Inverse design in Quantum Acoustics

Designing a Phononic Beamsplitter using Inverse Design with Adjoint Simulation

David Hambraeus

[DRAFT]

Inverse design in Quantum Acoustics:
Designing a Phononic Beamsplitter using Inverse Design with Adjoint Simulation

David Hambraeus
Department of Microtechnology and Nanoscience
Chalmers University of Technology

Abstract

Lorem ipsum dolor sit amet, consectetur adipisicing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Keywords: lorem, ipsum, dolor, sit, amet, consectetur, adipisicing, elit, sed, do.

Acknowledgements

Lorem ipsum dolor sit amet, consectetur adipisicing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

David Hambraeus, Gothenburg, April 2023

Table of contents

List of figures

List of tables

List of Todos

Todonotes are organized as follows:

General comment / question

Things that could be done now, no further simulations/consultation needed

Things that could be done now but I am not sure if I should, or how to do it

Things that can't be done yet because they depend on other things, e.g. results

Citation needed

1. Introduction

Introduction to quantum acoustics... I need to read more literature I think

Restructure a little... I would like to talk about inverse design first and quantum acoustics second. Talk about how inverse design is a concept that has been applied to nanophotonics but not to quantum acoustics yet. Then talk about why we care about quantum acoustics. It feels a little bit forced to do it in that order though, talking about quantum acoustics first might be a better idea, since that would naturally lead one to introduce the problem of design.

Conventionally, when designing these components, the designer comes up with a design through intuition and parametrizes it with a couple of parameters. For example they may believe that a structure with periodically placed circular holes should yield a device that performs the desired function. The parameters that are unknown might then be the distance between neighbouring holes and the radius of the holes. To find the optimal device they would then systematically test parameter values to see which give the best performance in a simulation of the device. This brute force method of design limits the possible number of parameters to a very small number. If there are 10 different values to test for each parameter, the even 6 parameters would require 1,000,000 simulations. One can of course use smarter optimization algorithms like bayesian optimization or particle swarm optimization to decrease the number of simulations needed, but it will still be of the same order.

cite something, check Ida's thesis maybe

A different approach that has been gaining some popularity is *inverse design with adjoint simulation.* The idea is that if the gradient of the figure of merit with respect to the parameters can be calculated, then we can use gradient based optimization methods, which converge much faster, even if the number of parameters is very large. With these methods, one hopes to be able to search among a much more general class of designs for the optimal one. Su, Vercruysse, Skarda, Sapra, Petykiewicz, and Vuckovic has developed software that successfully uses inverse design for nanophotonic devices [1].

cite the thing the danish guys cited

maybe cite *inverse design in nanophotonics*

With this thesis, we explore the possibility of extending this paradigm to acoustic devices. In order to do so, we attempt to design a phononic beam splitter.

1.1 Thesis outline

2. Theory

2.1 Acoustic waves and waveguides

In order to efficiently model the deformation and stresses in a solid material, a linear elasticity model is often assumed. For small deformations, solid materials obey Hooke's law which in it's full form looks like

$$\sigma_{ij} = C_{ijkl}\epsilon_{jl}$$

where σ is the stress tensor, C the elasticity tensor which is a property of the material, and $\epsilon := \nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T$ is the strain tensor. This equation is linear in $\boldsymbol{u}$, hence the name *linear* elasticity. Using this and newtons equations of motion, the equation governing the dynamics is obtained:

$$\rho \ddot{\boldsymbol{u}} = \nabla \cdot \sigma + \boldsymbol{F}.$$

where ρ is the density, $\boldsymbol{u}$ is the displacement and $\boldsymbol{F}$ is the externally applied force.

Proper derivation for equation below? It is relatively straightforward but requires some effort

Assuming a time harmonic solution $\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{u}(x)e^{i\omega t}$ and plugging this into the governing equations yields

$$-\rho\omega^2 u_i = \partial_j C_{ijkl} \partial_k u_l + F_i \tag{2.1}$$

written in index notation for clarity.

With no external forces we get traveling modes=eigenvalues. Explain how and why periodicity means only certain modes can propagate. Good resource in Chan's thesis, or maybe solid state physics book?

At some point write about phonons? I haven't really had to care about phonons so if I talk about it it's just for applications...

Show our mode as example of this, and include band diagram

Write about PML design and why we need it: Simulating infinite waveguides isn't possible because of the finite computing power. Also we don't care about stuff far away, just that there are no reflections that can interfere.

2.2 Inverse Design

Inverse design is a design paradigm where the design of a device is guided fully by the desired characteristics. These desired characteristics are quantified through what is called an objective function[1], which I will denote f_{obj}, that should be maximized. When coupled with *adjoint simulation*, which is a clever way to compute gradients, and gradient based optimization algorithms, this is a very powerful methodology.

An overview of the design process is as follows:

1. Initialize a random device design.
2. Calculate the gradient of the design through the adjoint method.
3. Update the device design using the gradient according to the optimization algorithm.
4. If the device performance is good enough, terminate optimization, else return to step 2.

2.2.1 Adjoint Simulation

Adjoint simulation is a way to compute the gradient of f_{obj} with respect to the design, which in our case means with respect to the material parameters. I will in this section first give a general derivation, followed by the case of inverse design in acoustics.

2.2.1.1 General Derivation

Let f_{obj} be a function which depends on some (large) vector v. The vector v can be calculated by solving the linear equation $Av = b$, where b is a fixed vector and A is a matrix that depends on a vector of design parameters p. The overall goal is to find the parameters p that maximize the objective function f_{obj}. The goal of adjoint simulation is to find $\frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}p}$. This can be expanded through the chain rule as

$$\frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}p} = \frac{\mathrm{d}f_{\text{obj}}}{\mathrm{d}v}\frac{\mathrm{d}v}{\mathrm{d}p}.$$

To find the latter factor we do

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}p}[Av = b] &\implies \frac{\mathrm{d}A}{\mathrm{d}p}v + A\frac{\mathrm{d}v}{\mathrm{d}p} = 0 \\ &\implies \frac{\mathrm{d}v}{\mathrm{d}p} = -A^{-1}\frac{\mathrm{d}A}{\mathrm{d}p}v\end{aligned}$$

[1] Also called *figure of merit (FoM)* by some.

which gives

$$\frac{\mathrm{d}f_{\mathrm{obj}}}{\mathrm{d}p} = -\frac{\mathrm{d}f_{\mathrm{obj}}}{\mathrm{d}v} A^{-1} \frac{\mathrm{d}A}{\mathrm{d}p} v \tag{2.2}$$

$$= -\left(A^{-T} \frac{\mathrm{d}f_{\mathrm{obj}}}{\mathrm{d}v}^T \right)^T \frac{\mathrm{d}A}{\mathrm{d}p} v \tag{2.3}$$

The first factor of this product is the solution to the *adjoint problem*

$$A^T \tilde{v} = \frac{\mathrm{d}f_{\mathrm{obj}}}{\mathrm{d}v}^T, \tag{2.4}$$

hence the name adjoint simulation. As it turns out, A is often symmetric which means that this is simply a normal simulation but with $\frac{\mathrm{d}f_{\mathrm{obj}}}{\mathrm{d}v}^T$ as the source. Thus, to obtain the derivative we just need to run an additional simulation with a different input.

Now you might be wondering: what have we gained by this? Let n be the dimension of v, m the dimension of p and l the dimension of b. This means that A is a matrix with dimension $l \times n$ and $\frac{\mathrm{d}A}{\mathrm{d}p}$ is a three-tensor with dimension $m \times l \times n$. Thus calculating $A^{-1}\frac{\mathrm{d}A}{\mathrm{d}p}$ directly involves solving $Ax = w$ for a three-tensor, and calculating $A^{-1}\left(\frac{\mathrm{d}A}{\mathrm{d}p}v\right)$ involves solving for a matrix, both of which are orders of magnitude more computationally expensive than solving for a vector.

2.2.1.2 Specific derivation with acoustics

Now we turn to the specific case of acoustic devices. Here $Av = b$ is replaced by the dynamic equation of linear elasticity:

dynamic equation? Better name

$$-\left(\rho\omega\delta_{il} + \partial_j C_{ijkl} \partial_k\right) u_l = F_i \tag{2.5}$$

Derive specific case (with functional analysis): borrowing heavily from the mathy notes is possible. Derivation is theoretically possible without specifying that the objective function is an overlap integral, only using equation (2.1), but the equations would be *a lot* longer and more abstruse, so I don't think that it is a good idea.

2.2.2 Optimization Algorithms

General paragraph on the benefits of gradient based optimization algorithms vs other algorithms? And general overview of the optimization process: simulate – compute gradient – step

Paragraph describing regular gradient descent

Paragraph describing the ADAM algorithm

3. Methods

The aim of this thesis is to use inverse design to find a phononic beamsplitter, a task that can be divided into three parts: First, some definitions of what should be designed and what constitutes a “good” design needs to be made. Second, we need a way to calculate the gradient of the “goodness” with respect to the design. And lastly, we need a gradient based optimization algorithm to find the optimal design. All of this will be described in this chapter.

3.1 Design

The device design to be optimized can be seen in figure 3.1

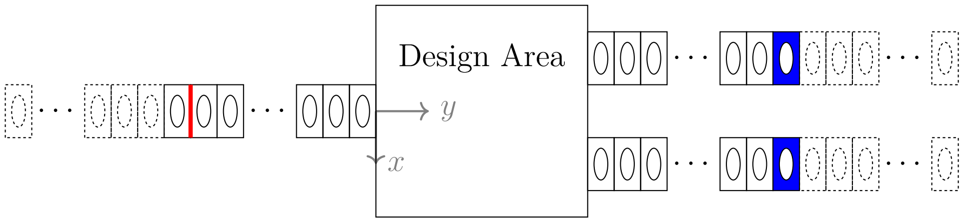

Figure 3.1: *Device design to be optimized. At the red line, a wave traveling right is excited. On the blue unit cells is where the output is measured. The dashed unit cells are PML*

Write about why we use the mode we use, and why I clamp the bottom. Can reference Johan and Pauls paper

3.1.1 Level-set

Description of what level-set is: A way of storing a boundary between two regions; and how it works: Signed distance function

Description of it’s advantages: Easily evolved (level-set equation), no connectivity issues, see level-set book

Write about how I use it? This feels like it should come after I’ve talked about computing the derivative.

3.1.2 Objective function

Maybe I'll only mention that f is an integral of the displacement field in the theory and here give the specific formula:

$$f_{\text{obj}} = \int_{\Omega_1} \boldsymbol{m}_{\mathbf{1}}^*(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x})\,\mathrm{d}x + \int_{\Omega_2} \boldsymbol{m}_{\mathbf{2}}^*(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x}) \tag{3.1}$$

Paragraph about pure part of objective function, enforcing the minimum feature size

3.2 Adjoint Simulation

Give the explicit formula for the gradient now that the objective function has been fully defined

3.3 Optimization

Describe what optimization algorithm was used, as well as how this changed during the simulation. E.g. first 200 iterations ADAM; next ADAM but with sigmoid function application; sigmoid + feature size; and finally level-set.

4. Results

5. Conclusion

References

[1] L. Su, D. Vercruysse, J. Skarda, N. V. Sapra, J. A. Petykiewicz, and J. Vuckovic, "Nanophotonic inverse design with spins: Software architecture and practical considerations," 2019. arXiv: 1910.04829 [physics.app-ph].

A. First appendix

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

B. Second appendix

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.