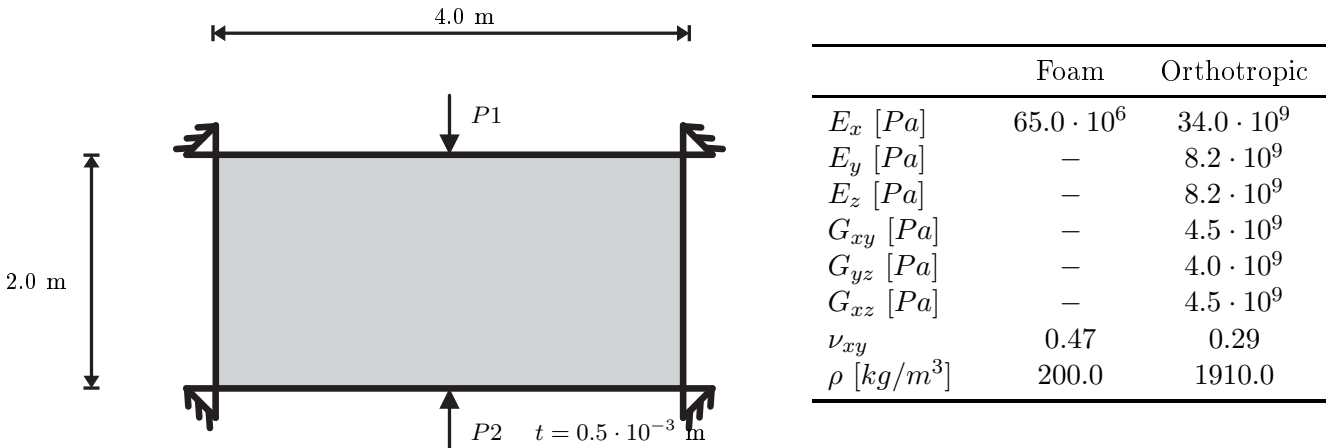


Figure 5: Example 8-9. Left: Domain geometry and boundary conditions. Loads act independently. Right: Material properties in principal material coordinate system for the candidate materials.

8.3 Examples 8-9

In these examples we solve plane problems with two independent load cases of equal importance ($w_1 = w_2 = 0.5$) and loads with equal magnitude ($|P1| = |P2|$) acting at midspan oppositely on each face. In both load cases the plate is hinged at all corners ($u_i = 0$), see Fig. 5. The physical domain within which the material is distributed is a rectangular disc of dimension $4.0m \times 2.0m \times 0.5 \cdot 10^{-3}m$. The domain is discretized by two different meshes, (20×10) and (40×20) respectively and in each design sub domain (=element) five candidate materials are possible. The first candidate material is a light and soft material representing e.g. isotropic polymeric foam and the remaining four candidate materials represent a heavier and stiffer orthotropic material oriented at four distinct directions ($-45^\circ, 0^\circ, 45^\circ$ or 90°). We set the mass constraint such that the heavy orthotropic materials can be chosen in at most 35% of the domain. The constitutive properties in the principal material coordinate system the orthotropic material and of the foam material are given in Fig. 5.

8.4 Example 10

The following very simple example illustrates the possibility of distributing a limited amount of material through the thickness of the domain as well as in the plane. A design domain is given in terms of a simply supported beam (discretized using shell elements) subjected to a uniform transverse pressure load in the vertical direction, see Fig. 6. The domain is discretized into 20 by 2 elements in the plane of the structure and five layers through the thickness. This discretization is used for the analysis as well as the design. The total volume of the design domain is $1.25m^3$. The mass density of the lightweight candidate material is $\rho = 200kg/m^3$ and that of the heavy candidate material is $\rho = 1910kg/m^3$. Thus with a total mass constraint of $1500kg$, heavy material can not be chosen in more than 58.5% of the total design domain corresponding to 116 element layers. The material properties of the candidate materials used in this example are identical to those shown in Fig. 5.

8.5 Examples 11-13

This set of examples demonstrates the ability to perform optimal multi-layered composite plate design. We solve the same design problem using different design discretizations through the thickness to investigate the influence on the optimal design. The physical domain within which the material is distributed is a quadratic plate of dimension $1.0m \times 1.0m \times 1.0 \cdot 10^{-2}m$. The plate is loaded at the center by a point load P and each corner is hinged ($u_i = 0$). A sketch of the problem is shown in Fig. 7. All three examples employ a (24×24) in-plane discretization. Example 11 is discretized through the thickness with 8 layers whereas example 12 and 13 have 4 layers. The candidate materials are identical to those in the previous example, i.e. a light and soft isotropic foam material and a heavy and stiff orthotropic material oriented at four distinct directions, see Fig. 5. For more information on the problem characteristics please consult

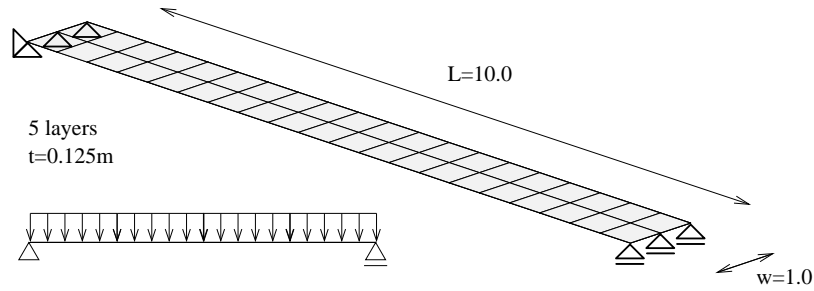


Figure 6: Example 10: Geometry: side lengths $10.0 \cdot 1.0 \text{ m}^2$, shell thickness 0.125 m ($= 5 \cdot 0.025 \text{ m}$), design discretization is identical to the analysis discretization (20×2 elements), transverse distributed pressure load and simply supported at each end.

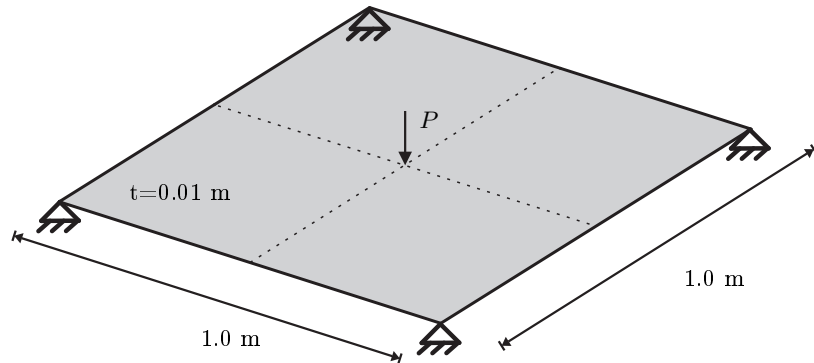


Figure 7: Example 11-13. Multi-layered (4 or 8) corner-hinged plate with point load applied at the center. See Fig. 5 for material properties.

Table 1.

8.6 Computational Experience

The 13 examples were used for setting 17 computational examples (in the case of examples 4, 5, 6 and 7, two different sets of material angle candidates were considered, generating one extra numerical sub-example for each of these ones). For each of these computational examples, 4 sets of numerical experiments were carried out. The first set of examples corresponds to the execution of the GBD algorithm without considering any heuristic procedure (GBD-1). The second set of examples corresponds to the execution of the GBD algorithm where the quadratic interpolation heuristic was used (GBD-2). The third set of examples corresponds to the use of the GBD-RENS heuristic procedure (GBD-3), and the fourth set of examples is the one combining these two heuristics before starting the GBD algorithm (GBD-4). The total CPU-time allowed for each example was 96 [h], and the algorithm is set to stop whenever the optimality gap reaches the tolerance of 1.0%. However, we consider as a satisfactory result, if the considered algorithm is able to find globally optimal solutions within an optimality tolerance of 5%. Besides, we set a maximum cpu-time of 3000[s] for the execution of each relaxed master problem. The reason for setting this limit value, is to avoid the MILP solver trying to solve to optimality the MILP problem which is too difficult and could take too many hours or even days.

9 Results

In this section, we present the computational results for the 13 (17) examples introduced in Sect. 8. In total 68 numerical examples were executed, which correspond to the execution of the 17 numerical examples described in Sect. 8, for each of the four methods described in Sect. 8.6 (GBD-1, GBD-2, GBD-3 and GBD-4).

The results for these sets of examples is shown in Tables 2, 3, 4, 5 respectively. These tables show

Prob.	Description	# Mat.	Design discr.	Variables	FE discr.	# LC's	\bar{M} (kg)
1	Parabolic Shell	5	P2x2x8L	160	E32x32	1	7.248
2	Parabolic Shell	5	P4x4x8L	640	E32x32	1	7.248
3	Parabolic Shell	5	P8x8x8L	2560	E32x32	1	7.248
4	Clamped Membrane	4/12	P4x4x1L	64	E32x32	1	n/a
5	Clamped Membrane	4/12	P8x8x1L	256	E32x32	1	n/a
6	Clamped Membrane	4/12	P16x16x1L	1024	E32x32	1	n/a
7	Clamped Membrane	4/12	P32x32x1L	4096	E32x32	1	n/a
8	Two Load Case	5	E20x10x1L	1000	E20x10	2	3.0
9	Two Load Case	5	E40x20x1L	4000	E40x20	2	3.0
10	Simply sup. beam	5	E20x2x5L	1000	E20x2	1	1500.0
11	LayeredPlate	5	E24x24x8L	23040	E24x24	1	6.8
12	LayeredPlate	5	E24x24x4L	11520	E24x24	1	6.8
13	LayeredPlate	5	E24x24x4L	11520	E24x24	1	10.6

Table 1: Summary of problem characteristics for the numerical examples.

the information about the best objective value attained by the algorithm *Best UB*, the objective value of the continuous relaxation solution (R) *Sol.*, the best value of the lower bound of the optimal solution obtained by the GBD method *GBD LB*, the final optimality gap at stop *O. Gap*, and the total number of valid GBD cuts included in total in the algorithm *# GBD cuts*.

For the set of examples executed with the algorithm GBD-1, 3 examples reached a final optimality gap smaller than 1.0%, 5 examples reached a gap < 3% (including the 3 that reached 1.0%), and 10 examples reached under 5.0%. For examples run with GBD-2, 4 examples reached the stop criteria 1.0%, 8 examples reached a gap < 3.0%, and 11 were under 5.0%. For the examples run with GBD-3, 3 examples reached the stop criteria 1.0%, 6 examples reached a gap < 3.0%, and 11 were under 5.0%. Finally, for the examples run with GBD-4, 4 examples reached the stop criteria 1.0%, 11 examples reached a gap < 3.0%, and 12 were under 5.0%. In addition, to make the comparison among the different algorithms more clear, Table 6 shows the final convergence gap *O. Gap* for each group of examples.

The comparison of the results in terms of convergence (*O. gap* at stop) for each set of numerical examples is presented in Table 6.

10 Discussion

In general, the performance shown of the four algorithms is satisfactory, and shows the general strengths of the GBD algorithm itself. The use of the presented heuristics shows how the method is able to find better designs, and therefore, is able to find more tight bounds for the assessment of global optimality of the algorithm, which is important specially when treating medium-large scale problems. The combination of the two presented heuristics showed the best results in the sense of obtaining solutions with the smallest objective value, and obtaining the lowest optimality gap among the examples not reaching the stop criterion of 1.0%.

Note that the combining heuristic procedures algorithm (GBD-4) reached a negative optimality gap at convergence for examples 4.1 and 5.1. This is nothing to worry about, since these values are subjected to the optimality tolerance for the solution of the master problem, obtained by the MILP solver. These values fall inside the usual optimality tolerance of any MILP solver. Thus, these numbers are perfectly reasonable.

Another important fact to point out, is the variation in the number of GBD cuts obtained through the different examples. In general, a number of around thousand GBD cuts is an reasonable number to consider in the algorithm. Above this number, the resolution of the master problem becomes fairly slow, and almost no further improvement in the lower bound is observed. Therefore, it is desired that the algorithm uses the best quality cuts in order to converge as early as possible. In Munoz (2010b) it was pointed out that the quality of the GBD cuts related to the compliance function depends strongly in

Prob.	Best UB	(R) Sol. LB	GBD LB	O. Gap	# GBD cuts
1	31.827	27.707	27.706	14.867	379
2	27.102	22.175	22.217	21.986	332
3	19.330	17.695	17.672	9.237	439
4.1	143.828	138.053	142.549	0.897	126
4.2	128.382	126.157	127.154	0.966	23
5.1	186.441	184.448	185.956	0.261	4
5.2	123.099	120.885	121.217	1.553	759
6.1	134.255	128.212	128.135	4.727	2029
6.2	121.809	116.903	116.879	4.197	1235
7.1	131.828	125.028	124.935	5.439	1225
7.2	117.337	113.506	113.460	3.376	479
8	568.568	22.017	22.092	2473.6	2501
9	825.281	22.718	22.672	340.19	595
10	163.273	160.178	161.354	1.189	467
11	30.108	28.760	28.691	4.688	241
12	68.842	34.841	34.725	97.587	694
13	21.356	20.529	20.520	4.024	503

Table 2: Numerical Results for GBD with out any Heuristics (GBD-1).

Prob.	Best UB	(R) Sol. LB	GBD LB	O. Gap	# GBD cuts
1	31.337	27.707	27.576	13.098	512
2	23.746	22.175	22.220	7.058	916
3	18.556	17.695	17.678	4.864	782
4.1	143.828	138.053	142.406	0.999	95
4.2	128.021	126.157	127.738	0.222	44
5.1	186.441	184.448	186.162	0.150	11
5.2	^a	120.885	^a	^a	^a
6.1	131.587	128.212	128.451	2.441	1186
6.2	120.012	116.903	116.867	2.659	1284
7.1	128.428	125.028	125.147	2.622	1009
7.2	116.032	113.506	113.642	2.103	1009
8	554.735	22.017	22.104	2409.6	993
9	840.459	22.718	22.671	3599.2	395
10	163.008	160.178	161.848	0.717	448
11	29.668	28.760	28.699	3.159	155
12	61.484	34.841	34.721	76.468	297
13	21.239	20.529	20.518	3.455	506

^a Example 5 needs to be re-run

Table 3: Numerical Results for the Modified Stiffness Matrix Heuristics (GBD-2).

Prob.	Best UB	(R) Sol. LB	GBD LB	O. Gap	# GBD cuts
1	31.834	27.707	27.574	14.892	179
2	24.025	22.175	22.185	7.230	677
3	18.734	17.695	17.675	5.873	649
4.1	143.828	138.053	142.609	0.855	103
4.2	128.021	126.157	127.511	0.400	29
5.1	186.441	184.448	186.411	0.016	13
5.2	123.163	120.885	121.181	1.636	699
6.1	132.205	128.212	128.156	3.114	949
6.2	120.799	116.903	116.928	3.311	449
7.1	129.662	125.028	124.991	3.707	799
7.2	117.304	113.506	113.499	3.346	449
8	35.767	22.017	22.096	61.870	1268
9	26.731	22.718	22.731	17.600	994
10	163.500	160.178	160.635	1.784	250
11	29.442	28.760	28.722	2.373	682
12	49.592	34.841	34.756	42.336	399
13	20.838	20.529	20.535	1.478	649

Table 4: Numerical Results for GBD-RENS Heuristics (GBD-3).

Prob.	Best UB	(R) Sol. LB	GBD LB	O. Gap	# GBD cuts
1	31.631	27.666	27.707	14.162	556
2	23.636	22.175	22.203	6.463	995
3	18.485	17.695	17.695	4.463	867
4.1	143.815	138.053	143.819	-0.002	129
4.2	128.021	126.157	128.021	0.0	58
5.1	186.441	184.448	186.537	-0.05	23
5.2	122.868	120.885	121.194	1.381	927
6.1	131.546	128.212	128.449	2.411	1975
6.2	119.784	116.903	116.880	2.464	1460
7.1	128.438	125.027	125.101	2.667	3593
7.2	116.075	113.506	113.506	2.264	1928
8	34.308	22.017	22.017	55.823	1230
9	26.537	22.718	22.718	16.810	298
10	162.675	160.178	162.208	0.288	902
11	29.327	28.760	28.730	1.974	93
12	45.133	34.841	34.805	29.539	1434
13	20.765	20.529	20.548	1.054	2615

Table 5: Numerical Results for GBD with Combining methods.

Prob.	GBD-1	GBD-2	GBD-3	GBD-4
1	14.867	<u>13.098</u>	14.892	14.162
2	21.986	7.058	7.230	<u>6.463</u>
3	9.237	4.864	5.873	<u>4.463</u>
4.1	0.897	0.416	0.855	<u>-0.003</u>
4.2	0.966	0.222	0.400	<u>0.000</u>
5.1	0.261	0.150	0.016	<u>-0.051</u>
5.2	1.553	727.2	1.636	<u>1.381</u>
6.1	5.696	2.441	3.114	<u>2.411</u>
6.2	4.197	2.659	3.311	<u>2.552</u>
7.1	5.439	<u>2.622</u>	3.707	2.667
7.2	3.376	<u>2.000</u>	3.346	2.303
8	2473.6	<u>2409.6</u>	61.870	<u>55.823</u>
9	532.8	3599.6	17.600	<u>16.810</u>
10	1.189	0.717	1.784	<u>0.288</u>
11	4.688	3.159	2.373	<u>1.974</u>
12	96.131	76.468	42.336	<u>29.539</u>
13	4.024	3.455	1.478	<u>1.054</u>

Table 6: Comparison of the convergence (O. Gap) attained by each algorithm. The smallest gap obtained among the four algorithms is underlined.

the compliance value. Thus, it is natural to expect that the better the solutions found, the less number of GBD cuts will be necessary for convergence of the GBD algorithm. Furthermore, we have chosen to compare the number of GBD-cuts, because it seems to be the most fair way to compare methods following different heuristic procedures in the context of the GBD algorithm. In fact, the best way to assess a heuristic procedure, is to determine the quality of the designs obtained by this procedure, in terms of objective value, and to count the number of candidate designs found by this heuristic. In this way, a heuristic providing for example 300 candidate designs to the GBD algorithm only could be compared in a fair way to the pure GBD algorithm, after the latter has reached 300 iterations since this can be considered as a different way of exploring this number of solutions. In this sense, heuristic procedures will most likely obtain the 300 candidate designs faster than the GBD algorithm, since the GBD algorithm needs to solve one MILP problem each time a new design is obtained. Besides that, the CPU time spent in solving the MILP is unpredictable, since it depends on the intrinsic combinatorial nature of each master problem.

Nevertheless, note that for small examples the use of any heuristic procedure may make the algorithm spend time in searching candidate designs and make the overall algorithm slow in comparison with the GBD algorithm alone (GBD-1). This situation is seen in example 4.1 (the case of four angle orientation candidates). For this example, the algorithm GBD-1 stopped right away after only 4 iterations, while the algorithm GBD-4 included 23 valid feasibility cuts. But this is nothing but the conclusion that for small problems, the use of heuristics is more likely to be unnecessary.

Another interesting remark is that none of the methods could treat satisfactory Examples 1, 8, 9 and 12. There could be many reasons for this fact. Since the algorithm has shown dependency in its performance according to the successful application of heuristics, we believe that for these examples, neither the algorithm, nor the heuristics were able to find good, or close to optimal designs. If another heuristic doing this job exists, then combined with the presented GBD algorithm, it will be able to obtain the best possible estimation of global convergence gap possible for the GBD algorithm. Therefore we believe that in general, the GBD method, combined with other heuristic methods, will reach better results in terms of the quality of both the obtained solution and the ability to assess the global optimality gap in numerical examples.

11 Conclusion

We have demonstrated the combined use of continuous relaxations, large neighborhood search heuristics and global integer optimization using Generalized Benders' Decomposition (GBD) for the solution of static minimum compliance multimaterial topology optimization problems with an emphasis on layered composite structures. On basis of the statement of the original nonlinear non-convex mixed-integer optimization problem, we make reformulations allowing us to solve the problem using GBD. One of the reformulations is a convex continuous relaxation on nested form which can be solved to optimality in a reasonable amount of time using a standard nonlinear programming algorithm giving both a lower bound as well as important information about the optimal solution to the original integer problem. The solution to the continuous relaxation is used within a starting heuristic in the sense that we formulate a sub-MINLP in the variables that did not obtain integer values in the continuous solution. This sub-MINLP is solved to optimality using GBD on a reduced problem and this solution is used to generate a good GBD cut in the global overall mixed-integer program. The idea of solving the reduced sub-MINLP is that the complexity of solving this problem is (hopefully) lower than solving the overall problem and by including the information obtained from its solution and the solution of the continuous relaxation, the convergence of the overall algorithm is increased compared to not including this information. Furthermore, we use a heuristic that uses a non-convex relaxation to generate cuts that lead to good, but not optimal solutions in a short amount of time. This information is also passed up to the global problem in order to speed up convergence.

The improvements in terms of the capability to solve larger problems compared to not using these heuristics are confirmed on a set of numerical examples where most instances are solved to global optimality within a tolerance $< 5\%$. The results illustrate the combined effect of improving the lower as well as the upper bound. It is observed that improving one bound may also lead to faster improvement of the other bound.

The improvements obtained using the presented heuristics are a contribution to the ability to solve larger discrete structural optimization problems to proven global optimality. Using information from the continuous relaxation is well suited for problems where the continuous solution contains a non-negligible amount of integer-valued variables. This is often the case in structural optimization and thereby it is possible to obtain good roundings of continuous solutions.

To the authors' knowledge, the use of the RENS heuristic within a GBD (GBD-RENS) framework has not been presented before and it is our belief that the approach may be used with success with GBD for other nonlinear mixed-integer problems as well. This question remains to be investigated further by attacking and solving broader classes of different problems from e.g. some of the standard test problems for MINLP. Furthermore the use of other heuristics that (in a cheap manner) generate good cuts for the overall GBD procedure could be interesting to pursue, especially in the realm of parallel processing where individual processes could work on different heuristics and sub-problems whose information can be passed back to the overall problem and thereby improve the overall algorithm.

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Paper C

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Material interpolation schemes for unified topology and multi-material optimization

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Abstract This paper presents two multi-material interpolation schemes as direct generalizations of the well-known SIMP and RAMP material interpolation schemes originally developed for isotropic mixtures of two isotropic material phases. The new interpolation schemes provide generally applicable interpolation schemes between an arbitrary number of pre-defined materials with given (anisotropic) properties. The method relies on a large number of sparse linear constraints to enforce the selection of at most one material in each design subdomain. Topology and multi-material optimization is formulated within a unified parametrization.

Keywords Material interpolation · Topology optimization · Multi-material parametrization · Composite materials

1 Introduction

Since the seminal papers by Bendsøe and Kikuchi (1988) and Bendsøe (1989) on topology optimization considered as a material distribution problem, the field of structural topology optimization has gained momentum and the ideas of optimal material distribution using the so-called density approach have been extended to other applications and physics as well, see e.g. Bendsøe and Sigmund (2003) and Bendsøe et al. (2005).

The basic question addressed in two-phase topology optimization is; how to distribute a limited amount of material within a spatial reference domain so as to optimize some objective function. In other words the question is whether or not to put material at any given point within the fixed reference domain. The natural extension of this question is; given a number of materials with different properties, how should they be distributed to optimize some objective function under a constraint on the total amount of material or constraints on the amount of the individual phases? In this paper we address the problem with a constraint on the total amount of material, but the other question with constraints on the amount of each phase is not too different.

The topology problem may be modeled as a (non)linear mixed 0–1 program and solved using global optimization techniques, see e.g. Stolpe and Svanberg (2003), Muñoz and Stolpe (2010) and Muñoz (2010). In theory these approaches are able to determine a global optimum but in practice they are limited by their ability to cope with large scale problems.

In classic solid-void topology optimization the use of material interpolation schemes such as SIMP (Solid Isotropic Material with Penalization) is probably the most popular approach and has proven successful for a large number of applications, see Bendsøe and Sigmund (2003) and Eschenauer and Olhoff (2001). The idea of approximating the 0–1 problem using penalized intermediate densities was originally proposed by Bendsøe (1989). Another material interpolation scheme is the RAMP scheme (Rational Approximation of Material Properties) (Stolpe and Svanberg 2001) which is similar to the SIMP scheme in its basic concept.

Extensions of the SIMP scheme to multiple phases were presented by Sigmund and Torquato (1997) and Gibiansky and Sigmund (2000) who designed material microstructures

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having extreme properties using a three-phase (two materials and void) topology optimization approach. In these papers one variable controls the topology by determining the pointwise amount of material while the other variable controls the mixture between the two material phases. The ideas of using topology optimization techniques to choose between multiple phases were extended to any number of phases by Lund and Stegmann (2005), Stegmann (2004) and Stegmann and Lund (2005) using the so-called Discrete Material Optimization (DMO) approach for the design of laminated composite structures. They proposed generalizations of the SIMP scheme where weighting functions with penalization of intermediate selections control the selection of each phase. Each weighting function is affected by all design variables (associated with the subdomain) such that an increase of one weight results in a decrease in all other weights. This interdependency in combination with a SIMP-like penalization typically leads to a distinct material selection. Different variations of these schemes were shown; one with the property that the weights sum to unity and another scheme where the weights sum to less than unity for intermediate values of the design variables.

In Yin and Ananthasuresh (2001) a peak function approach is used where the effective material properties for mixtures of an arbitrary number of phases are interpolated using one density variable. The approach uses Gaussian distribution “peak functions” as weights on each phase. The peaks corresponding to selection of a given material are separated such that selection of a given material is obtained if the density variable attains the value corresponding to a material peak. The width (mean deviation) of the peaks is a parameter and continuation is used to sharpen the peaks gradually in order to obtain distinct choices.

Another way to parametrize multi-phase problems is the so-called color level set approach (Wang and Wang 2004, 2005; Wang et al. 2005) where material regions are represented by unions of different level sets of implicit functions. The idea is to separate the design domain into regions representing the sub domains containing one of the material phases and design changes are imposed by letting the interfaces evolve so as to obtain an optimal subdivision of the design domain into distinct material regions.

In Setoodeh et al. (2005) a combined SIMP and cellular automata approach was proposed for combined topology and continuous fiber angle optimization for 2D continua though the approach in this work is not exactly a multi-material parametrization. To some extent the results obtained in that work (simultaneous fiber angle and topology) are comparable to some of those presented in the present paper.

Recently a new multi-material parametrization has been proposed in Bruyneel (2011) where bilinear finite element

shape functions act as weights in a weighted interpolation between the candidate materials. The approach uses two variables to interpolate between four materials leading to fewer design variables compared to other approaches. The idea was demonstrated for four materials and could maybe be generalized to more phases, though it is not clear how non-negativity of the weight functions is assured for higher-order interpolations.

In this paper we generalize the SIMP and RAMP schemes so as to parametrize simultaneous topology and multi-materials design within a unified parametrization. The approach relies on a large number of sparse linear constraints limiting the selection of a material to at most one in each domain. The approach is demonstrated on the minimum compliance (maximum stiffness) problem, but the basic idea of the parametrization is applicable to any material distribution design problem involving an arbitrary number of candidate materials/phases.

2 Problem formulation

We consider the minimum compliance material distribution problem representing multi-material selection (and topology design) problem within a fixed reference domain in two or three dimensions with an optional constraint on the total mass.

2.1 Design parametrization

In the following we describe the parametrization of multi-material selection problems as well as simultaneous topology and multi-material selection problems, respectively.

A fixed reference domain $\Omega \in \mathbb{R}^2$ or \mathbb{R}^3 is divided into a number of design subdomains Ω_j , $j = 1, 2, \dots, n^d$ within which we want to select the optimal material given a number of possible candidates. A design subdomain may be e.g. a layer in a finite element, a layer covering multiple elements, multiple layers within a single element, a collection of elements for which the same material should be chosen etc. The definition of design subdomains may be chosen to coincide with the finite element discretization but a design subdomain may also contain multiple elements in a so-called patch. Patches may be used due to manufacturing reasons if it is not allowable to have changes in material or fiber orientations at the level of the finite element discretization.

Within each design subdomain a number of candidate materials is given and the selection of these is parametrized using a *binary* selection variable x_{ij} whose value determines

the selection of a given material within the subdomain of interest

$$x_{ij} = \begin{cases} 1 & \text{if material } i \text{ is chosen in design} \\ & \text{subdomain } j \\ 0 & \text{if not} \end{cases} \quad (1)$$

To be physically meaningful this variable should only attain the values 0 or 1. However, this requirement leads to non-linear binary/integer programming problems which would limit the size of tractable problems significantly. A popular technique for solving large scale instances of such problems is the so-called density approach; the variables are treated as continuous and can attain intermediate values during the optimization process. To obtain physically valid integer solutions intermediate choices are made unfavorable by the use of penalization techniques. The advantage is that gradient information can be used efficiently in the search for a solution which significantly increases the size of computationally tractable problems.

The number of candidate materials may differ between the design subdomains, and thus the total number of design variables n is given as the sum of the number of candidate materials over all subdomains, $n = \sum_{j=1}^{n^d} n_j^c$. Typically, and throughout this paper, we have the same number of candidate materials n^c in all subdomains and therefore the total number of design variables is simply given by $n = n^c n^d$.

2.1.1 Simultaneous topology and multi-material optimization

The simultaneous topology and material selection problem considers the following question in every design subdomain; which material, if any, should be chosen given a number of possible candidates? It has been customary to treat this question by having one variable controlling the topology by scaling the contribution of the variables controlling the material selection, see e.g. Sigmund and Torquato (1997) and Gibiansky and Sigmund (2000). We propose to parametrize the topology question as follows. With the parametrization from (1) in mind we know that at most one material can be chosen in each design subdomain. Thus, in every subdomain we allow *at most* one material to be chosen, but we also allow no candidate to be chosen. This condition is expressed by the following inequality constraints.

$$\sum_{i=1}^{n^c} x_{ij} \leq 1, \quad \forall j \quad (2)$$

Together with the constraints (1) this constraint ensures that at most one material is chosen in each design subdomain. If

the sum of the binary selection variables is zero, none of the corresponding materials have been chosen and a base material (representing “void”) is chosen. If any variable entering the sum attains one (i.e. the corresponding material is chosen) the remaining variables necessarily must be zero for the inequality to be satisfied.

2.1.2 Multi-material optimization

Requiring *exactly* one material to be chosen (and hence not allowing holes) is imposed through a linear equality constraint in each subdomain.

$$\sum_{i=1}^{n^c} x_{ij} = 1, \quad \forall j \quad (3)$$

Satisfying this constraint ensures that exactly one of the candidates $i = 1, 2, \dots, n^c$ is chosen and the remaining candidates are automatically not chosen within the subdomain in question.

2.2 Material parametrization

The effective material properties are parametrized using the material selection variables. The effective mass density for the j 'th subdomain, $\rho_j(x) \in \mathbb{R}$, is given by

$$\rho_j(x) = \rho_0 + \sum_{i=1}^{n^c} x_{ij} \Delta \rho_{ij}, \quad \forall j \quad (4)$$

where $\Delta \rho_{ij} = \rho_{ij} - \rho_0$. As explained above the 0'th phase typically is an ersatz material representing void. In case it is massless, the void mass density is of course zero and consequently $\Delta \rho_{ij} = \rho_{ij}$. The n^c materials with an associated selection variable are the candidate materials among which we want to choose. If a variable is 1 and (2) or (3) is fulfilled, the effective mass density is that of the corresponding material. If all variables are 0 the effective properties are those of the 0'th phase, void.

Similarly the effective stiffness tensor is represented by a symmetric matrix $E_j(x) \in \mathbb{R}^{6 \times 6}$

$$E_j(x) = E_0 + \sum_{i=1}^{n^c} x_{ij} \Delta E_{ij}, \quad \forall j \quad (5)$$

where $\Delta E_{ij} = E_{ij} - E_0 \in \mathbb{R}^{6 \times 6}$. Again phase 0 typically is given properties representing or approximating those of void, and the properties of the remaining phases are those of the physical candidate materials. We assume that $0 < E_0 < E_{ij}$ from which it follows that $\Delta E_{ij} := E_{ij} - E_0 > 0$.

With the proposed approach we can formulate both multi-material selection problems, and simultaneous multi-material and topology problems within the same parametrization with the only difference being if the sparse linear constraints are inequality constraints (2) or equality constraints (3).

Actually it is possible to parameterize multi-material selection using (2) by letting one of the candidates be the 0'th phase and thereby save one design variable per design subdomain. However, using the 0'th phase for a physical candidate in combination with penalization is not invariant with respect to phase ordering. Thus it is not advisable to use this approach. It is also possible to parametrize simultaneous topology and material selection using (3) by letting void be one of the phases that can be selected with an associated variable. For the reasons explained above we choose the unified parametrization since it leads to invariance with respect to the ordering of the phases when penalization is applied as shown later.

2.3 Original problem

The original problem is modeled as a non-convex mixed-integer problem; the design variables physically can only attain integer values, i.e. $x_{ij} \in \{0, 1\}$. We assume quasi-static loading applied to the non-restrained nodes $f \in \mathbb{R}^d$ where d is the number of non-restrained finite element degrees of freedom. The unknown optimal nodal displacements $u \in \mathbb{R}^d$ are continuous. We consider the problem

$$\underset{x \in \mathbb{R}^n, u \in \mathbb{R}^d}{\text{minimize}} \quad c(x) = f^T u(x) \quad (6a)$$

$$\text{subject to} \quad K(x)u = f \quad (6b)$$

$$\sum_{i,j} x_{ij} \rho_i V_j \leq \bar{M} \quad (6c)$$

$$\sum_{i=1}^{n^c} x_{ij} = 1 \text{ OR } \sum_{i=1}^{n^c} x_{ij} \leq 1, \quad \forall j \quad (6d)$$

$$x_{ij} \in \{0, 1\}, \quad \forall (i, j) \quad (6e)$$

where ρ_i is the mass density of material i , V_j is the volume of the j 'th design subdomain and \bar{M} is a resource constraint limiting the total mass of the structure. The mass constraint is only relevant for multi-material problems where the candidate materials have different mass density. In the case of pure fiber angle optimization modeled using an orthotropic material oriented at a number of distinct directions as candidate materials, the mass constraint is redundant. $K(x) \in \mathbb{R}^{d \times d}$ is the design dependent (global

level) stiffness matrix. The stiffness matrix is parametrized in the following manner

$$K(x) = \sum_j K_j = \sum_j \int_{\Omega_j} B_j^T E_j(x) B_j d\Omega_j \quad (7)$$

where the summation denotes assembly of the stiffness matrix. $E_j(x) \in \mathbb{R}^{6 \times 6}$ is the design dependent constitutive tensor given in (5) and B_j is the standard finite element strain-displacement matrix.

If $K(x)$ is non-singular, the original non-convex 0–1 problem may be reformulated as a 0–1 problem with a convex objective function in so-called nested form where the nodal displacements are eliminated by use of the equilibrium equations, i.e. $u(x) = K(x)^{-1} f$ to obtain an equivalent optimization problem in the design variables x only.

2.4 Nested continuous problem formulation

We relax the binary requirement on the variables and introduce material interpolations for the discrete material parametrization as shown in Sections 3.1 and 3.2. The relaxed problem we consider is given by

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad c(x) = f^T K(x)^{-1} f \quad (8a)$$

$$\text{subject to} \quad \sum_{i,j} x_{ij} \rho_i V_j \leq \bar{M} \quad (8b)$$

$$\sum_{i=1}^{n^c} x_{ij} = 1 \text{ OR } \sum_{i=1}^{n^c} x_{ij} \leq 1, \quad \forall j \quad (8c)$$

$$x_{ij} \geq 0, \quad \forall i, j \quad (8d)$$

where $K(x) \in \mathbb{R}^{d \times d}$ is now the design dependent (global level) stiffness matrix as shown in (7) with the interpolated constitutive tensors $E_j(x)$ as given in relation (9) or (12). In the following section we describe the material interpolation schemes in more detail. We use adjoint sensitivity analysis for the objective function (8a), see e.g. Bendsøe and Sigmund (2003) for details.

3 Material interpolation schemes

Material interpolation schemes allow intermediate material choices during the solution process but should at the same time penalize intermediate choices so as to obtain distinct choices eventually honoring the original binary requirement on the selection variables (1). It is often argued that the popular material interpolation schemes for certain parameter

intervals violate variational bounds on the attainable properties of material mixtures, see discussion in Bendsøe and Sigmund (1999). The use of interpolations is regarded as a heuristic method that is viable as long as the final solution honors the binary condition (for which there should be no ambiguity regarding the effective properties). Intermediate solutions are merely an artifact that we use to obtain distinct solutions.

3.1 Multiphase ‘‘SIMP’’

We put SIMP in quotation marks since the effective material properties in our approach are not necessarily isotropic, e.g. when interpolating between anisotropic materials. The scheme is a direct generalization of the original scheme proposed for interpolation between void and solid. We take the discrete parametrization from (5) and raise the, now relaxed, design variable to a power $p \geq 1$. We keep the generalized upper bound constraints and obtain the following interpolation scheme for the full constitutive tensor

$$E_j^S(x) = E_0 + \sum_{i=1}^{n^c} \underbrace{x_{ij}^p}_{w_{ij}} \Delta E_{ij}, \quad p \geq 1, \quad \forall j \quad (9)$$

For $p = 1$ the sum of the weights controlling the contribution from each stiffness phase add to unity if the design variables do. For $p > 1$ intermediate material selections are unfavorable since the total stiffness contribution is reduced in the sense that the weights do not sum to unity for intermediate choices, even if the design variables do. Thus intermediate choices intrinsically are penalized.

Note that for $n^c = 1$, the generalized scheme (9) reduces to the well-known two-phase SIMP scheme. For this particular case, however, only the generalized upper bound inequality (2) is relevant and requiring (3) would lead to a trivial problem. The sensitivity of (9) with respect to a design variable affecting the interpolation is

$$\frac{\partial E_j^S(x)}{\partial x_{ij}} = p x_{ij}^{p-1} \Delta E_{ij}, \quad \forall i, j \quad (10)$$

It follows that for $p > 1$ the sensitivity of the stiffness tensor vanishes if the corresponding design variable is zero,

$$\frac{\partial E_j^S(x_{ij} = 0)}{\partial x_{ij}} = p 0^{p-1} \Delta E_{ij} = 0, \quad p > 1, \quad \forall i, j \quad (11)$$

3.2 Multiphase RAMP

In Stolpe and Svanberg (2001) the so-called RAMP scheme was proposed as an alternative interpolation scheme for two-phase topology optimization. The idea of the scheme is that

for isotropic two-phase interpolation a certain value of the penalization parameter yields a concave objective function increasing the probability of obtaining a distinct solution. We propose a generalization to multiple materials similar to the SIMP generalization (9).

The interpolation scheme for the constitutive tensor is given by

$$E_j^R(x) = E_0 + \sum_{i=1}^{n^c} \underbrace{\frac{x_{ij}}{1 + q(1 - x_{ij})}}_{w_{ij}} \Delta E_{ij}, \quad q \geq 0, \quad \forall j \quad (12)$$

The effect of the penalization parameter q is analogous to that of p in the SIMP scheme; it makes intermediate selections unfavorable by reducing the net material contribution in the stiffness interpolation. The sensitivity of (12) with respect to a design variable affecting the interpolation is

$$\frac{\partial E_j^R(x)}{\partial x_{ij}} = \frac{1 + q}{(1 + q(1 - x_{ij}))^2} \Delta E_{ij} > 0, \quad \forall i, j \quad (13)$$

3.3 Penalizing effect

For both schemes the penalizing effect of feasible intermediate densities fulfilling (2) or (3) comes from the fact that the sum of the penalized weights is less than unity. In the following we address different issues affecting the penalization and derive relations for the parameters such that it is possible to control the amount of penalization and prescribe comparably penalizing parameters for the SIMP and the RAMP scheme, respectively. We compare the amount of penalization for uniform mixtures; $\bar{x}_{ij} = \frac{1}{n^c}$, $\forall i, j$, whereby all weights are equal.

3.3.1 Number of candidates

For a fixed penalization parameter the number of candidate materials has an influence on the sum of the penalized weights. Thus, different values of the penalization parameters may be necessary to obtain comparable penalization in problems with different number of candidate materials. In the following we obtain relations between the number of candidates and the sum of the weights for uniform mixtures. Looking at the weights within a subdomain, the sum of the weights for a uniform mixture with the SIMP scheme is

$$\sum_{i=1}^{n^c} w_i(\bar{x}_{ij}) = \sum_{i=1}^{n^c} \left(\frac{1}{n^c}\right)^p = n^c \left(\frac{1}{n^c}\right)^p, \quad p \geq 1 \quad (14)$$

For $p = 1$ it is seen that the sum of weights equals unity. For $p > 1$ the sum depends on the number of candidate materials such that a larger number of candidates leads to a smaller sum for fixed penalization p . Thus with many candidates the penalization acts stronger compared to penalization of fewer candidates. Similarly for the RAMP scheme the uniform mixture weights sum as

$$\begin{aligned} \sum_{i=1}^{n^c} w_i(\bar{x}_{ij}) &= \sum_{i=1}^{n^c} \frac{\frac{1}{n^c}}{1 + q \left(1 - \frac{1}{n^c}\right)} \\ &= \frac{1}{1 + q \left(1 - \frac{1}{n^c}\right)}, \quad q \geq 0 \end{aligned} \tag{15}$$

For $q = 0$ the uniform mixture weight sum is independent of the number of materials whereas the penalized weight sum (for $q > 0$) depends on the number of candidate materials. The effect of the number of candidates is equivalent to the behaviour of the SIMP scheme.

3.3.2 SIMP/RAMP equivalent penalization

The effect of the penalization parameters in the generalized SIMP and RAMP scheme, respectively, is different and in order to compare the amount of penalization of the schemes we now derive relations for the parameters that give the same sum of weights for uniform mixtures of the phases. This yields sets of parameters that give comparable amounts of penalization for both schemes.

For a uniform mixture of materials $\bar{x}_{ij} = \frac{1}{n^c}$, $\forall i, j$, all weights are equal. Now equating the weights in the SIMP scheme to those in the RAMP scheme, we obtain a value for the RAMP penalization parameter that yields the same sum of the weights for uniform mixtures as the SIMP scheme does,

$$\left(\frac{1}{n^c}\right)^{\bar{p}} = \frac{\frac{1}{n^c}}{1 + \bar{q} \left(1 - \frac{1}{n^c}\right)} \Leftrightarrow \tag{16}$$

$$\bar{q} = \frac{\left(\frac{1}{n^c}\right)^{-\bar{p}} - n^c}{n^c - 1} \tag{17}$$

The opposite expression for \bar{p} in terms of \bar{q} and n^c is

$$\bar{p} = -\frac{\ln(n^c + n^c \bar{q} - \bar{q})}{\ln\left(\frac{1}{n^c}\right)} \tag{18}$$

These expressions can be used to assign sets of parameter values yielding comparable penalization. In Fig. 1 we show the sum of the penalized weights for $n^c = 2$ for a range of penalization parameters for both schemes. We

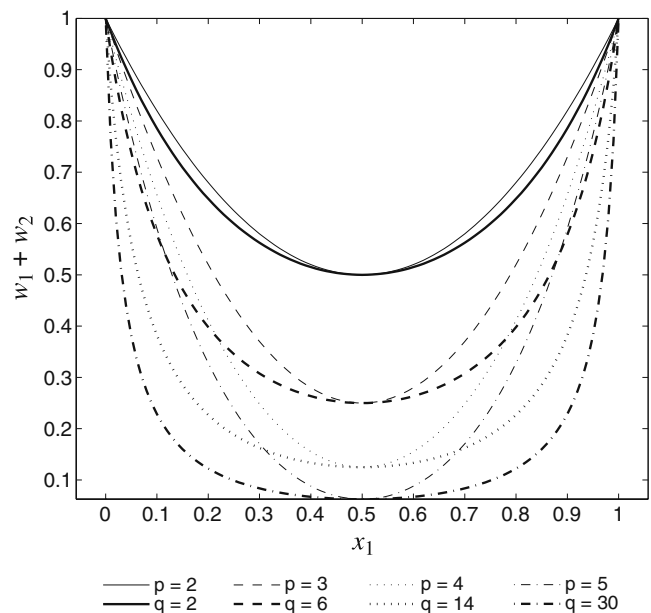


Fig. 1 Sum of penalized stiffness weights for $n^c = 2$ for the SIMP and the RAMP interpolation scheme for various penalization parameters

use $x_1 + x_2 = 1$ to eliminate x_2 and plot the sum of the penalized weights, e.g. for the SIMP weights $w_1 + w_2 = x_1^p + x_2^p = x_1^p + (1 - x_1)^p$. Table 1 shows the result of (17), i.e. the equivalent RAMP penalization parameter \bar{q} for various number of candidates n^c and given SIMP penalization parameters \bar{p} .

From the table it is seen the value of q should be set significantly higher than that of p in order to obtain comparable penalization. As seen from Fig. 1 the RAMP scheme seems to penalize mixtures over a larger range compared to the SIMP scheme.

3.3.3 Remarks on penalization and continuation strategy

We start out solving a convex relaxation without any penalization (i.e. $p = 1$ or $q = 0$) and use the result of this problem as an initial guess for a penalized problem that should yield a distinct material selection eventually. In the problems solved in this paper, the solution to the convex problem often has many variables within a subdomain equal

Table 1 Equivalent uniform mixture penalization; RAMP parameter \bar{q} for given SIMP parameter \bar{p} and number of phases n^c

n^c	\bar{p}	1	2	3	4	5
2	\bar{q}	0	2	6	14	30
3	\bar{q}	0	3	12	79.5	120
4	\bar{q}	0	4	20	254.7	340
5	\bar{q}	0	5	30	623.75	780

to zero and non-zero values only for two or three of the materials. Thus to penalize equally in the SIMP and the RAMP scheme we select the equivalent penalization parameters obtained for $n^c = 2$ instead of those for the actual number of candidate phases. In case of use of the schemes for problems where experience shows other behavior, it may be useful or necessary to adjust the penalization parameters accordingly.

We first solve the convex problem to optimality (see next section) and then use this solution as a starting guess in a penalized subproblem where we raise the SIMP penalization p to 2 then 3 and finally 4. For the RAMP scheme we increase q to 3 then 6 and finally 14. All subproblems are solved to optimality which is usually around 60–70 iterations for the convex problem and typically less than 20 for each of the penalized problems.

3.4 Implementation

The procedure proposed in this paper is implemented in our in-house finite element and optimization code MUST (MULTidisciplinary Synthesis Tool) mainly written in Fortran 90. MUST takes a finite element discretization as input from e.g. ANSYS and together with a few additional lines of information defining the optimization problem, the problem is set up.

All examples solved in this paper are discretized using nine-node degenerated shell elements with five degrees of freedom per node (three translational and two rotational), see e.g. Ahmad et al. (1970) and Panda and Natarajan (1981). For purely plane problems such elements are unnecessarily complicated and computationally expensive, but these examples illustrate that the proposed approach is able to solve the material distribution problem within the plane of the structure as well as through the thickness in layered structures. Note that the method may be used with any kind of finite elements.

The optimization problems are solved using the sequential quadratic programming algorithm SNOPT 7.2-9 (Sparse Nonlinear OPTimizer), see Gill et al. (2005, 2008). SNOPT uses first-order gradient information and exploits sparsity in the problem in combination with a limited-memory quasi-Newton approximation to the Hessian of the Lagrangian. Linear mass and material selection constraints are treated as such which is utilized within SNOPT in the sense that linear constraints are always satisfied before calling the non-linear functions. In SNOPT default parameter settings are used except for the so-called “New Superbasics Limit” which is set to 100.000, the “Major iterations limit” to 200, the “Minor iterations limit” to 10.000, and we explicitly specify “QPSolver CG”. The “Major optimality tolerance” is set to $2.0 \cdot 10^{-4}$.

4 Illustrative example

The following example demonstrates properties of the material interpolation schemes proposed in this paper and illustrates the effect of penalization. We investigate the influence of the penalization in combination with the applied loading and candidate materials on the likelihood of obtaining a distinct material selection.

Usually for solid void topology optimization the ability of the SIMP (and RAMP) scheme to obtain 0/1 solutions is attributed to its penalized stiffness relative to the full contribution in the mass/volume constraint at intermediate densities. However, the situation is quite different if we are to select between different materials with the same mass density but different directional properties, i.e. anisotropic or orthotropic materials.

The following example is constructed so as to remove the influence of the mass constraint completely; both materials have the same mass density and thus the mass constraint plays no role. Furthermore the two candidate materials are instances of the same orthotropic material but oriented differently. The idea is to study different stress states for which we know the optimal solution in terms of a distinct material choice and observe which solution the interpolation schemes would lead to.

Consider the bi-axial plane stress state as shown in Fig. 2. Different characteristic stress states are obtained by varying the principal stress ratio; $-1 \leq \frac{\sigma_{II}}{\sigma_I} \leq 1$. The design problem that we address is that of choosing between two distinct orientations of an orthotropic material. This problem we regard as a material selection problem with two candidate materials in the sense that each material orientation represents a candidate material. The first candidate material that we consider is an orthotropic material with its principal material direction coincident with the first principal stress direction (i.e. $\theta = 0^\circ$) and the second candidate material has the principal material direction coincident with the second principal stress direction ($\theta = 90^\circ$). The compliance of the structure is directly linked to the pointwise stress energy density

$$u^c(x_1) = \frac{1}{2} \sigma^T E(x_1)^{-1} \sigma \quad (19)$$

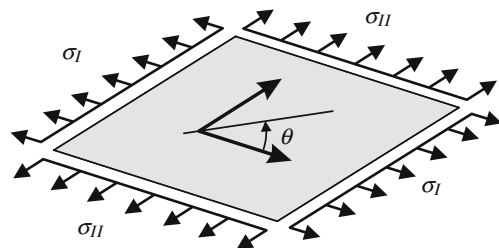


Fig. 2 Bi-axial stress states with coordinate system

Now, for a given stress state σ and two candidate materials we explore the design space for different interpolations. We want to investigate the interpolation scheme in terms of its behaviour when selecting between two materials and thus we eliminate the topology question by requiring (3) to hold. This furthermore makes it possible to eliminate one variable whereby the problem is parametrized in x_1 only. Thus, $x_1 = 1$ means that the orthotropic material oriented at $\theta = 0^\circ$ is chosen and for $x_1 = 0$ the same material at $\theta = 90^\circ$ is chosen.

4.1 SIMP scheme

Using the simplifications described above the generalized SIMP scheme in (9) reduces to

$$E(x_1) = x_1^p E_{0^\circ} + (1 - x_1)^p E_{90^\circ} \tag{20}$$

For $p > 1$ the sum of the weighting of the individual phases is less than or equal to one, $w_1 + w_2 \leq 1$ for $0 < x_1 < 1$. Thereby mixtures are penalized in the sense that the amount of stiffness contributing material effectively is reduced. In Fig. 3 the resulting stress energy density is shown for different principal stress ratios and

different values of the penalization parameter p . From the figure we observe a number of properties for this scheme

- For a distinct material selection, i.e. $x_1 = 0.0$ or $x_1 = 1.0$ the scheme yields the same objective function value, regardless of the value of p .
- For $p = 1.0$ the compliance is *convex* in x_1 . For all loads except the uni-directional load ($\frac{\sigma_{II}}{\sigma_I} = 0.0$), the optimum is a mixture.
- For large p the compliance level generally is higher for mixtures. This is due to the fact that the weights on the phases do not sum to unity meaning that intermediate choices also encompass choosing less material in total.
- For large p the compliance is non-convex with several local minima and hence a non-integer point may be a local optimum.
- The scheme is indifferent with respect to ordering of the phases, i.e. the ordering does not bias the tendency to select any of the phases over the other.

Note that for a plane problem as is the case here, E may be interpreted as the equivalent membrane stiffness of a material consisting of two layers, one with material

Fig. 3 Stress energy density for different fixed bi-axial stress states obtained using the SIMP interpolation (20)

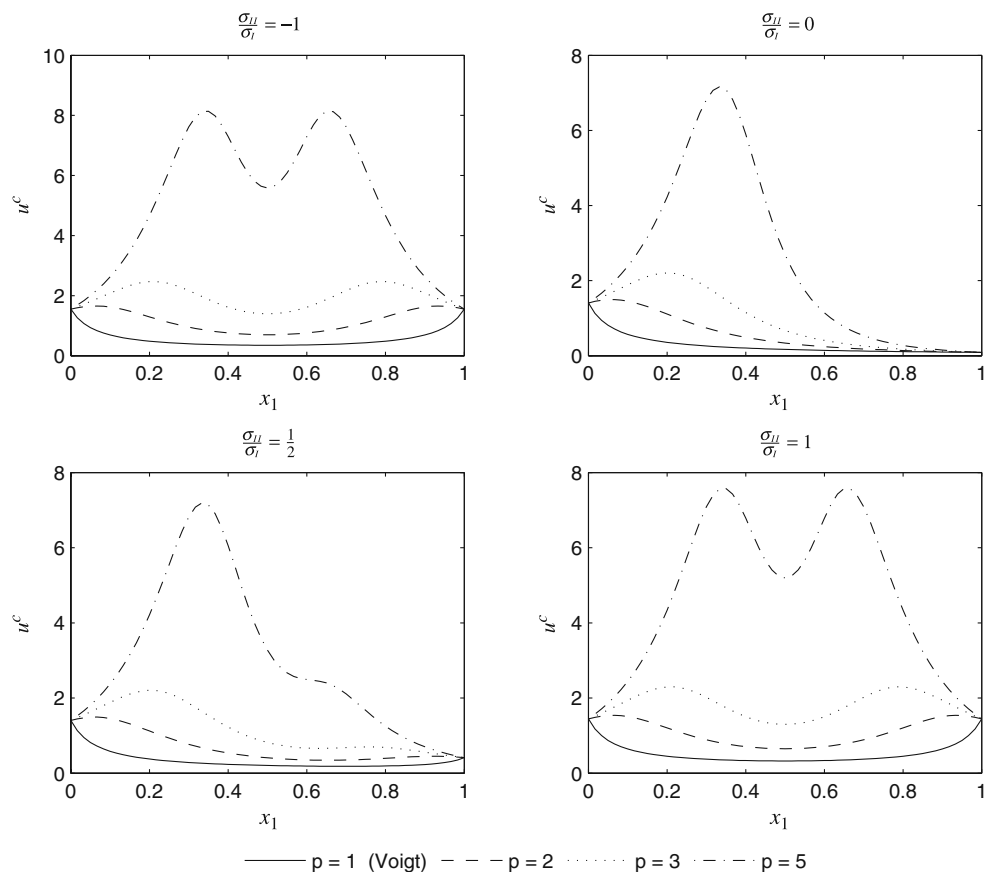
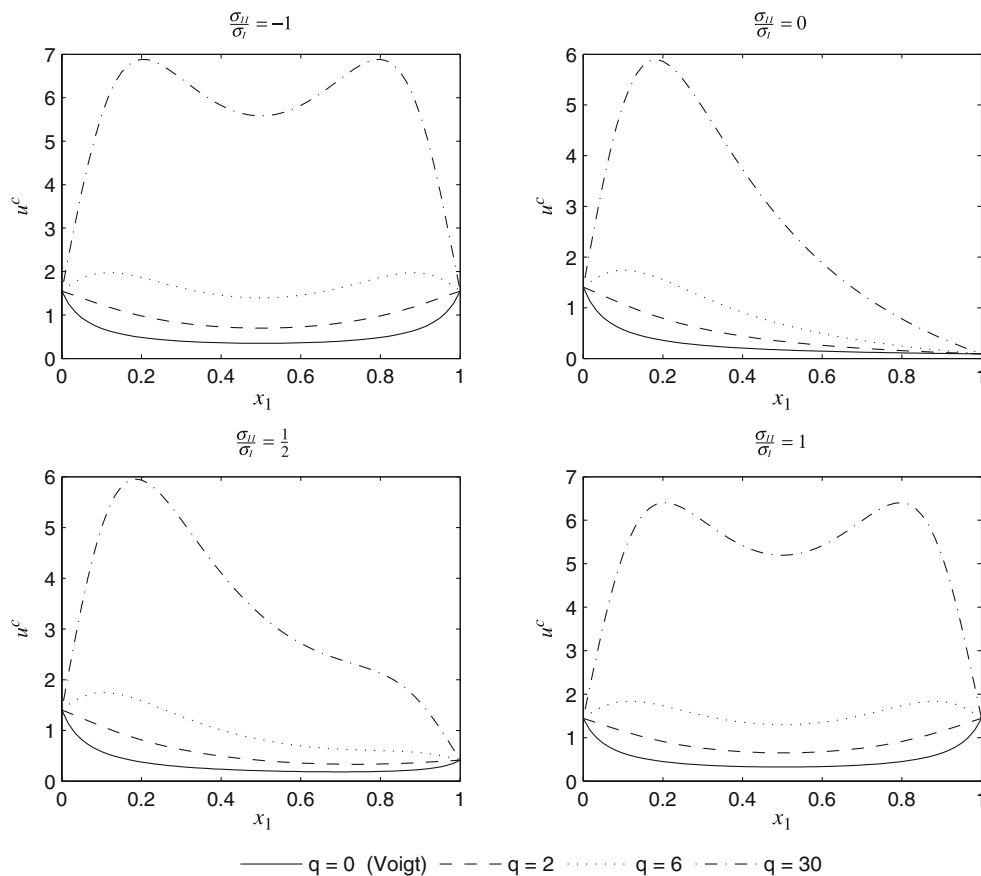


Fig. 4 Stress energy density for different fixed bi-axial stress states obtained using the RAMP interpolation (21)



E_{0° , the other with material E_{90° , of thicknesses x_1^p and $(1 - x_1)^p$, respectively. For $p > 1$ the total thickness of the layers is less than unity for intermediate designs, and thereby penalization favors distinct choices since only distinct choices achieve unit total thickness. For $p = 1$ the total thickness adds to unity and the design variables may be interpreted directly as the layer thicknesses and for this case the parametrization itself does not penalize intermediate thicknesses.

4.2 RAMP scheme

Using the equality selection constraint (3) the RAMP scheme in (12) reduces to

$$E(x_1) = \frac{x_1}{1 + q(1 - x_1)} E_{0^\circ} + \frac{1 - x_1}{1 + qx_1} E_{90^\circ} \quad (21)$$

where $q \geq 0$ is the penalization parameter used to make intermediate choices unfavorable. The observations made for the SIMP scheme carry over to the RAMP scheme, see Fig. 4 for plots of resulting stress energy density for different fixed bi-axial stress states. Actually, for $q = 0$ the RAMP scheme is identical to the SIMP scheme for $p = 1$. The overall shapes of the curves are similar except for some

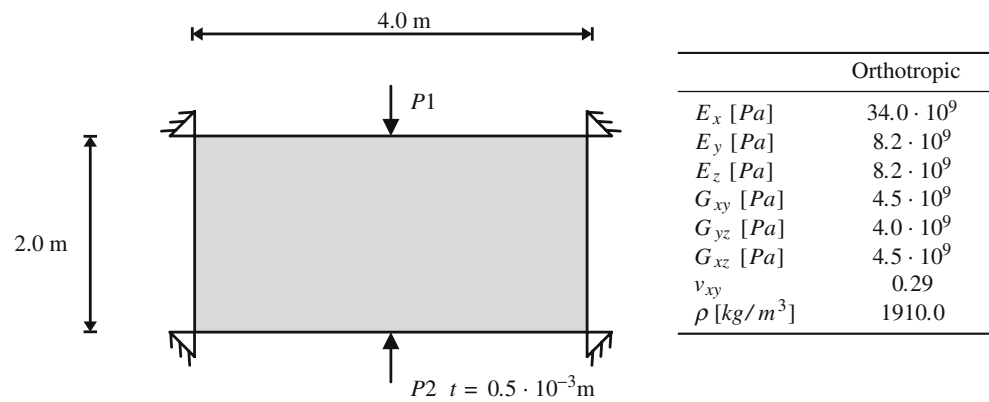
minor differences in slope and curvature near 0 and 1 where the RAMP scheme in general is steeper. Note that the curves shown take into account the sum to unity equality constraint eliminating x_2 , and thereby the slope of the curves rather represents the reduced gradient than the pure derivative wrt. x_1 . Therefore the expected vanishing slope of the SIMP scheme is not observed at $x_1 = 0$.

5 Numerical examples

In the following we describe numerical examples illustrating the possibilities using the new generalized multi-material interpolation schemes. In particular we address the ability of the schemes to obtain discrete solutions and compare the solutions obtained using the two new schemes. We show how it is possible to formulate and solve optimal orientation of orthotropic materials that are limited to a number of distinct directions. Furthermore we show examples of simultaneous material selection and orientation between multiple different materials where some of them may be anisotropic or orthotropic. Some of the examples addressed in this paper were investigated in an earlier paper by the authors using quadratic penalization of intermediate

Fig. 5 *Left:* Domain geometry and boundary conditions. Loads act independently.

Right: Material properties in principal material coordinate system for the candidate materials



densities to obtain distinct solutions (Hvejsel et al. 2011). Results are presented in Section 6.

5.1 Plane two load case example

This example illustrates simultaneous topology and discrete orientation optimization on a plane continuum subjected to two independent load cases of equal importance and loads with equal magnitude ($|P1| = |P2|$) and was originally proposed by Bendsøe et al. (1995). The multiple load case extension is treated using a weighted sum formulation of the individual load case compliances. In both load cases the structure is hinged at all corners ($u_i = 0$), see Fig. 5. The physical domain in which the material is distributed is a rectangular domain with dimensions $4.0 \text{ m} \times 2.0 \text{ m} \times 0.5 \cdot 10^{-3} \text{ m}$. The domain is discretized by 40×20 elements and in each element four candidate materials are possible. The four candidate materials represent the same orthotropic material oriented at four distinct directions, -45° , 0° , 45° or 90° . We set the mass constraint such that material can be chosen in 32.7% of the domain (i.e. 261.8 elements) meaning that void must be chosen in the remaining elements. The constitutive properties of the orthotropic material are given in material coordinate system in the table of Fig. 5.

5.2 Layered composite multi-material plate

This example illustrates multi-material design optimization with a lightweight polymeric foam and a limited amount of heavy and stiff orthotropic material oriented in four predefined distinct directions.

The candidate materials are the same as in Section 5.1 but the design domain consists of a quadratic plate within which we want to distribute and orient the materials, see Fig. 6.

5.3 Clamped membrane

This example is a plane problem which we treat first as an optimal orientation selection problem and subsequently as

a simultaneous topology and optimal orientation problem. The problem has previously been solved in Bruyneel (2011) who used a finite element shape function parametrization (SFP) to select between multiple materials and a separate topology density variable. The problem consists of a plane domain as shown in Fig. 7.

5.3.1 Discrete orientation selection

First we address the problem of choosing the optimal distinct orientation out of four possible at which an orthotropic material may be oriented, -45° , 0° , 45° or 90° . Each direction is considered a distinct material and the mass constraint is redundant for this problem. Thus we solve the optimization problem using the equality constraint in (3).

5.3.2 Simultaneous topology and discrete orientation optimization

This problem solves the orientation problem as well as the topology problem with a constraint on the total amount of available material. The total amount of material is limited such that material can only be present in 11 out of the 16 design subdomains, and in each design subdomain we include the possibility of choosing no material as modeled by the inequality constraint in (2).

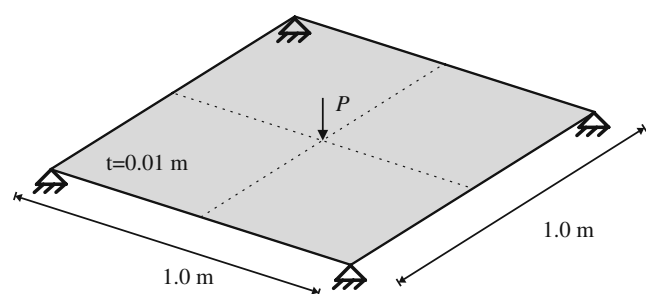
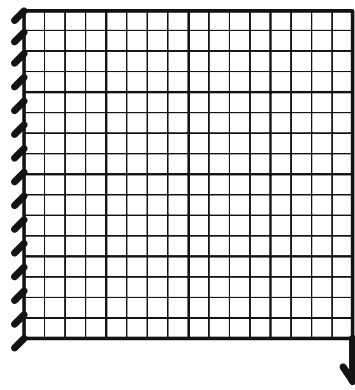


Fig. 6 Eight layer corner-hinged plate with point load applied at the center. See Fig. 5 for material properties

Fig. 7 *Left*: Problem sketch of plane domain clamped at left edge and loaded vertically downward at lower right corner. Note that finite element discretization differs from design discretization indicated in *greyscale*. *Right*: Material properties for clamped membrane example from Bruyneel (2011)



	Orthotropic
$E_x [Pa]$	$146.86 \cdot 10^9$
$E_y [Pa]$	$10.62 \cdot 10^9$
$E_z [Pa]$	$10.62 \cdot 10^9$
$G_{xy} [Pa]$	$5.45 \cdot 10^9$
$G_{yz} [Pa]$	$3.99 \cdot 10^9$
$G_{xz} [Pa]$	$5.45 \cdot 10^9$
ν_{xy}	0.33
$\rho [kg/m^3]$	1600.0

Fig. 8 Two load case plane disc, SIMP solution: interpolated mass density and chosen fiber orientation, penalized compliance ($p = 4$): 26.12. Please note that in this plot the *lightest grey* corresponds to orthotropic material with a bit of void. Compare density scale with that in Fig. 9

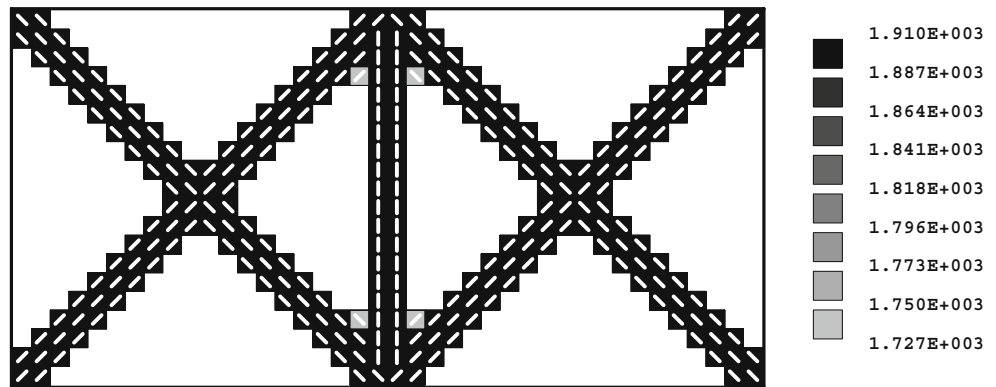


Fig. 9 Two load case plane disc, RAMP solution: interpolated mass density and chosen fiber orientation, penalized compliance ($q = 14$): 26.32. Please note that in this plot the *lightest grey* corresponds to a bit of orthotropic material mixed with void. Compare density scale with that in Fig. 8

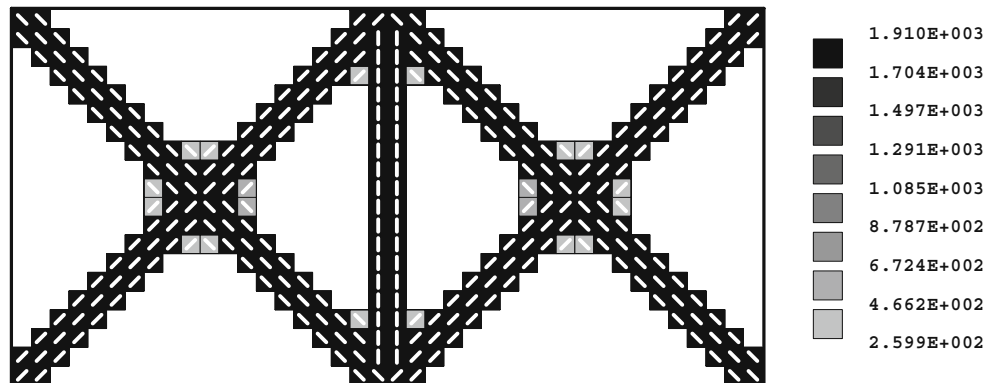
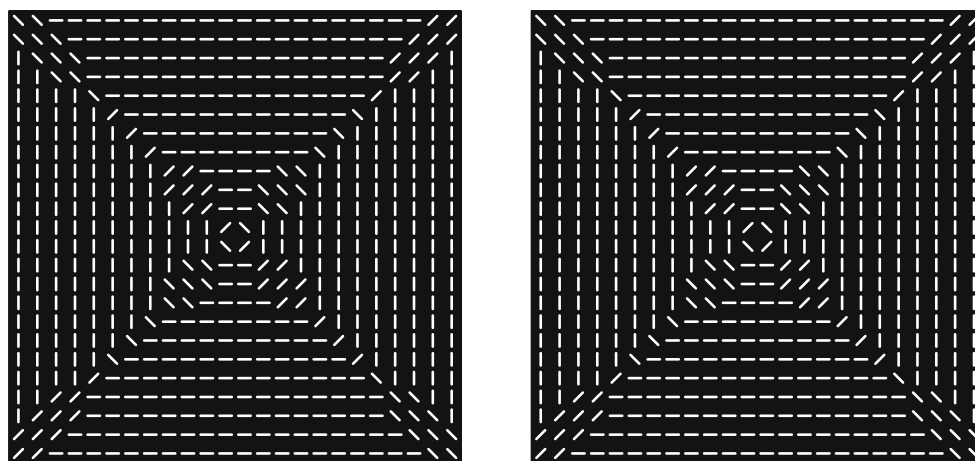


Fig. 10 Identical SIMP (*left*) and RAMP (*right*) solution in layer 1 (and 8): interpolated mass density and chosen fiber orientation



6 Results

6.1 Plane two load case example

The topology and material directions obtained using the proposed interpolation schemes are shown in Figs. 8 and 9, respectively. The interpolated mass density and the chosen direction of the orthotropic material is indicated in elements with orthotropic material. Elements where all design variables are at their lower bound are removed to clarify the topology of the structure.

It is seen that the topologies are virtually identical and for both solutions the convergence to a distinct material selection is quite clear. The SIMP scheme obtains a more distinct solution compared to the RAMP solution. A non-distinct interpolated mass density is only observed in a few elements in both solutions and the reason for this is that the mass constraint is set (more or less arbitrarily) to a value in between the distinct jumps corresponding to the mass increase when switching one element from void to material. Thus, the algorithm employs material until the mass constraint is active

in order to gain the stiffness increase obtained by choosing more of the heavy material. Mixture between orthotropic materials of same mass density is not visible by inspection from the given figures, but from the underlying results it is seen that all elements with orthotropic material fully contain the indicated one. Since the solutions have converged almost to 0/1 solutions, the penalized compliance is comparable to the non-penalized compliance.

A similar example was addressed by Bendsøe et al. (1995), Hörnlein et al. (2001) and Bodnár (2009), where the design problem was investigated using Free Material Optimization (FMO). The results obtained using FMO are not directly comparable to those obtained in this paper due to the full freedom of design of the material tensor in FMO compared to the setting of DMO where the design is restricted to a set of physically available materials. Nevertheless, the results obtained here have similarities to those obtained by FMO in the sense that stiff material is chosen in the same areas where the FMO results indicate a need for stiffness, and also the fiber orientations obtained here resemble those shown by Bodnár (2009).

Fig. 11 SIMP (*left*) and RAMP (*right*) solution in layer 2; *light grey*: pure foam, *dark grey*: mixture of foam and orthotropic material, *black*: pure orthotropic material

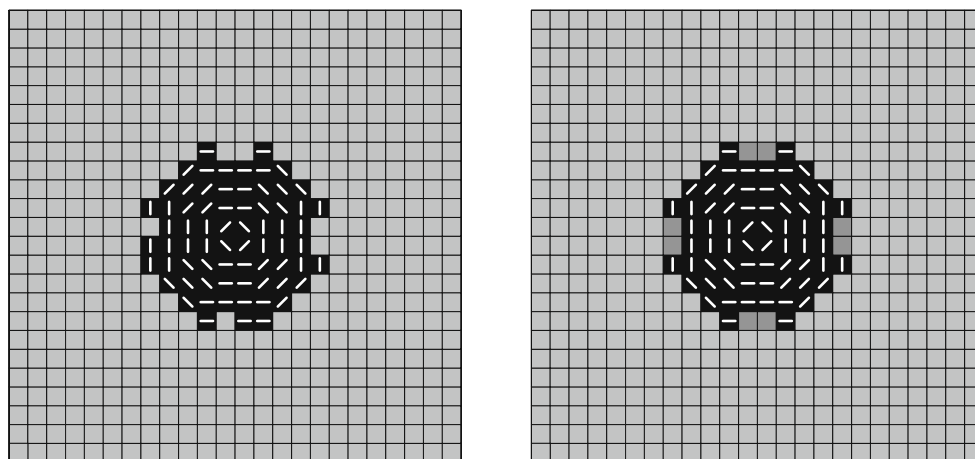
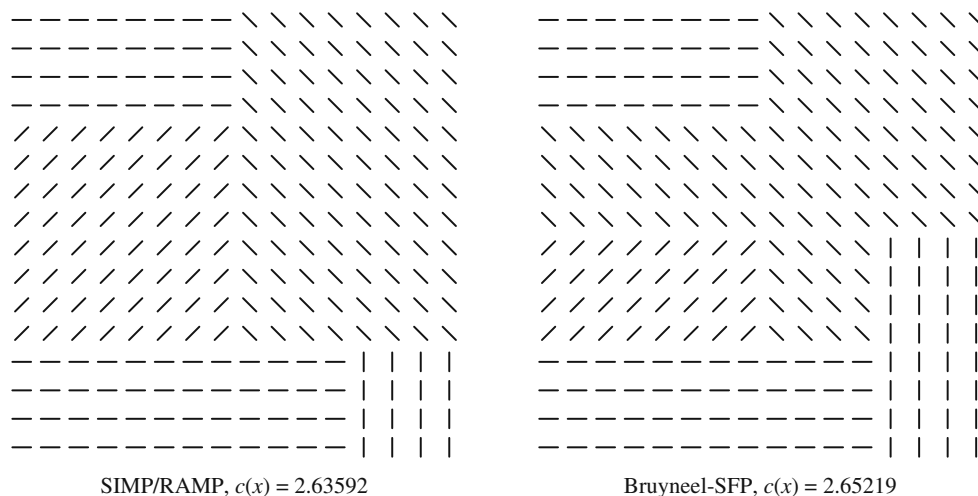


Fig. 12 Discrete orientation selection. *Left:* SIMP/RAMP solution. *Right:* SFP solution from Bruyneel (2011) evaluated using our code



6.2 Layered composite multi-material plate

We use the same conventions for plotting the solution as for the previous example. In the four innermost layers the light and compliant foam material has been chosen throughout as expected. In Fig. 10 we see the outer layers (symmetric) where it is observed that the stiff material is chosen throughout and at the same time oriented so as to make use of the orthotropy. Note that the sandwich structure with stiff outer layers and a compliant core comes out as a result of the optimization. This result agrees well with the expectations for a stiffness optimal lightweight structure for bending.

In most elements the material choice has converged to a distinct solution. In terms of material distribution and orientation the RAMP solution is perfectly symmetric around all planes of symmetry, see right column of Figs. 10 and 11. Almost all elements contain a distinct material selection and the only non-distinct elements are found in layer 2 and 7 where a few elements symmetrically arranged around the region of stiff material contain mixture of light and stiff

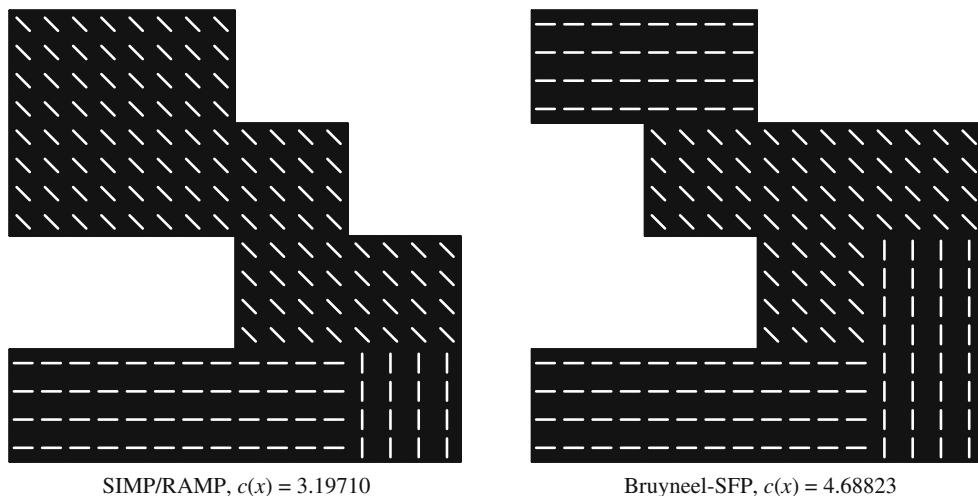
material, see Fig. 11(right). The SIMP solution is very similar to the RAMP solution but slightly more converged in terms of distinct material selection where the elements that contained mixture in the RAMP solution now have become distinct at the price of breaking the perfect symmetries, see Fig. 11(left). Both designs have almost the same objective function.

6.3 Clamped membrane

6.3.1 Discrete orientation selection

For this problem the SIMP and the RAMP solution are identical and the solution in terms of orientation of the orthotropic material is shown in Fig. 12. The solution is slightly different from the one obtained by Bruyneel (2011). The reason for this may be the differences in the finite element formulations employed in either approach. To compare with the solution obtained by Bruyneel we reevaluated

Fig. 13 Simultaneous topology and discrete orientation selection. *Left:* SIMP/RAMP solution. *Right:* SFP solution from Bruyneel (2011) evaluated using our code



the design presented in Bruyneel (2011) using our finite element code; the result was that Bruyneel's solution performed slightly worse than the one obtained using the approach presented in this paper. It is perfectly possible that the solution obtained by Bruyneel is the optimal solution for the finite element formulation employed in that paper. Therefore one should be cautious drawing conclusions about the merits of either approach. The optimal solution depends on the finite element formulation employed and therefore it is difficult to draw conclusions about the methods based on this comparison only.

6.3.2 Simultaneous topology and discrete orientation optimization

As for the previous solution the SIMP and the RAMP solution are identical. This example was also solved by Bruyneel, but this time our solution differs more than in the previous problem. In Fig. 13 both solutions are shown and differences are observed in the topology as well as in the material orientation in the coincident elements. Again we have reevaluated the design from Bruyneel (2011) using our finite element code, and this time the performance is significantly different. The solution obtained using our approach outperforms the one using the SFP approach primarily due to a better topology where our solution makes better use of the support on the left edge by placing material there instead of adding material above the diagonal stair-like connection.

7 Conclusion and future work

This paper has presented natural generalizations of the well-known two phase material interpolation schemes so as to include any number of possibly anisotropic materials/phases. The generalization of the SIMP and RAMP schemes to multiple phases is made possible through a large number of linear (in-)equality constraints that ensure that at most one (2) or exactly one (3) material is chosen in each design subdomain. This modeling of the problem is viable using modern optimizers that handle the many sparse linear constraints efficiently. The presented parametrization enables topology design combined with discrete material optimization within the same problem formulation and changing from one type to the other only requires a change of the linear equality constraints to linear inequality constraints, or vice versa.

The penalizing effect of the new schemes has been analyzed in the setting of equal mass density orthotropic materials subject to different states of stress, and the penalizing effect is attributed to the fact that the sum of weights is less

than unity for the penalized problems and hence intermediate densities are prevented. An alternative to the approach presented in this paper could be to require the *weights* (the penalized design variables) to sum to unity. However, this would destroy the linearity of the constraints and possibly the penalizing effect. This formulation has not been investigated further but it is known from the original DMO weighting schemes that distinct choices are more difficult for schemes with the sum to unity property, see Lund and Stegmann (2005) and Stegmann and Lund (2005).

Dual algorithms in combination with convex separable approximations such as the method of moving asymptotes (MMA), see Svanberg (1987, 2002), have been the natural choice for two-phase topology optimization problems with a large number of variables and few constraints. The large number of sparse linear constraints in the present approach should be possible to treat efficiently with such algorithms as it is done in e.g. SNOPT. To the authors' best knowledge no such MMA implementation currently exists and it could be interesting to see how the parametrization shown in this paper behaves numerically using MMA-like optimizers modified to handle the many sparse linear constraints. Another alternative could be to use interior-point methods such as IPOPT, see Wächter and Biegler (2006).

The presented generalization of the SIMP and the RAMP schemes to an arbitrary number of phases opens up for a large number of possibilities for topology and multi-material design optimization. Many of the ideas and developments from two-phase topology optimization in terms of governing physics, problem formulations, solution techniques, regularization/filtering, etc. may now be extended directly to multi-material problems.

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