NumBAT Documentation

Release 2.0.0

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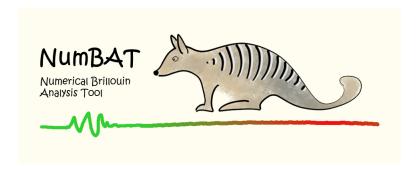
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CHAPTER

ONE

INTRODUCTION



1.1 Introduction

NumBAT, the Numerical Brillouin Analysis Tool, integrates electromagnetic and acoustic mode solvers to calculate the interactions of optical and acoustic waves in waveguides.

1.2 Goals

NumBAT is designed primarily to calculate the optical gain response from stimulated Brillouin scattering (SBS) in integrated waveguides. It uses finite element algorithms to solve the electromagnetic and acoustic modes of a wide range of 2D waveguide structures. It can account for photoelastic/electrostriction and moving boundary/radiation pressure effects, as well as uniaxial optical anisotropy and general acoustic anisotropy.

NumBAT also supports user-defined material properties and we hope its creation will drive a community-driven set of standard properties and geometries which will allow all groups to test and validate each other's work.

A full description of the NumBAT physics and numerical algorithms is available in an arxiv paper submitted in September 2017.

NumBAT is open-source software and the authors welcome additions to the code. Details for how to contribute are available in *Contributing to NumBAT*.

1.3 Development team

NumBAT was developed by Bjorn Sturmberg, Kokou Dossou, Blair Morrison, Chris Poulton and Michael Steel in a collaboration between Macquarie University, the University of Technology Sydney, and the University of Sydney, as part of the Australian Research Council Discovery Project DP160101691.

1.4 Release notes

1.4.1 Version 2.0

A number of API changes have been made in NumBAT 2.0 to tidy up the interface and make plotting and analysis simpler and more powerful. You will need to make some changes to existing files to run in NumBAT 2.0. Your best guide to new capabilities and API changes is to look through the code in the tutorial examples.

Some key changes you will need to make are as follows:

- The waveguide class *Struct* has been renamed to *Structure*.
- The interface for creating materials has changed. You now call the *materials. make_material(*name*)* function. For example *material_a = materials.make_material('Vacuum')*
- To access an existing material in an existing *Struture* object (usually in a variable called *wguide*), use *wguide.get_material(*label*)*. For example, *mat_a = wguide.get_material('b')*, where the allowed labels are *bkg*, and the letters *a* to *r*.
- The member name for refractive in a *Material* object has changed from *n* to *refindex_n*.
- The member name for density in a Material object has changed from n to rho.

CHAPTER

TWO

INSTALLATION

2.1 Installation

The source code for NumBAT is hosted here on Github. Please download the latest release from here.

NumBAT has been developed on Ubuntu 18.04 with the following package versions: Python 3.6.9, Numpy 1.19.4, Suitesparse 4.4.6, and Gmsh 3.0.6. The integration with Gmsh has a history of version dependence - the first test script runs independently of Gmsh, so if this passes and the second script fails, look into Gmsh version issues. It has also been successfully installed by users on Debian, RedHat and on Windows 10 (installing Ubuntu after enabling the Windows Subystem for Linux - steps 3 here https://msdn.microsoft.com/en-au/commandline/wsl/install_guide) and with different versions of packages, but these installations have not been as thoroughly documented so may require user testing.

In general, you can simply download the git repository and run the setup script

```
$ git clone https://github.com/michaeljsteel/NumBAT.git
$ cd NumBAT/
$ ./setup.sh
```

or, depending on your system configuration as

```
$ sudo ./setup.sh
```

Before doing so you may wish to update your system

```
$ sudo apt-get update
$ sudo apt-get upgrade
```

Or, if you prefer to do things manually, this is equivalent to

```
$ sudo apt-get install -y <dependencies>
$ cd backend/fortran/
$ make
$ cd ../../tests/
$ nosetests3
```

where the <dependencies> packages are listed dependencies.txt. Note that it is safer to pip install matplotlib than apt-get'ing as will install matplotlib 2.0 without conflicting older versions.

For optimal results

```
$ cp NumBAT/backend/NumBATstyle.mplstyle ~/.config/matplotlib/stylelib/
```

or replace plt.style.use('NumBATstyle') in NumBAT/backend/plotting.py with your own prefered matplotlib style file.

This is all there is, there isn't any more.

Well there's more if you want to change it up.

The Fortran components (NumBAT source code and libraries) have been successfully compiled with intel's ifortran as well as open-source gfortran. In this documentation we use gfortran, but this can be easily adjusted in NumBAT/backend/fortran/Makefile

On non-ubuntu OSes you may also need to compile a local version of Suitesparse, which is described in the next section.

2.1.1 Manual installation of SuiteSparse

The FEM routine used in NumBAT makes use of the highly optimised UMFPACK (Unsymmetric MultiFrontal Package) direct solver for sparse matrices developed by Prof. Timothy A. Davis. This is distributed as part of the SuiteSparse libraries under a GPL license. It can be downloaded from https://www.cise.ufl.edu/research/sparse/SuiteSparse/

This is the process we have used in the past, however this was some years ago and may need to be modified.

Unpack SuiteSparse into NumBAT/backend/fortran/, it should create a directory there; SuiteSparse/ Make a directory where you want SuiteSparse installed, in my case SS_installed

```
$ mkdir SS_installed/
```

edit SuiteSparse/SuiteSparse_config/SuiteSparse_config.mk for consistency across the whole build; i.e. if using intel fortran compiler

```
line 75 F77 = gfortran --> ifort
```

set path to install folder:

```
line 85 INSTALL_LIB = /$Path_to_EMustack/NumBAT/backend/fortran/SS_installed/lib
line 86 INSTALL_INCLUDE = /$Path_to_EMustack/NumBAT/backend/fortran/SS_installed/include
```

line 290ish commenting out all other references to these:

```
F77 = ifort
CC = icc
BLAS = -L/apps/intel-ct/12.1.9.293/mkl/lib/intel64 -lmkl_rt
LAPACK = -L/apps/intel-ct/12.1.9.293/mkl/lib/intel64 -lmkl_rt
```

Now make new directories for the paths you gave 2 steps back:

```
$ mkdir SS_installed/lib SS_installed/include
```

Download metis-4.0 and unpack metis into SuiteSparse/ Now move to the metis directory:

```
$ cd SuiteSparse/metis-4.0
```

Optionally edit metis-4.0/Makefile.in as per SuiteSparse/README.txt plus with -fPIC:

```
CC = gcc

or

CC = icc

OPTFLAGS = -03 -fPIC
```

Now make metis (still in SuiteSparse/metis-4.0/):

```
$ make
```

Now move back to NumBAT/backend/fortran/

```
$ cp SuiteSparse/metis-4.0/libmetis.a SS_installed/lib/
```

and then move to SuiteSparse/ and execute the following:

```
$ make library
$ make install
$ cd SuiteSparse/UMFPACK/Demo
$ make fortran64
$ cp SuiteSparse/UMFPACK/Demo/umf4_f77zwrapper64.o into SS_installed/lib/
```

Copy the libraries into NumBAT/backend/fortran/Lib/ so that NumBAT/ is a complete package that can be moved across machine without alteration. This will override the pre-compiled libraries from the release (you may wish to save these somewhere).:

```
$ cp SS_installed/lib/*.a NumBAT/backend/fortran/Lib/
$ cp SS_installed/lib/umf4_f77zwrapper64.o NumBAT/backend/fortran/Lib/
```

NumBAT Makefile

Edit NumBAT/backend/fortran/Makefile to reflect what compiler you are using and how you installed the libraries. The Makefile has further details.

Then finally run the setup.sh script!

2.1.2 Contributing to NumBAT

NumBAT is open source software licensed under the GPL with all source and documentation available at github.com. We welcome additions to NumBAT code, documentation and the materials library. Interested users should fork the standard release from github and make a pull request when ready. For major changes, we strongly suggest contacting the NumBAT team before starting work at michael.steel@mq.edu.au.

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CHAPTER

THREE

BASIC USAGE

3.1 Simulation Procedure

Simulations with NumBAT are generally carried out using a python script file. This file is kept in its own directory which is placed in the NumBAT directory. All results of the simulation are automatically created within this directory. This directory then serves as a complete record of the calculation. Often, we will also save the simulation objects within this folder for future inspection, manipulation, plotting, etc.

Throughout the tutorial the script file will be called simo.py.

These files can be edited using your choice of text editor (for instance running the following in the terminal \$ nano simo.py) or an IDE (for instance pycharm) which allow you to run and debug code within the IDE.

To start a simulation open a terminal and change into the directory containing the simo.py file.

To start we run an example simulation from the tutorials directory. To move to this directory in the terminal enter:

```
$ cd <path to installation>/NumBAT/tutorials
```

To run this script execute:

```
$ python3 simo.py
```

To save the results from the simulation that are displayed upon execution (the print statements in simo.py) use:

```
$ python3 ./simo.py | tee log-simo.log
```

This may require you to update the permissions for the simo.py file to make it executable. This is done in the terminal as:

```
$ chmod +x simo.py
```

To have direct access to the simulation objects upon the completion of the script use:

```
$ python3 -i simo.py
```

This will execute the simo.py script and then return you into an interactive python session within the terminal. This terminal session provides the user experience of an ipython type shell where the python environment and all the simulation objects are as in the simo.py script. In this session you can access the docstrings of objects, classes and methods. For example:

```
>>> from pydoc import help
>>> help(objects.Struct)
```

where we have accessed the docstring of the Struct class from objects.py.

3.2 Script Structure

As will be seen in the tutorials below, most NumBAT scripts proceed with a standard structure:

- · defining materials
- defining waveguide geometries and associating them with material properties
- solving electromagnetic and acoustic modes
- · calculating gain and other derived quantities

The following section provides some information about specifying material properties and waveguide structures, as well as the key parameters for controlling the finite-element meshing. Information on how to add new structures to NumBAT is provided in *Making New Mesh*.

3.3 Materials

In order to calculate the modes of a structure we must specify the acoustic and optical properties of all constituent materials.

In NumBAT, this data is read in from json files, which are stored in <runo</pre>root>/NumBAT/backend/material_data.

These files not only provide the numerical values for optical and acoustic variables, but record how these variables have been arrived at. Often they are taken from the literature.

The intention of this arrangement is to create a library of materials that can we hope can form a standard amongst the research community. They also allow users to check the sensitivity of their results on particular parameters for a given material.

At present, the material library contains:

- Vacuum
- As2S3_2016_Smith
- As2S3_2017_Morrison
- As2S3_2021_Poulton
- GaAs_2016_Smith
- Si_2013_Laude
- Si_2015_Van_Laer
- Si_2016_Smith
- Si_2021_Poulton
- SiO2_2013_Laude
- SiO2_2015_Van_Laer
- SiO2_2016_Smith
- SiO2_2021_Smith
- Si_test_anisotropic

All available materials are loaded into NumBAT into the materials.materials_dict dictionary, whose keys are the json file names. Materials can easily be added to this by copying any of these files as a template and modifying the properties

to suit. The Si_test_anisotropic file contains all the variables that NumBAT is setup to read. We ask that stable parameters (particularly those used for published results) be added to the NumBAT git repository using the same naming convention.

3.4 Waveguide Geometries

The following figures give some examples of how material types and physical dimensions are represented in the mesh geometries. These can also be found in the directory:

```
>>> NumBAT/docs/msh_type_lib
```

as a series of .png files. The captions below also list the mesh geometry template files in NumBAT/backend/fortran/msh of the form refix>_msh_template.geo which define the structures and can give ideas for developing new structure files.

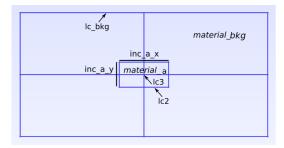


Fig. 3.1: Rectangular waveguide using shape rectangular (template oneincl_msh).

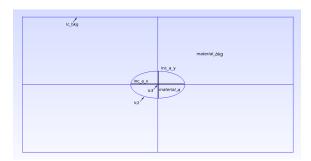


Fig. 3.2: Elliptical waveguide using shape circular (template oneincl_msh).

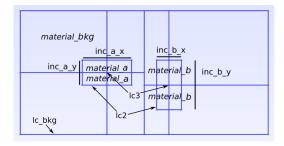


Fig. 3.3: Coupled rectangular waveguides using shape rectangular (template twoincl_msh).

Fig. 3.4: Coupled circular waveguides using shape circular (template twoincl_msh).

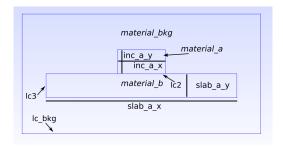


Fig. 3.5: A conventional rib waveguide using shape rib (template rib).

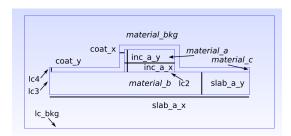


Fig. 3.6: A coated rib waveguide using shape rib_coated (template rib_coated).

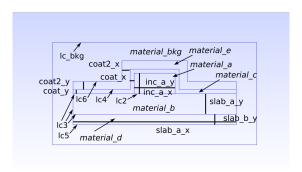


Fig. 3.7: A rib waveguide on two substrates using shape rib_double_coated (template rib_double_coated).

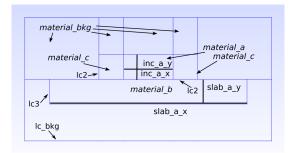


Fig. 3.8: A slot waveguide using shape slot (material_a is low index) (template slot).

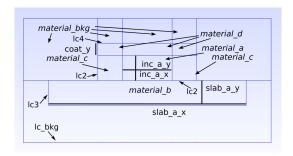


Fig. 3.9: A coated slot waveguide using shape slot_coated (material_a is low index) (template slot).

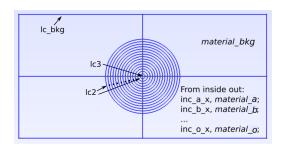


Fig. 3.10: A many-layered concentric structure using shape onion.

Fig. 3.11: A two-layered concentric structure with background using shape onion2.

 $Fig.\ 3.12:\ A\ two-layered\ concentric\ structure\ with\ background\ using\ shape\ {\tt onion3}.$

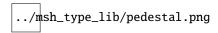


Fig. 3.13: A supported pedestal structure using shape pedestal.

The parameters lc_bkg, lc_refine_1, lc_refine_2 to be encountered below set the fineness of the FEM mesh. lc_bkg sets the reference background mesh size, larger lc_bkg = larger (more coarse) mesh. In NumBAT it is also possible to refine the mesh near interfaces and near select points in the domain, as highlighted in the figures above. This is done using the lc_refine_commands, which we now discuss. At the interface between materials the mesh is refined to be lc_bkg/lc_refine_1, therefore larger lc_refine_1 = finer mesh at these interfaces. The meshing program automatically adjusts the mesh size to smoothly transition from a point that has one mesh parameter to points that have other meshing parameters. The mesh is typically also refined at the centers of important regions, such as in the center of a waveguide, which is done with lc_refine_2, which analogously to lc_refine_1, refines the mesh size at these points as lc_bkg/lc_refine_2. For definition of lc_refine_3+ parameters see the particular .geo file.

Choosing appropriate values of lc_bkg, lc_refine_1, lc_refine_2 is crucial for NumBAT to give accurate results. The values depend strongly on the type of structure being studied, and so it is recommended to carry out a convergence test before delving into new structures (see Tutorial 5) starting from similar parameters as used in the tutorial simulations. In NumBAT the x-dimension of the unit cell is traditionally normalised to unity, in which case there will be lc_bkg mesh elements along the horizontal outside edge; in other words the outside edge is divided into lc_bkg elements.

You can also visually check the resolution of your mesh by setting plt_mesh=True or check_mesh=True when you define your objects.Struct - the first saves a png of the mesh (in NumBAT/backend/fortran/msh/) the second opens mesh in gmsh - (see Tutorial 1). The NumBAT generated .msh file is stored in NumBAT/backend/fortran/msh/ which can be viewed by running the following command

```
NumBAT/backend/fortran/msh$ gmsh <msh_name>.msh
```

Users on WSL will need to first run an X listener (such as XMING) in Windows in order for the "plt_mesh=True" feature to work. Once the X listener is running, execute the following in the terminal:

```
$ sudo apt-get install x11-apps
$ export DISPLAY=:0
$ xclock
```

where the last command is simply to check the setup. Once this is confirmed to be operating smoothly, the "plt_mesh=True" command will then run as anticipated and generate two png files (one for the geometry and one for the mesh) in NumBAT/backend/fortran/msh/. Note the X windows that open must be manually closed for the calculation to continue, and after unexpected restarts the X window may no longer display output but the png files will contain the necessary features.

In the remainder of this chapter we go through a number of example simo.py files. But before we do, another quick tip about running simulations within screen sessions, which allow you to disconnect from servers leaving them to continue your processes.

3.5 Screen Sessions

screen

is an extremely useful little linux command. In the context of long-ish calculations it has two important applications; ensuring your calculation is unaffected if your connection to a remote machine breaks, and terminating calculations that have hung without closing the terminal. For more information see the manual:

```
$ man screen
```

or see online discussions here, and here.

The screen session or also called screen instance looks just like your regular terminal/putty, but you can disconnect from it (close putty, turn off your computer etc.) and later reconnect to the screen session and everything inside of this will have kept running. You can also reconnect to the session from a different computer via ssh.

3.5.1 Basic Usage

To install screen:

```
$ sudo apt-get install screen
```

To open a new screen session:

```
$ screen
```

\$ top

We can start a new calculation here:

```
$ cd NumBAT/tutorials/
$ python simo-tut_01-first_calc.py
```

We can then detach from the session (leaving everything in the screen running) by typing:

```
Ctrl +a
Ctrl +d
```

We can now monitor the processes in that session:

Where we note the numerous running python processes that NumBAT has started. Watching the number of processes is useful for checking if a long simulation is near completion (which is indicated by the number of processes dropping to less than the specified num_cores).

We could now start another screen and run some more calculations in this terminal (or do anything else). If we want to access the first session we 'reattach' by typing:

```
Ctrl +a +r
```

Or entering the following into the terminal:

```
$ screen -r
```

If there are multiple sessions use:

3.5. Screen Sessions 15

\$ screen -ls

to get a listing of the sessions and their ID numbers. To reattach to a particular screen, with ID 1221:

\$ screen -r 1221

To terminate a screen from within type:

Ctrl+d

Or, taking the session ID from the previous example:

screen -X -S 1221 kill

3.5.2 Terminating NumBAT simulations

If a simulation hangs, we can kill all python instances upon the machine:

\$ pkill python3

If a calculation hangs from within a screen session one must first detach from that session then kill python, or if it affects multiple instances, you can kill screen. A more targeted way to kill processes is using their PID:

\$ kill PID

Or if this does not suffice be a little more forceful:

\$ kill -9 PID

The PID is found from one of two ways:

\$ top

\$ ps -fe | grep username

EXAMPLES AND TUTORIALS

This chapter provides several resources for learning NumBAT, exploring its applications and validating it against literature results. You should begin by working through the sequence of tutorial exercises which are largely based on literature results. You may then select from examples drawn from a recent tutorial paper by Dr Mike Smith and colleagues, and a range of other literature studies.

4.1 Tutorial

In this section we walk through a number of simple simulations that demonstrate the basic use of NumBAT. *Literature Examples* looks at a number of literature examples taken from many of the well-known groups in this field. The full Python interface is documented in *Python Interface*.

4.1.1 Tutorial 1 – Basic SBS Gain Calculation

This example, contained in tutorials/simo-tut_01-first_calc.py calculates the backward SBS gain for a rectangular silicon waveguide surrounded by air.

The sequence of operations (annotated in the source code below as Step 1, Step 2, etc) is:

- 1. Import NumBAT modules
- 2. Define the structure shape and dimensions
- 3. Specify the electromagnetic and acoustic modes to be solved for
- 4. Construct the waveguide with objects.Struct
- 5. Solve the electromagnetic problem. mode_calcs.calc_EM_modes() returns an object containing electromagnetic mode profiles, propagation constants, and potentially other data which can be accessed through various methods.
- 6. Display the propagation constants in units of m^{-1} of the EM modes using mode_calcs.kz_EM_all()
- 7. Obtain the effective index of the fundamental mode using mode_calcs.neff()
- 8. Identify the desired acoustic wavenumber from the difference of the pump and Stokes propagation constants and solve the acoustic problem. mode_calcs.calc_AC_modes() returns an object containing the acoustic mode profiles, frequencies and potentially other data at the propagation constant k_AC.
- 9. Display the acoustic frequencies in Hz using mode_calcs.nu_AC_all().
- 10. Calculate the total SBS gain, contributions from photoelasticity and moving boundary effects, and the acoustic loss using integration.gain_and_qs().

```
""" Calculate the backward SBS gain for modes in a
   silicon waveguide surrounded in air.
# Step 1
import time
import datetime
import numpy as np
import sys
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k_AC: acoustic wavevector
start = time.time()
print('\n\nCommencing NumBAT tutorial 1')
# Step 2
# Geometric Parameters - all in nm.
wl_nm = 1550 # Wavelength of EM wave in vacuum.
# Unit cell must be large to ensure fields are zero at boundary.
unitcell_x = 2.5*wl_nm
unitcell_y = unitcell_x
# Waveguide widths.
inc_a_x = 300
inc_a_y = 280
# Shape of the waveguide.
inc_shape = 'rectangular'
# Step 3
# Number of electromagnetic modes to solve for.
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
# Number of acoustic modes to solve for.
num\_modes\_AC = 20
# The EM pump mode(s) for which to calculate interaction with AC modes.
# Can specify a mode number (zero has lowest propagation constant) or 'All'.
EM_ival_pump = 0
# The EM Stokes mode(s) for which to calculate interaction with AC modes.
EM_ival_Stokes = 0
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
```

(continues on next page)

```
# Step 4
# Use specified parameters to create a waveguide object.
# to save the geometry and mesh as png files in backend/fortran/msh/
wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("Si_2016_Smith"),
                        lc_bkg=1, # in vacuum background
                        lc_refine_1=600.0, # on cylinder surfaces
                        lc_refine_2=300.0) # on cylinder center
# Note use of rough mesh for demonstration purposes by turning this line on.
#wguide.plot_mesh()
# Explicitly remind ourselves what data we're using.
print('\nUsing material data: ', wguide.get_material('a'))
# Step 5
# Estimate expected effective index of fundamental guided mode.
n_eff = wguide.get_material('a').refindex_n-0.1
# Calculate the Electromagnetic modes of the pump field.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
# Display the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of electromagnetic modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# Calculate the Electromagnetic modes of the Stokes field.
# For an idealised backward SBS simulation the Stokes modes are identical
# to the pump modes but travel in the opposite direction.
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
# # Alt
# sim_EM_Stokes = wguide.calc_EM_modes(wl_nm, num_modes_EM_Stokes, n_eff, Stokes=True)
# Find the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("\n Fundamental optical mode ")
print(" n_eff = ", np.round(n_eff_sim, 4))
# Acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(0) - sim_EM_Stokes.kz_EM(0))
print('\n Acoustic wavenumber (1/m) = ', np.round(k_AC, 4))
# Step 7
# Calculate Acoustic modes, using the mesh from the EM calculation.
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
# Print the frequencies of AC modes.
```

(continues on next page)

```
v_nu=sim_AC.nu_AC_all()
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_n): print('\{0:3d\} {1:.5f}'.format(i, np.real(nu)*1e-9))
# Do not calculate the acoustic loss from our fields, instead set a Q factor.
set_q_factor = 1000.
# Step 8
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB. Also calculate acoustic loss alpha.
SBS_gain_tot, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.

    gain_and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, EM_ival_pump=EM_ival_pump,
   EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_Q=set_q_factor)
# SBS_gain_tot, SBS_gain_PE, SBS_gain_MB are 3D arrays indexed by pump, Stokes and,
→acoustic mode
# Extract those of interest as a 1D array:
SBS_gain_PE_ij = SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:]
SBS_gain_MB_ij = SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:]
SBS_gain_tot_ij = SBS_gain_tot[EM_ival_pump,EM_ival_Stokes,:]
# Print the Backward SBS gain of the AC modes.
print("\nContributions to SBS gain [1/(WM)]")
print("Acoustic Mode number | Photoelastic (PE) | Moving boundary(MB) | Total")
for (m, gpe, gmb, gt) in zip(range(num_modes_AC), SBS_gain_PE_ij, SBS_gain_MB_ij, SBS_
print('{0:8d} {1:18.6e} {2:18.6e} {3:18.6e}'.format(m, gpe, gmb, gt))
#with np.printoptions(formatter={ % 'float': '{: 12.4e}'.format, 'int': '{: 12d}'.format }
⇔):
    print(np.array([ range(num_modes_AC), SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:],
                     SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], SBS_gain[EM_ival_pump,
→EM_ival_Stokes,:]]
                      ).T)
#print("\n SBS_gain [1/(Wm)] PE contribution \n", SBS_gain_PE[EM_ival_pump,EM_ival_
→Stokes,:])
#print("SBS_gain [1/(Wm)] MB contribution \n", SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,
#print("SBS_gain [1/(Wm)] total \n", SBS_gain[EM_ival_pump,EM_ival_Stokes,:])
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.where(np.abs(SBS_gain_PE_ij)>threshold, SBS_gain_PE_ij, 0)
masked_MB = np.where(np.abs(SBS_gain_MB_ij)>threshold, SBS_gain_MB_ij, 0)
masked_tot = np.where(np.abs(SBS_gain_tot_ij)>threshold, SBS_gain_tot_ij, 0)
print("\n Displaying gain results with negligible components masked out:")
```

(continues on next page)

```
print("AC Mode number | Photoelastic (PE) | Moving boundary(MB) | Total")
for (m, gpe, gmb, gt) in zip( range(num_modes_AC), masked_PE, masked_MB, masked_tot):
    print('{0:12d} {1:19.6e} {2:19.6e} {3:16.6e}'.format(m, gpe, gmb, gt))
end = time.time()
print("\nSimulation time: {0:10.3f} secs.".format(end - start))
print('\n\n')
```

4.1.2 Tutorial 2 - SBS Gain Spectra

This example, contained in tutorials/simo-tut_02-gain_spectra-npsave.py considers the same silicon-in-air structure but adds plotting of fields, gain spectra and techniques for saving and reusing data from earlier calculations.

Here are some elements to note:

- 1. np.savez() and np.load() allow storage of arbitrary data in numpy .npz files between simulations to accelerate subsequent calculations. Use the flag recalc_fields to determine whether to recalculate the data from scratch or load data from an existing .npz file. The data is recovered as a :Simmo: object by calling the tolist() method. Note that numpy requires the allow_pickle=True flag for loading array data from file.
- 2. This tutorial and many subsequent ones can be made to run faster at the expense of accuracy by appending the argument fast=1 to the command line. This has the effect of specifying a coarser FEM grid. In this case, the output data and fields directory begin with ftut_02 rather than tut_02.
- 3. Both electric and magnetic fields can be selected using EM_E or EM_H as the value of EM_AC in plotting. mode_fields. These fields are stored in a folder tut_02-fields/ within the tutorial folder.
- 4. By default, plots are exported as png format. Pass the option pdf_png=pdf to plot functions to generate a pdf output.
- 5. Plots of both spectra and modes are generated with a best attempt at font sizes, line widths etc, but the range of potential cases make it impossible to find a selection that works in all cases. Most plot functions therefore support the passing of a plotting. Decorator object that can vary the settings of these parameters and also pass additional commands to write on the plot axes. See the plotting API for details. This should be regarded as a relatively advanced NumBAT feature.
- 6. The suppress_imimre option suppresses plotting of the Im[x], Im[y] and Re[z] components of the fields which in a lossless non-leaky problem should normally be zero at all points and therefore not useful to plot.
- 7. Vector field plots often require tweaking to get an attractive set of vector arrows. The quiver_points option controls the number of arrows drawn along each direction.
- 8. The plot functions and the Decorator class support many options. Consult the API chapter for details on how to fine tune your plots.

```
""" Calculate the backward SBS gain spectra of a silicon waveguide surrounded in air.

Show how to save simulation objects (eg. EM mode calcs) to expedite the process of altering later parts of simulations.

Show how to implement integrals in python and how to load data from Comsol.

"""

import time import datetime import numpy as np import sys

sys.path.append("../backend/") import materials import objects import mode_calcs
```

(continues on next page)

```
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 2.5*wl_nm
unitcell_y = unitcell_x
inc_a_x = 300
inc_a_y = 280
inc_shape = 'rectangular'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 25
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate_
→calculation
  prefix_str = 'ftut_02-'
 refine_fac=1
else:
 prefix_str = 'tut_02-'
  refine_fac=5
print('\nCommencing NumBAT tutorial 2\n')
# Use of a more refined mesh to produce field plots.
wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("Si_2016_Smith"),
                        lc_bkg=1, lc_refine_1=120.0*refine_fac, lc_refine_2=60.0*refine_
بfac)
# Estimate expected effective index of fundamental guided mode.
n_eff = wguide.get_material('a').refindex_n-0.1
recalc_fields=True
                       # run the calculation from scratch
#recalc_fields=False # reuse saved fields from previous calculation
if recalc_fields:
  # Calculate Electromagnetic modes.
  sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
  sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
 print('\nSaving EM fields')
```

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```
sim_EM_pump.save_simulation('wguide_data')
  sim_EM_Stokes.save_simulation('wguide_data2')
else:
  # Once npz files have been saved from one simulation run.
  # set recalc_fields=True to use the saved data
  sim_EM_pump = mode_calcs.load_simulation('wguide_data')
  sim_EM_Stokes = mode_calcs.load_simulation('wguide_data2')
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# Plot the E fields of the EM modes fields - specified with EM_AC='EM_E'.
# Zoom in on the central region (of big unitcell) with xlim_, ylim_ args,
# which specify the fraction of the axis to remove from the plot.
# For instance xlim_min=0.4 will remove 40% of the x axis from the left outer edge
# to the center. xlim_max=0.4 will remove 40% from the right outer edge towards the...
⇔center.
# This leaves just the inner 20% of the unit cell displayed in the plot.
# The ylim variables perform the equivalent actions on the y axis.
# Let's plot fields for only the fundamental (ival = 0) mode.
#decorator=plotting.Decorator()
#decorator.set_multiplot_axes_property('subplots_wspace',.4)
#Plot the E field of the pump mode
print('\nPlotting EM fields')
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.4, xlim_max=0.4, ylim_min=0.4,
                         ylim_max=0.4, ivals=[EM_ival_pump], contours=True,
                         EM_AC='EM_E',
                         prefix_str=prefix_str, ticks=True,
                         comps=['Ex', 'Ey', 'Ez', 'Et'])
#Repeat this plot in pdf output format
#plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.4, xlim_max=0.4, ylim_min=0.4,
#
                          ylim_max=0.4, ivals=[EM_ival_pump], contours=True, #EM_AC='EM_E
                          pdf_png='pdf', prefix_str=prefix_str, ticks=True)
# Plot the H fields of the EM modes - specified with EM_AC='EM_H'.
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.4, xlim_max=0.4, ylim_min=0.4,
                         ylim_max=0.4, ivals=[EM_ival_pump], EM_AC='EM_H',
                         prefix_str=prefix_str, ticks=True, suppress_imimre=False)
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff", np.round(n_eff_sim, 4))
# Acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(0) - sim_EM_Stokes.kz_EM(0))
```

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```
if recalc fields:
  # Calculate and save acoustic modes.
  sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
  print('Saving AC fields')
  sim_AC.save_simulation('wguide_data_AC')
else:
  sim_AC = mode_calcs.load_simulation('wguide_data_AC')
# Print the frequencies of AC modes.
v_nu=sim_AC.nu_AC_all()
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('\{0:3d\} {1:.5f}'.format(i, np.real(nu)*1e-9))
# Plot the AC modes fields, important to specify this with EM_AC='AC'.
# The AC modes are calculated on a subset of the full unitcell.
# which excludes vacuum regions, so there is usually no need to restrict the area plotted
# with xlim_min, xlim_max etc.
print('\nPlotting acoustic modes')
plotting.plot_mode_fields(sim_AC, #EM_AC='AC',
        contours=True, prefix_str=prefix_str,
    ticks=True, quiver_points=20, ivals=[0])
if recalc_fields:
  # Calculate the acoustic loss from our fields.
  # Calculate interaction integrals and SBS gain for PE and MB effects combined,
  # as well as just for PE, and just for MB.
  SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
   sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, EM_ival_pump=EM_ival_pump,
   EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
  # Save the gain calculation results
  np.savez('wguide_data_AC_gain', SBS_gain=SBS_gain, SBS_gain_PE=SBS_gain_PE,
            SBS_gain_MB=SBS_gain_MB, linewidth_Hz=linewidth_Hz)
else:
 npzfile = np.load('wguide_data_AC_gain.npz', allow_pickle=True)
  SBS_gain = npzfile['SBS_gain']
  SBS_gain_PE = npzfile['SBS_gain_PE']
  SBS_gain_MB = npzfile['SBS_gain_MB']
  linewidth_Hz = npzfile['linewidth_Hz']
# The following function shows how integrals can be implemented purely in python,
# which may be of interest to users wanting to calculate expressions not currently
# included in NumBAT. Note that the Fortran routines are much faster!
# Also shows how field data can be imported (in this case from Comsol) and used.
comsol_ivals = 5 # Number of modes contained in data file.
SBS_gain_PE_py, alpha_py, SBS_gain_PE_comsol, alpha_comsol = integration.gain_python(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, 'comsol_ac_modes_1-5.dat',
   comsol_ivals=comsol_ivals)
# Print the PE contribution to gain SBS gain of the AC modes.
```

(continues on next page)

```
print("\n Displaying results of first five modes with negligible components masked out")
# Mask negligible gain values to improve clarity of print out.
threshold = -1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:comsol_ivals],__
\rightarrow0, threshold)
print("SBS_gain [1/(Wm)] PE NumBAT default (Fortran)\n", masked_PE)
masked = np.ma.masked_inside(SBS_gain_PE_py[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
print("SBS_gain [1/(Wm)] python integration routines \n", masked)
masked = np.ma.masked_inside(SBS_gain_PE_comsol[EM_ival_pump,EM_ival_Stokes,:], 0,...
→threshold)
print("SBS_gain [1/(Wm)] from loaded Comsol data \n", masked)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = np.real(sim_AC.nu_AC_all()[0])*1e-9 - 2 # GHz
freq_max = np.real(sim_AC.nu_AC_all()[-1])*1e-9 + 2 # GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
    EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str)
# Repeat this plot focusing on one frequency range
freq_min = 12 # GHz
freq_max = 14 \# GHz
plotting gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='_zoom')
end = time.time()
print("\nSimulation time: {0:10.3f} secs.".format(end - start))
print('\n\n')
```

The following figures show a selection of electromagnetic and acoustic mode profiles produced in this example.

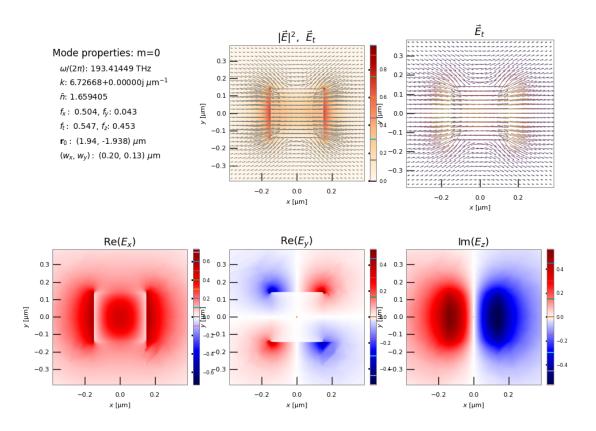


Fig. 4.1: Fundamental optical mode fields.

Fig. 4.2: Acoustic mode with high gain due to moving boundary effect.

Fig. 4.3: Acoustic mode with high gain due to moving boundary effect.

This example also generates gain spectra.

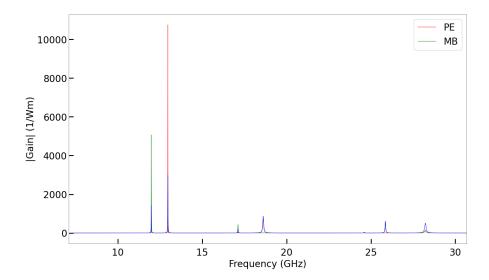


Fig. 4.4: Gain spectra showing gain due to the photoelastic effect, gain due to moving boundary effect, and the total gain.

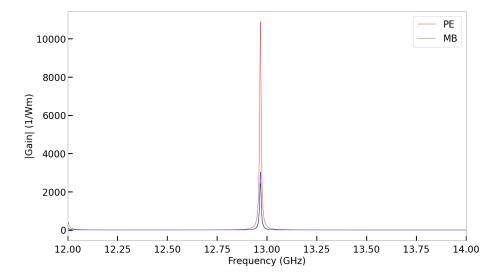


Fig. 4.5: Zoomed-in gain spectra from Gain spectra showing gain due to the photoelastic effect, gain due to moving boundary effect, and the total gain.

4.1.3 Tutorial 3a – Investigating Dispersion and np.save/np.load

This example, contained in tutorials/simo-tut_03_1-dispersion-npload.py calculates the acoustic dispersion diagram for the problem in the previous tutorial and classifies the modes according to the point group symmetry class.

```
""" Calculate a dispersion diagram of the acoustic modes
    from k\_AC \sim 0 (forward SBS) to k\_AC = 2*k\_EM (backward SBS).
   Load EM mode data from simo_tut_02.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
print('\n\nCommencing NumBAT tutorial 3a')
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 2.5*wl_nm
unitcell_y = unitcell_x
inc_a_x = 300
inc_a_y = 280
inc_shape = 'rectangular'
# Choose modes to include.
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 25
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("Si_2016_Smith"),
                        lc_bkg=1, lc_refine_1=600.0, lc_refine_2=300.0)
# Expected effective index of fundamental guided mode.
```

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```
n_eff = wguide.get_material('a').refindex_n-0.1
# Assuming this calculation is run directly after simo-tut_02
# we don't need to recalculate EM modes, but can load them in.
sim_EM_pump = mode_calcs.load_simulation('wguide_data')
sim_EM_Stokes = mode_calcs.load_simulation('wguide_data2')
# Will scan from forward to backward SBS so need to know k_AC of backward SBS.
k_AC = np.real(sim_EM_pump.kz_EM(0) - sim_EM_Stokes.kz_EM(0))
# Number of wavevector steps.
nu_ks = 20
plt.clf()
plt.figure(figsize=(10,6))
ax = plt.subplot(1,1,1)
for i_ac, q_ac in enumerate(np.linspace(0.0,k_AC,nu_ks)):
    sim_AC = wguide.calc_AC_modes(num_modes_AC, q_ac, EM_sim=sim_EM_pump)
   prop_AC_modes = np.array([np.real(x) for x in sim_AC.nu_AC_all() if abs(np.real(x)) >
\rightarrow abs(np.imag(x))])
    sym_list = integration.symmetries(sim_AC)
    for i in range(len(prop_AC_modes)):
        Om = prop_AC_modes[i]*1e-9
        if sym_list[i][0] == 1 and sym_list[i][1] == 1 and sym_list[i][2] == 1:
            sym_A, = plt.plot(np.real(q_ac/k_AC), Om, 'or')
        if sym_list[i][0] == -1 and sym_list[i][1] == 1 and sym_list[i][2] == -1:
            sym_B1, = plt.plot(np.real(q_ac/k_AC), Om, 'vc')
        if sym_list[i][0] == 1 and sym_list[i][1] == -1 and sym_list[i][2] == -1:
            sym_B2, = plt.plot(np.real(q_ac/k_AC), Om, 'sb')
        if sym_list[i][0] == -1 and sym_list[i][1] == -1 and sym_list[i][2] == 1:
            sym_B3, = plt.plot(np.real(q_ac/k_AC), Om, '^g')
   print("Wavevector loop", i_ac+1, "/", nu_ks)
ax.set_ylim(0,25)
ax.set_xlim(0,1)
plt.legend([sym_A, sym_B1, sym_B2, sym_B3],['A',r'B$_1$',r'B$_2$',r'B$_3$'], loc='lower_
⇔right')
plt.xlabel(r'Axial wavevector (normalised)')
plt.ylabel(r'Frequency (GHz)')
plt.savefig('tut_03_1-dispersion_npload_symmetrised.png', bbox_inches='tight')
plt.close()
end = time.time()
print("\nSimulation time: {0:10.3f} secs.".format(end - start))
print('\n\n')
```

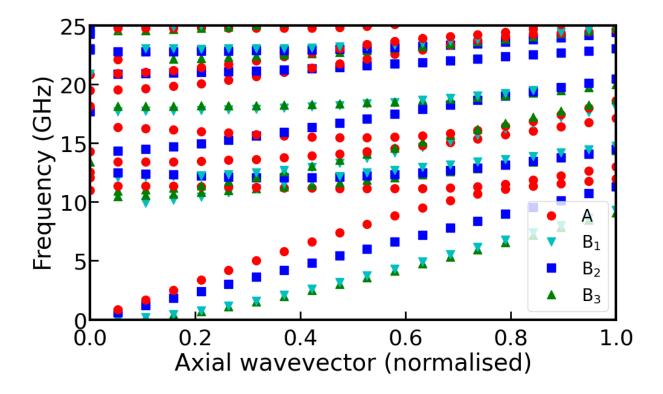


Fig. 4.6: Acoustic dispersion diagram with modes categorised by symmetry as in Table 1 of "Formal selection rules for Brillouin scattering in integrated waveguides and structured fibers" by C. Wolff, M. J. Steel, and C. G. Poulton https://doi.org/10.1364/0E.22.032489

4.1.4 Tutorial 3b - Investigating Dispersion and multiprocessing

This tutorial, contained in tutorials/simo-tut_03_2-dispersion-multicore.py continues the study of acoustic dispersion and demonstrates the use of Python multiprocessor calls to increase speed.

```
""" Calculate a dispersion diagram of the acoustic modes
    from k\_AC \sim 0 (forward SBS) to k\_AC = 2*k\_EM (backward SBS).
    Use python's (embarrassing parallel) multiprocessing package.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
from multiprocessing import Pool
import threading
import os
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 3.0*wl_nm
unitcell_y = unitcell_x
inc_a_x = 800.
inc_a_y = 220.
inc_shape = 'rectangular'
# Choose modes to include.
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 60
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate_
prefix_str = 'ftut_03-2-'
  refine_fac=1
```

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```
print('\n\nCommencing NumBAT tutorial 3b - fast mode')
else:
  prefix_str = 'tut_03-2-'
  refine_fac=5
  print('\n\nCommencing NumBAT tutorial 3b')
# Note that this mesh is quite fine, may not be required if purely using dispersive sims
wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("Si_2016_Smith"),
                        lc_bkg=1, lc_refine_1=24.0*refine_fac, lc_refine_2=12.0*refine_
\rightarrowfac)
# Estimated effective index of fundamental guided mode.
n_eff = wguide.get_material('a').refindex_n-0.1
# Calculate Electromagnetic modes.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
# Will scan from forward to backward SBS so need to know k_AC of backward SBS.
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
# Rather than calculating with a loop we can use pool to do a multi core sim
def ac_mode_freqs(k_ac):
   thread_nm = threading.current_thread().name
   print('PID: %d, Thread %s: commencing mode calculation for k_ac = %f'% (
        os.getpid(), thread_nm, k_ac))
    # Calculate the modes, grab the output frequencies only and convert to GHz
    sim_AC = wguide.calc_AC_modes(num_modes_AC, k_ac, EM_sim=sim_EM_pump)
   prop_AC_modes = np.array([np.real(nu) for nu in sim_AC.nu_AC_all() if abs(np.
\rightarrowreal(nu)) > abs(np.imag(nu))])
   mode_freqs = np.real(sim_AC.nu_AC_all()) *1.e-9 # convert to GHz
    # Clear memory
   sim\_AC = None
   print('PID: %d, Thread %s: completed mode calculation for width a_x = %f'%(
        os.getpid(), thread_nm, k_ac))
    # Return the frequencies and simulated k_ac value in a list
   return mode_freqs
# Now we utilise multi-core calculations to perform parallel simulations and speed up.
→the simulation
test_name = 'dispersion_multicore'
nu_ks = 10  # start with a low number of k_ac values to get an idea
acoustic_ks = np.linspace(5., k_AC*1.1, nu_ks)
num_cores = 8 # should be appropriate for individual machine/vm, and memory!
```

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```
pool = Pool(num_cores)
pooled_mode_freqs = pool.map(ac_mode_freqs, acoustic_ks)
# Note pool.map() doesn't pass errors back from fortran routines very well.
# It's good practise to run the extrema of your simulation range through map()
# before launcing full multicore simulation.
# We will pack the above values into a single array for plotting purposes, initialise...
\hookrightarrow first
freq_arr = np.empty((nu_ks, num_modes_AC))
for i_w, sim_freqs in enumerate(pooled_mode_freqs):
    # Set the value to the values in the frequency array
    freq_arr[i_w] = sim_freqs
# Now that we have packed will save to a numpy file for better plotting and reference
file_name = 'tut_03-2-freq_array_200'
np.save(file_name, freq_arr)
np.save(file_name+'_qs', acoustic_ks) # and the q values
# Also plot a figure for reference
plot_range = num_modes_AC
plt.clf()
plt.figure(figsize=(10,6))
ax = plt.subplot(1,1,1)
for idx in range(plot_range):
    # slicing in the row direction for plotting purposes
    freq_slice = freq_arr[:, idx]
   plt.plot(acoustic_ks/k_AC, freq_slice, 'r')
# Set the limits and plot axis labels
ax.set_ylim(0,35)
ax.set_xlim(0,1.1)
plt.xlabel(r'Axial wavevector (normalised)')
plt.ylabel(r'Frequency (GHz)')
plt.savefig(prefix_str+test_name+'.pdf', bbox_inches='tight')
plt.savefig(prefix_str+test_name+'.png', bbox_inches='tight')
plt.close()
# Output the normalisation k value for reference
print("The phonon wavevector 2*kp = %f" % k_AC)
end = time.time()
print("\nSimulation time: {0:10.3f} secs.".format(end - start))
print('\n\n')
```

../../tutorials/tut_03_2-dispersion_multicore.png

Fig. 4.7: Acoustic dispersion diagram ploted as lines.

4.1.5 Tutorial 4 - Parameter Scan of Widths

This tutorial, contained in tutorials/simo-tut_04_scan_widths.py demonstrates use of a parameter scan, in this case of the width of the silicon rectangular waveguide, to understand the behaviour of the Brillouin gain.

```
""" Calculate the backward SBS gain spectra as a function of
    waveguide width, for silicon waveguides surrounded in air.
   Also shows how to use python multiprocessing library.
import os
import time
import datetime
import numpy as np
import sys
from multiprocessing import Pool
import threading
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib.collections import PolyCollection
from matplotlib.colors import colorConverter
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Select the number of CPUs to use in simulation.
num_cores = 6
# Geometric Parameters - all in nm.
wl_nm = 1550
inc_shape = 'rectangular'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 20
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate_
→calculation
```

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```
prefix_str = 'ftut_04-'
  refine_fac=1
  print('\n\nCommencing NumBAT tutorial 4 - fast mode')
  prefix_str = 'tut_04-'
  refine_fac=5
  print('\n\nCommencing NumBAT tutorial 4')
# Width previous simo's done for, with known meshing params
known\_geo = 315.
def modes_n_gain(wguide):
    thread_nm = threading.current_thread().name
   print ('Process %d, thread %s : commencing mode calculation for width a_x = %f' % (
        os.getpid(), thread_nm, wguide.inc_a_x))
    # Expected effective index of fundamental guided mode.
   n_eff = (wguide.get_material('a').refindex_n-0.1) * wguide.inc_a_x/known_geo
    # Calculate Electromagnetic modes.
   sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
    sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
   k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
    # Calculate Acoustic modes.
    sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
    # Calculate interaction integrals and SBS gain.
    SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.
→gain_and_qs(
        sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
        EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
   print ('Process %d, thread %s: completed mode calculation for width a_x = %.3f' % (
        os.getpid(), thread_nm, wguide.inc_a_x))
   return [sim_EM_pump, sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC]
nu\_widths = 6
waveguide_widths = np.linspace(300,350,nu_widths)
l_wguides = []
# Scale meshing to new structures.
for width in waveguide_widths:
   msh_ratio = (width/known_geo)
   unitcell_x = 2.5*wl_nm*msh_ratio
   unitcell_y = unitcell_x
   inc_a_x = width
   inc_a_y = 0.9*inc_a_x
   wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,
                            inc_a_y, inc_shape,
                            material_bkg=materials.make_material("Vacuum"),
                            material_a=materials.make_material("Si_2016_Smith"),
```

```
lc_bkg=1, lc_refine_1=120.0*refine_fac, lc_refine_2=60.
→0*refine_fac)
   l_wguides.append(wguide)
new_calcs=True # fixme
if new_calcs:
  # Run widths in parallel across num_cores CPUs using multiprocessing package.
  pool = Pool(num_cores)
  # Note pool.map() doesn't pass errors back from fortran routines very well.
  # It's good practise to run the extrema of your simulation range through map()
  # before launching full multicore simulation.
  l_width_data = pool.map(modes_n_gain, l_wguides)
  v_width_data = np.array(l_width_data, dtype=object)
 np.savez('%s_simo_results'%prefix_str, width_objs=v_width_data) # This generates a_
→warning abut ragged nested sequences. Is there an option to pool.map that would clean
→this up?
else:
  npzfile = np.load('%s_simo_results.npz'%prefix_str, allow_pickle=True)
  v_width_data = np.array(npzfile['width_objs'].tolist())
n_effs = []
freqs_gains = []
interp_grid_points = 10000
int min = 10
int max = 26
interp_grid = np.linspace(int_min, int_max, interp_grid_points)
for i_w, width_obj in enumerate(v_width_data):
    interp_values = np.zeros(interp_grid_points)
   sim_EM = width_obj[0]
    sim_AC = width_obj[1]
   SBS_gain = width_obj[2]
   SBS_gain_PE = width_obj[3]
   SBS_gain_MB = width_obj[4]
   linewidth_Hz = width_obj[5]
   k_AC = width_obj[6]
    # Calculate the EM effective index of the waveguide (k_AC = 2*k_EM).
   n_{eff_sim} = np.round(np.real((k_AC/2.)*((wl_nm*1e-9)/(2.*np.pi))), 4)
   n_effs.append(n_eff_sim)
    # Construct the SBS gain spectrum, built from Lorentzian peaks of the individual.
⊶modes.
    freq_min = np.real(sim_AC.nu_AC_all()[0])*1e-9 - 5 # GHZ
    freq_max = np.real(sim_AC.nu_AC_all()[-1])*1e-9 + 5 # GHz
   plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
        EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
       prefix_str=prefix_str, suffix_str='_scan%i' % i_w)
```

(continues on next page)

```
# Repeat calc to collect data for waterfall plot.
    tune\_steps = 50000
    tune_range = 10 # GHz
   detuning_range = np.append(np.linspace(-1*tune_range, 0, tune_steps),
                       np.linspace(0, tune_range, tune_steps)[1:])*1e9 # GHz
    # Linewidth of Lorentzian is half the FWHM style linewidth.
   linewidth = linewidth_Hz/2
    for AC_i in range(len(linewidth_Hz)):
        gain_list = np.real(SBS_gain[EM_ival_Stokes,EM_ival_pump,AC_i]
                     *linewidth[AC_i]**2/(linewidth[AC_i]**2 + detuning_range**2))
        freq_list_GHz = np.real(sim_AC.nu_AC(AC_i) + detuning_range)*1e-9
        interp_spectrum = np.interp(interp_grid, freq_list_GHz, gain_list)
        interp_values += interp_spectrum
    freqs_gains.append(list(zip(interp_grid, abs(interp_values))))
print('Widths', waveguide_widths)
print('n_effs', n_effs)
# Plot a 'waterfall' plot.
#fig = plt.figure()
#ax = fig.gca(projection='3d')
ax = plt.figure().add_subplot(projection='3d')
poly = PolyCollection(freqs_gains)
poly.set_alpha(0.7)
ax.add_collection3d(poly, zs=waveguide_widths, zdir='y')
ax.set_xlabel('Frequency (GHz)', fontsize=14)
ax.set_xlim3d(int_min,int_max)
ax.set_ylabel('Width (nm)', fontsize=14)
ax.set_ylim3d(waveguide_widths[0], waveguide_widths[-1])
ax.set_zlabel('|Gain| (1/Wm)', fontsize=14)
ax.set_zlim3d(0,1500)
# We change the fontsize of minor ticks label
plt.tick_params(axis='both', which='major', labelsize=12, pad=-2)
plt.savefig(prefix_str+'gain_spectra-waterfall.png')
plt.close()
end = time.time()
print("\nSimulation time: {0:10.3f} secs.".format(end - start))
print('\n\n')
```

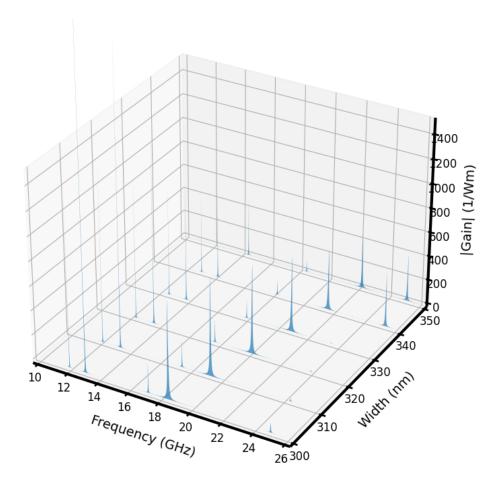


Fig. 4.8: Gain spectra as function of waveguide width.

4.1.6 Tutorial 5 – Convergence Study

This tutorial, contained in tutorials/simo-tut_05_convergence_study.py demonstrates a scan of numerical parameters for our standard silicon-in-air problem to test the convergence of the calculation results.

```
print("Calculation times (secs.): ", ', '.join(map(lambda s:'%.2f',time_list)))
""" Calculate the convergence as a function of FEM mesh for
   backward SBS gain spectra of a silicon waveguide
    surrounded in air.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Geometric Parameters - all in nm.
wl nm = 1550
unitcell_x = 2.5*wl_nm
unitcell_y = unitcell_x
inc_a_x = 300
inc_a_y = 280
inc_shape = 'rectangular'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 20
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
prefix_str = 'tut_05-'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate...
prefix_str = 'ftut_05-'
 refine_fac=1
 print('\n\nCommencing NumBAT tutorial 5 - fast mode')
  prefix_str = 'tut_05-'
  refine_fac=5
```

```
print('\n\nCommencing NumBAT tutorial 5')
# Warning: The fine grids in this list will take considerable time to run!
\#1c\_1ist = [20, 100, 500, 1000, 1500, 2000, 2500]
lc_list = [4,20,100,200,300,400,500]
nu_lcs = len(lc_list)
lc_bkg_list = 1*np.ones(nu_lcs)
x_axis = lc_list
conv_list = []
time_list = []
# Do not run in parallel, otherwise there are confusions reading the msh files!
for i_lc, lc_ref in enumerate(lc_list):
    start = time.time()
   print("\n Running simulation", i_lc+1, "/", nu_lcs)
   lc_refine_2 = lc_ref/2
   lc_bkg = lc_bkg_list[i_lc]
   wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,
                            inc_a_y,inc_shape,
                            material_bkg=materials.make_material("Vacuum"),
                            material_a=materials.make_material("Si_2016_Smith"),
                            lc_bkg=lc_bkg, lc_refine_1=lc_ref*refine_fac, lc_refine_2=lc_
→refine_2*refine_fac, force_mesh=True)
    # Expected effective index of fundamental guided mode.
   n_eff = wguide.get_material('a').refindex_n-0.1
    # Calculate Electromagnetic modes.
   sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
    sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
    # Calculate Acoustic modes.
   k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
   sim_AC = wquide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
    # Calculate interaction integrals and SBS gain.
    SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.

→gain_and_qs(
        sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
        EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
   conv_list.append([sim_EM_pump, sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB])
    end = time.time()
    time_list.append(end - start)
# It is crucial that you preselect modes with significant gain!
# Otherwise you will observe large relative errors similar to dividing by zero.
rel_modes = [3,4,8,10]
# If you do not know the mode numbers of the significant AC modes you may wish to simply.
⇒plot them all
# by uncommenting the line below and check if the modes with large gain have low_
→relative errors.
```

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```
# rel_modes = np.linspace(0,num_modes_AC-1,num_modes_AC)
rel_mode_kz_EM = np.zeros(nu_lcs,dtype=complex)
rel_mode_freq_AC = np.zeros((nu_lcs,len(rel_modes)),dtype=complex)
rel_mode_gain = np.zeros((nu_lcs,len(rel_modes)),dtype=complex)
rel_mode_gain_MB = np.zeros((nu_lcs,len(rel_modes)),dtype=complex)
rel_mode_gain_PE = np.zeros((nu_lcs,len(rel_modes)),dtype=complex)
for i_conv, conv_obj in enumerate(conv_list):
   rel_mode_kz_EM[i_conv] = conv_obj[0].kz_EM(0)
    for i_m, rel_mode in enumerate(rel_modes):
        rel_mode_freq_AC[i_conv,i_m] = conv_obj[1].nu_AC(rel_mode)
        rel_mode_gain[i_conv,i_m] = conv_obj[2][EM_ival_Stokes,EM_ival_pump,rel_mode]
        rel_mode_gain_PE[i_conv,i_m] = conv_obj[3][EM_ival_Stokes,EM_ival_pump,rel_mode]
        rel_mode_gain_MB[i_conv,i_m] = conv_obj[4][EM_ival_Stokes,EM_ival_pump,rel_mode]
xlabel = "Mesh Refinement Factor"
fig = plt.figure()
plt.clf()
ax1 = fig.add\_subplot(1,1,1)
ax2 = ax1.twinx()
ax2.yaxis.tick_left()
ax2.yaxis.set_label_position("left")
EM_plot_Mk = rel_mode_kz_EM*1e-6
error0 = np.abs((np.array(EM_plot_Mk[0:-1])-EM_plot_Mk[-1])/EM_plot_Mk[-1])
ax2.plot(x_axis[0:-1], error0, 'b-v',label='Mode #%i'%EM_ival_pump)
ax1.plot(x_axis, np.real(EM_plot_Mk), 'r-.o',label=r'EM k$_z$')
ax1.yaxis.tick_right()
ax1.spines['right'].set_color('red')
ax1.yaxis.label.set_color('red')
ax1.yaxis.set_label_position("right")
ax1.tick_params(axis='y', colors='red')
handles, labels = ax2.get_legend_handles_labels()
ax2.legend(handles, labels)
ax1.set_xlabel(xlabel)
ax1.set_ylabel(r"EM k$_z$ ($\times 10^6$ 1/m)")
ax2.set_ylabel(r"Relative Error EM k$_z$")
ax2.set_yscale('log')#, nonposx='clip')
plt.savefig(prefix_str+'convergence-freq_EM.png', bbox_inches='tight')
plt.close()
fig = plt.figure()
plt.clf()
ax1 = fig.add\_subplot(1,1,1)
ax2 = ax1.twinx()
ax2.yaxis.tick_left()
ax2.yaxis.set_label_position("left")
for i_m, rel_mode in enumerate(rel_modes):
   rel_mode_freq_AC_plot_GHz = rel_mode_freq_AC[:,i_m]*1e-9
    error0 = np.abs((np.array(rel_mode_freq_AC_plot_GHz[0:-1])-rel_mode_freq_AC_plot_
\rightarrowGHz[-1])/rel_mode_freq_AC_plot_GHz[-1])
    ax2.plot(x_axis[0:-1], error0, '-v',label='Mode #%i'%rel_mode)
```

```
ax1.plot(x_axis, np.real(rel_mode_freq_AC_plot_GHz), '-.o',label=r'AC Freq mode #%i'
→%rel_mode)
ax1.yaxis.tick_right()
ax1.spines['right'].set_color('red')
ax1.yaxis.label.set_color('red')
ax1.yaxis.set_label_position("right")
ax1.tick_params(axis='y', colors='red')
handles, labels = ax2.get_legend_handles_labels()
ax2.legend(handles, labels)
ax1.set_xlabel(xlabel)
ax1.set_ylabel(r"AC Freq (GHz)")
ax2.set_ylabel(r"Relative Error AC Freq")
ax2.set_yscale('log')#, nonposx='clip')
plt.savefig(prefix_str+'convergence-freq_AC.png', bbox_inches='tight')
plt.close()
fig = plt.figure()
plt.clf()
ax1 = fig.add\_subplot(1,1,1)
ax2 = ax1.twinx()
ax2.yaxis.tick_left()
ax2.yaxis.set_label_position("left")
for i_m, rel_mode in enumerate(rel_modes):
    rel_mode_gain_plot = rel_mode_gain[:,i_m]
    error0 = np.abs((np.array(rel_mode_gain_plot[0:-1])-rel_mode_gain_plot[-1])/rel_mode_
\rightarrowgain_plot[-1])
    ax2.plot(x_axis[0:-1], error0, '-v',label=r'Mode #%i'%rel_mode)
    ax1.plot(x_axis, np.real(rel_mode_gain_plot), '-.o',label=r'Gain mode #%i'%rel_mode)
ax1.yaxis.tick_right()
ax1.spines['right'].set_color('red')
ax1.yaxis.label.set_color('red')
ax1.yaxis.set_label_position("right")
ax1.tick_params(axis='y', colors='red')
handles, labels = ax2.get_legend_handles_labels()
ax2.legend(handles, labels)
ax1.set_xlabel(xlabel)
ax1.set_ylabel(r"Gain")
ax2.set_ylabel(r"Relative Error Gain")
ax2.set_yscale('log')#, nonposx='clip')
plt.savefig(prefix_str+'convergence-Gain.pdf', bbox_inches='tight')
plt.savefig(prefix_str+'convergence-Gain.png', bbox_inches='tight')
plt.close()
fig = plt.figure()
plt.clf()
ax1 = fig.add\_subplot(1,1,1)
ax2 = ax1.twinx()
ax2.yaxis.tick_left()
ax2.yaxis.set_label_position("left")
for i_m, rel_mode in enumerate(rel_modes):
   rel_mode_gain_PE_plot = rel_mode_gain_PE[:,i_m]
    error0 = np.abs((np.array(rel_mode_gain_PE_plot[0:-1])-rel_mode_gain_PE_plot[-1])/
```

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```
→rel_mode_gain_PE_plot[-1])
    ax2.plot(x_axis[0:-1], error0, '-v',label=r'Mode #%i'%rel_mode)
    ax1.plot(x_axis, np.real(rel_mode_gain_PE_plot), '-.o',label=r'Gain mode #%i'%rel_
→mode)
ax1.yaxis.tick_right()
ax1.spines['right'].set_color('red')
ax1.yaxis.label.set_color('red')
ax1.yaxis.set_label_position("right")
ax1.tick_params(axis='y', colors='red')
handles, labels = ax2.get_legend_handles_labels()
ax2.legend(handles, labels)
ax1.set_xlabel(xlabel)
ax1.set_ylabel(r"Gain (PE)")
ax2.set_ylabel(r"Relative Error Gain (PE)")
ax2.set_yscale('log')#, nonposx='clip')
plt.savefig(prefix_str+'convergence-Gain_PE.pdf', bbox_inches='tight')
plt.savefig(prefix_str+'convergence-Gain_PE.png', bbox_inches='tight')
plt.close()
fig = plt.figure()
plt.clf()
ax1 = fig.add\_subplot(1,1,1)
ax2 = ax1.twinx()
ax2.yaxis.tick_left()
ax2.yaxis.set_label_position("left")
for i_m, rel_mode in enumerate(rel_modes):
    rel_mode_gain_MB_plot = rel_mode_gain_MB[:,i_m]
    error0 = np.abs((np.array(rel_mode_gain_MB_plot[0:-1])-rel_mode_gain_MB_plot[-1])/
→rel_mode_gain_MB_plot[-1])
    ax2.plot(x_axis[0:-1], error0, '-v',label=r'Mode #%i'%rel_mode)
    ax1.plot(x_axis, np.real(rel_mode_gain_MB_plot), '-.o',label=r'Gain mode #%i'%rel_
→mode)
ax1.yaxis.tick_right()
ax1.spines['right'].set_color('red')
ax1.yaxis.label.set_color('red')
ax1.yaxis.set_label_position("right")
ax1.tick_params(axis='y', colors='red')
handles, labels = ax2.get_legend_handles_labels()
ax2.legend(handles, labels)
ax1.set_xlabel(xlabel)
ax1.set_ylabel(r"Gain (MB)")
ax2.set_ylabel(r"Relative Error Gain (MB)")
ax2.set_yscale('log')#, nonposx='clip')
plt.savefig(prefix_str+'convergence-Gain_MB.pdf', bbox_inches='tight')
plt.savefig(prefix_str+'convergence-Gain_MB.png', bbox_inches='tight')
plt.close()
print("Calculation times (secs.): ", ', '.join(map(lambda s:'%.2f',time_list)))
```

Fig. 4.9: Convergence of optical mode frequencies.

Fig. 4.10: Convergence of acoustic mode frequencies.

Fig. 4.11: Convergence of photoelastic gain.

Fig. 4.12: Convergence of moving boundary gain.



Fig. 4.13: Convergence of total gain.

4.1.7 Tutorial 6 - Silica Nanowire

In this tutorial, contained in tutorials/simo-tut_06_silica_nanowire.py we start to explore some different structures, in this case a silica nanowire surrounded by vacuum.

```
""" We've now covered most of the features of NumBAT.
    In the following tutorials we'll show how to study different
    geometries and materials.
    Calculate the backward SBS gain spectra of a silicon waveguide
    surrounded by vacuum (air).
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 5*wl_nm
unitcell_y = unitcell_x
inc_a_x = 550
inc_a_y = inc_a_x
inc_shape = 'circular'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 40
EM_ival_pump = 0
EM_ival_Stokes = 0
AC ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate...
→calculation
 prefix_str = 'ftut_06-'
  refine_fac=1
  print('\n\nCommencing NumBAT tutorial 6 - fast mode')
```

```
else:
  prefix_str = 'tut_06-'
  refine_fac=5
  print('\n\nCommencing NumBAT tutorial 6')
wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("SiO2_2016_Smith"),
                        lc_bkg=1, lc_refine_1=120.0*refine_fac, lc_refine_2=40.0*refine_
\hookrightarrowfac)
# Expected effective index of fundamental guided mode.
n_eff = 1.4
                       # run the calculation from scratch
recalc_fields=True
#recalc fields=False # reuse saved fields from previous calculation
# Calculate Electromagnetic Modes
if recalc_fields:
    sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
    sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
    sim_EM_pump.save_simulation('tut_06_pump')
    sim_EM_Stokes.save_simulation('tut_06_stokes')
else:
   sim_EM_pump = mode_calcs.load_simulation('tut_06_pump')
    sim_EM_Stokes = mode_calcs.load_simulation('tut_06_stokes')
sim_EM_pump.set_r0_offset(0, -0.5e-9*unitcell_y) # ensure plots identify centre as (0,0)
sim_EM_Stokes.set_r0_offset(0, -0.5e-9*unitcell_y) # ensure plots identify centre as (0,
\hookrightarrow 0)
print('\nPlotting EM fields')
plotting.plot_mode_fields(sim_EM_pump, EM_AC='EM_E',
        xlim_min=0.4, xlim_max=0.4, ylim_min=0.4, ylim_max=0.4,
        prefix_str=prefix_str, suffix_str='NW')
#plotting.plot_mode_fields(sim_EM_pump, EM_AC='EM_E', prefix_str=prefix_str, suffix_str='NW
')
# Display the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} {1:.4e}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff = {0:.4e}".format(n_eff_sim))
# Acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
shift Hz = 4e9
```

(continues on next page)

```
# Calculate Acoustic modes.
if recalc_fields:
    sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_
→Hz)
    sim_AC.save_simulation('tut_06_acoustic')
else:
    sim_AC = mode_calcs.load_simulation('tut_06_acoustic')
sim_AC.set_r0_offset(0, -0.5e-9*unitcell_y) # ensure plots identify centre as (0,0)
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, suffix_str='NW')
# Print the frequencies of AC modes.
v_nu=sim_AC.nu_AC_all()
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('{0:3d} {1:.5f}'.format(i, np.real(nu)*1e-9))
set_q_factor = 1000.
print('\nCalculating gains')
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_
→Q=set_q_factor)
# np.savez('wguide_data_AC_gain', SBS_gain=SBS_gain, SBS_gain_PE=SBS_gain_PE, SBS_gain_
→MB=SBS_gain_MB, alpha=alpha)
# npzfile = np.load('wguide_data_AC_gain.npz')
# SBS_gain = npzfile['SBS_gain']
# SBS_gain_PE = npzfile['SBS_gain_PE']
# SBS_gain_MB = npzfile['SBS_gain_MB']
# alpha = npzfile['alpha']
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 5 # GHz
freq_max = 12 # GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='_Si02_NW')
end = time.time()
print("\nSimulation time: {0:10.3f}".format(end - start))
print('\n\n')
```



../../tutorials/tut_06-gain_spectra-MB_PE_comps_Si02_NW.png

Fig. 4.14: Gain spectra showing gain due to photoelastic effect, gain due to moving boundary effect, and total gain.

4.1.8 Tutorial 7 – Slot Waveguide

This tutorial, contained in, tutorials/simo-tut_07-slot.py examines backward SBS in a more complex structure: chalcogenide soft glass (As_2S_3) embedded in a silicon slot waveguide on a silica slab.

```
print('\n\n')
""" Calculate the backward SBS gain spectra of a Si
    slot waveguide containing As2S3 on a SiO2 slab.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 4*wl_nm
unitcell_y = 0.3*unitcell_x
inc_shape = 'slot'
inc_a_x = 150
inc_a_y = 190
inc_b_x = 250
# Current mesh template assume inc_b_y = inc_a_y
slab_a_x = 2000
slab_a_y = 100
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 40
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate...
→calculation
 prefix_str = 'ftut_07-'
  refine_fac=1
  print('\n\nCommencing NumBAT tutorial 7 - fast mode')
```

```
else:
  prefix_str = 'tut_07-'
  refine_fac=4
  print('\n\nCommencing NumBAT tutorial 7')
wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        slab_a_x=slab_a_x, slab_a_y=slab_a_y, inc_b_x=inc_b_x,
                        material_bkg=materials.make_material("Vacuum"),
                                                                                    #_
→background
                        material_a=materials.make_material("As2S3_2017_Morrison"), # slot
                                                                                    # slab
                        material_b=materials.make_material("SiO2_2013_Laude"),
                        material_c=materials.make_material("Si_2016_Smith"),
→walls of slot
                        lc_bkg=.05, lc_refine_1=20.0*refine_fac, lc_refine_2=10.0*refine_
\rightarrowfac)
wguide.plot_mesh(prefix_str)
# Move origin to nominal centre of waveguide, y adjustment needs refinement based on.
→mesh template.
# Note different shifts are allowed for EM and acoustic, because acoustic domain.
→excludes vacuum regions
# Shifts are in nm
wguide.set_xyshift_em(-unitcell_x*.5, unitcell_y*.5)
wguide.set_xyshift_ac(-unitcell_x*.5, unitcell_y*.5)
# Expected effective index of fundamental guided mode.
n_eff = wguide.get_material('a').refindex_n-0.1
recalc_fields=True
                       # run the calculation from scratch
#recalc_fields=False # reuse saved fields from previous calculation
# Calculate Electromagnetic modes.
if recalc fields:
    sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
    sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
    sim_EM_pump.save_simulation('tut_07_pump')
    sim_EM_Stokes.save_simulation('tut_07_stokes')
else:
    sim_EM_pump = mode_calcs.load_simulation('tut_07_pump')
    sim_EM_Stokes = mode_calcs.load_simulation('tut_07_stokes')
plotting.plot_mode_fields(sim_EM_pump, quiver_points = 20, xlim_min=0.2, xlim_max=0.2,
                           ylim_min=0.0, ylim_max=0.0, EM_AC='EM_E',
                           prefix_str=prefix_str, suffix_str='slot')
# Display the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('{0:3d} {1:.4e}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
```

(continues on next page)

```
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff = ", np.round(n_eff_sim, 4))
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
# Specify the expected acoustic frequency (slightly low balled).
shift_Hz = 4e9
# Calculate Acoustic modes.
if recalc_fields:
    sim_AC = wquide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_
    sim_AC.save_simulation('tut_07_acoustic')
    sim_AC = mode_calcs.load_simulation('tut_07_acoustic')
plotting.plot_mode_fields(sim_AC, quiver_points=20, xlim_min=0.3, xlim_max=0.3,
                           ylim_min=0.0, ylim_max=0.0, EM_AC='AC',
                           prefix_str=prefix_str, suffix_str='slot')
# Print the frequencies of AC modes.
v_nu=sim_AC.nu_AC_all()
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('\{0:3d\} {1:.5f}'.format(i, np.real(nu)*1e-9))
set_q_factor = 1000.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_
→Q=set_q_factor)
# np.savez('wguide_data_AC_gain', SBS_gain=SBS_gain, SBS_gain_PE=SBS_gain_PE, SBS_gain_
→ MB=SBS_gain_MB, alpha=alpha)
# npzfile = np.load('wguide_data_AC_gain.npz', allow_pickle=True)
# SBS_gain = npzfile['SBS_gain']
# SBS_gain_PE = npzfile['SBS_gain_PE']
# SBS_gain_MB = npzfile['SBS_gain_MB']
# alpha = npzfile['alpha']
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = np.real(sim_AC.nu_AC_all()[0])*1e-9 - 2 # GHz
freq_max = np.real(sim_AC.nu_AC_all()[-1])*1e-9 + 2 # GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='_slot')
end = time.time()
print("\nSimulation time: {0:10.3f} (secs.)".format(end - start))
print('\n\n')
```



../../tutorials/tut_07-gain_spectra-MB_PE_comps_slot.png

Fig. 4.15: Gain spectra showing gain due to photoelastic effect, gain due to moving boundary effect, and total gain.

4.1.9 Tutorial 8 – Slot Waveguide Scan Covering

This tutorial, contained in, tutorials/simo-tut_08-slot_coated-scan.py continues the study of the previous slot waveguide, by examining the thickness dependence of a silica capping layer.

```
""" Calculate the backward SBS gain spectra of a Si
    slot waveguide containing As2S3 on a SiO2 slab.
    This time include a capping layer of SiO2 and
    investigate the effect of this layer's thickness.
import time
import datetime
import numpy as np
import sys
from multiprocessing import Pool
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 4*wl_nm
unitcell_y = 0.3*unitcell_x
inc_shape = 'slot_coated'
inc_a_x = 150
inc_a_y = 190
inc_b_x = 250
# Current mesh template assume inc_b_y = inc_a_y
slab_a_x = 1000
slab_a_y = 100
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 40
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate_
→calculation
```

```
prefix_str = 'ftut_08-'
  refine_fac=1
  print('\n\nCommencing NumBAT tutorial 8 - fast mode')
  prefix_str = 'tut_08-'
  refine_fac=4
  print('\n\nCommencing NumBAT tutorial 8')
# Function to return ac freqs for given coating thickness
def ac_mode_freqs(coat_v):
   print('Commencing mode calculation for coat_y = %f'% coat_y)
   wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                            slab_a_x=slab_a_x, slab_a_y=slab_a_y, inc_b_x=inc_b_x,
                            coat_y=coat_y,
                            material_bkg=materials.make_material("Vacuum"),
                                                                                        #.
→background
                            material_a=materials.make_material("As2S3_2017_Morrison"), #_
\hookrightarrowslot
                            material_b=materials.make_material("Si02_2013_Laude"),
∽slab
                            material_c=materials.make_material("Si_2016_Smith"),
                                                                                        #__
→walls of slot
                            material_d=materials.make_material("SiO2_2013_Laude"),
lc_bkg=1, lc_refine_1=100.0*refine_fac, lc_refine_2=50.
→0*refine_fac)
    # Expected effective index of fundamental guided mode.
   n_eff = wguide.get_material('a').refindex_n-0.1
    # Calculate Electromagnetic modes.
   sim_EM_pump = wquide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
   sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
   k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
   shift_Hz = 4e9
    # Calculate Acoustic modes.
   sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_
→Hz)
    # plotting.plot_mode_fields(sim_AC, xlim_min=0.4, xlim_max=0.4,
                                ylim_min=0.7, ylim_max=0.0, EM_AC='AC',
                                prefix_str=prefix_str, suffix_str='_%i' %int(coat_y))
    set_q_factor = 1000.
   SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.
→gain_and_qs(
        sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
```

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```
EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_
→Q=set_q_factor)
    # Construct the SBS gain spectrum, built from Lorentzian peaks of the individual.
    freq_min = 4 # np.real(sim_AC.nu_AC_all()[0])*1e-9 - 2 # GHz
    freq_max = 14 # np.real(sim_AC.nu_AC_all()[-1])*1e-9 + 2 # GHz
   plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
        EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
        prefix_str=prefix_str, suffix_str='_%i' %int(coat_y))
    # Convert to GHz
   mode_freqs = sim_AC.nu_AC_all()*1.e-9
    # Clear memory
   wguide = sim_EM_pump = sim_EM_Stokes = sim_AC = None
   SBS_gain = SBS_gain_PE = SBS_gain_MB = linewidth_Hz = Q_factors = alpha = None
   print('Completed mode calculation for coating coat_y = %f'% coat_y)
    # Return the frequencies and simulated k_ac value in a list
   return mode_freqs
nu\_coats = 5
coat_min = 5
coat_max = 200
coat_y_list = np.linspace(coat_min,coat_max,nu_coats)
num_cores = 5 # should be appropriate for individual machine/vm, and memory!
pool = Pool(num_cores)
pooled_mode_freqs = pool.map(ac_mode_freqs, coat_y_list)
# Note pool.map() doesn't pass errors back from fortran routines very well.
# It's good practise to run the extrema of your simulation range through map()
# before launching full multicore simulation.
# We will pack the above values into a single array for plotting purposes, initialise.
\hookrightarrow first
freq_arr = np.empty((nu_coats, num_modes_AC))
for i_w, sim_freqs in enumerate(pooled_mode_freqs):
    # Set the value to the values in the frequency array
    freq_arr[i_w] = np.real(sim_freqs)
# Also plot a figure for reference
plot_range = num_modes_AC
plt.clf()
plt.figure(figsize=(10,6))
ax = plt.subplot(1,1,1)
for idx in range(plot_range):
    # slicing in the row direction for plotting purposes
    freq_slice = freq_arr[:, idx]
   plt.plot(coat_y_list, freq_slice, 'g')
```

```
# Set the limits and plot axis labels
ax.set_xlim(coat_min,coat_max)
plt.xlabel(r'Coating Thickness (nm)')
plt.ylabel(r'Frequency (GHz)')
plt.savefig(prefix_str+'freq_changes.pdf', bbox_inches='tight')
plt.savefig(prefix_str+'freq_changes.png', bbox_inches='tight')
plt.close()
end = time.time()
print("\nSimulation time: {0:10.3f} (secs.)".format(end - start))
print('\n\n')
```

../../tutorials/tut_08-freq_changes.png

Fig. 4.16: Acoustic frequencies as function of covering layer thickness.

4.1.10 Tutorial 9 – Anisotropic Elastic Materials

This tutorial, contained in, tutorials/simo-tut_09-anisotropy.py improves the treatment of the silicon rectangular waveguide by accounting for the anisotropic elastic properties of silicon (simply by referencing a different material file for silicon).

```
""" Sanity check implementation of fully anisotropic
    tensors by feeding in same parameters of simo_tut_01.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl nm = 1550
unitcell_x = 2.5*wl_nm
unitcell_y = unitcell_x
inc_a_x = 314.7
inc_a_y = 0.9*inc_a_x
inc_shape = 'rectangular'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 20
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate...

→ calculation

 print('\n\nCommencing NumBAT tutorial 9 - fast mode')
 prefix_str = 'ftut_09-'
 refine_fac=1
  print('\n\nCommencing NumBAT tutorial 9')
 prefix_str = 'tut_09-'
  refine_fac=5
```

```
# Use of a more refined mesh to produce field plots.
wguide = objects.Structure(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("Si_test_anisotropic"),
                        lc_bkg=1, lc_refine_1=200.0*refine_fac, lc_refine_2=1.0*refine_
\hookrightarrowfac)
# Expected effective index of fundamental guided mode.
n_eff = wguide.get_material('a').refindex_n-0.1
# Calculate the Electromagnetic modes of the pump field.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
# Display the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} {1:.4e}'.format(i, np.real(kz)))
# Calculate the Electromagnetic modes of the Stokes field.
# For an idealised backward SBS simulation the Stokes modes are identical
# to the pump modes but travel in the opposite direction.
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
# # Alt
# sim_EM_Stokes = wguide.calc_EM_modes(wl_nm, num_modes_EM_Stokes, n_eff, Stokes=True)
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("\n Fundamental optical mode ")
print(" n_eff = ", np.round(n_eff_sim, 4))
# Acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
print('\n AC wavenumber (1/m) = ', np.round(k_AC, 4))
# Calculate Acoustic modes, using the mesh from the EM calculation.
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
# Print the frequencies of AC modes.
v_nu=sim_AC.nu_AC_all()
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('{0:3d} {1:.4e}'.format(i, np.real(nu)*1e-9))
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB. Also calculate acoustic loss alpha.
SBS_gain_tot, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.

    gain_and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# SBS_gain_tot, SBS_gain_PE, SBS_gain_MB are 3D arrays indexed by pump, Stokes and.
→acoustic mode
```

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```
# Extract those of interest as a 1D array:
SBS_gain_PE_ij = SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:]
SBS_gain_MB_ij = SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:]
SBS_gain_tot_ij = SBS_gain_tot[EM_ival_pump,EM_ival_Stokes,:]
# Print the Backward SBS gain of the AC modes.
print("\nContributions to SBS gain [1/(WM)]")
print("AC Mode number | Photoelastic (PE) | Moving boundary(MB) | Total")
for (m, gpe, gmb, gt) in zip(range(num_modes_AC), SBS_gain_PE_ij, SBS_gain_MB_ij, SBS_
→gain_tot_ij):
   print('{0:12d} {1:19.6e} {2:19.6e} {3:16.6e}'.format(m, gpe, gmb, gt))
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.where(np.abs(SBS_gain_PE_ij)>threshold, SBS_gain_PE_ij, 0)
masked_MB = np.where(np.abs(SBS_gain_MB_ij)>threshold, SBS_gain_MB_ij, 0)
masked_tot = np.where(np.abs(SBS_gain_tot_ij)>threshold, SBS_gain_tot_ij, 0)
print("\n Displaying gain results with negligible components masked out:")
print("AC Mode number | Photoelastic (PE) | Moving boundary(MB) | Total")
for (m, gpe, gmb, gt) in zip( range(num_modes_AC), masked_PE, masked_MB, masked_tot):
   print('{0:12d} {1:19.6e} {2:19.6e} {3:16.6e}'.format(m, gpe, gmb, gt))
end = time.time()
print("\nSimulation time: {0:10.3f} (secs.)".format(end - start))
print('\n\n')
```

4.1.11 Tutorial 10 – Multilayered 'Onion'

This tutorial, contained in, tutorials/simo-tut_10-onion.py shows how to create multi-layered circular structures.

```
""" Example showing how the 'onion' geometry template can be used
   to simulate a circular Si waveguide clad in SiO2.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl nm = 1550
unitcell_x = 3.5*wl_nm
unitcell_y = unitcell_x
inc_a_x = 800
inc_b_x = 500
inc_shape = 'onion'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 20
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate...

→ calculation

 print('\n\nCommencing NumBAT tutorial 10 - fast mode')
 prefix_str = 'ftut_10-'
 refine_fac=1
  print('\n\nCommencing NumBAT tutorial 10')
 prefix_str = 'tut_10-'
  refine_fac=5
```

(continues on next page)

```
# Use of a more refined mesh to produce field plots.
wguide = objects.Structure(unitcell_x,inc_a_x,inc_shape=inc_shape,
                        inc_b_x=inc_b_x,
                        unitcell_y=unitcell_y,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("Si_2016_Smith"),
                        material_b=materials.make_material("SiO2_2016_Smith"),
                        lc_bkg=.1, lc_refine_1=2.0*refine_fac, lc_refine_2=2.0*refine_
\hookrightarrowfac)
wguide.check_mesh()
# Move origin to nominal centre of waveguide, y adjustment needs refinement based on.
→mesh template.
# Note different shifts are allowed for EM and acoustic, because acoustic domain.
→excludes vacuum regions
# Shifts are in nm
wguide.set_xyshift_em(-unitcell_x*.5, unitcell_y*.5)
wguide.set_xyshift_ac(-unitcell_x*.5, unitcell_y*.5)
#wguide.plot_mesh()
# Expected effective index of fundamental guided mode.
n_eff = wguide.get_material('a').refindex_n-0.1
new_calcs=True
# Calculate Electromagnetic modes.
if new_calcs:
  sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
  sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
  sim_EM_pump.save_simulation('tut_10_pump')
  sim_EM_Stokes.save_simulation('tut_10_stokes')
else:
  sim_EM_pump = mode_calcs.load_simulation('tut_10_pump')
  sim_EM_Stokes = mode_calcs.load_simulation('tut_10_stokes')
# Display the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff", np.round(n_eff_sim, 4))
# # Plot the E fields of the EM modes fields - specified with EM_AC='EM_E'.
# # Zoom in on the central region (of big unitcell) with xlim_, ylim_ args.
# # Only plot fields of fundamental (ival = 0) mode.
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.3, xlim_max=0.3, ylim_min=0.3,
                         ylim_max=0.3, ivals=range(10), contours=True, EM_AC='EM_E',
                         prefix_str=prefix_str, ticks=True, quiver_points=20)
```

```
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.3, xlim_max=0.3, ylim_min=0.3,
                         ylim_max=0.3, ivals=range(10), contours=True, EM_AC='EM_H',
                         prefix_str=prefix_str, ticks=True, quiver_points=20)
# Acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
# Calculate Acoustic modes.
if new_calcs:
  sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
  sim_AC.save_simulation('tut_10_acoustic')
else.
  sim_AC = mode_calcs.load_simulation('tut_10_acoustic')
# Print the frequencies of AC modes.
v_nu=sim_AC.nu_AC_all()
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('\{0:3d\} {1:.4e}'.format(i, np.real(nu)*1e-9))
plotting.plot_mode_fields(sim_AC, EM_AC='AC', pdf_png='png', contours=False,
                         prefix_str=prefix_str, ticks=True, ivals=[0], quiver_points=20)
# Calculate the acoustic loss from our fields.
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, EM_ival_pump=EM_ival_pump,
   EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = np.real(sim_AC.nu_AC_all()[0])*1e-9 - 2 # GHz
freq_max = np.real(sim_AC.nu_AC_all()[-1])*1e-9 + 2 # GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
    EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str)
end = time.time()
print("\nSimulation time: {0:10.3f} (secs.)".format(end - start))
print('\n\n')
```

4.1.12 Tutorial 11 – Two-layered 'Onion'

This tutorial, contained in, tutorials/simo-tut_11a-onion2.py demonstrates use of the two layered onion structure which generates a more efficient mesh than the full onion template.

```
""" Example showing how the 'onion2' geometry template can be used
    to simulate a circular Si waveguide clad in SiO2 surrounded by air.
   Uses the two-layer onion structure which with vacuum surrounds makes a three.
→material structure.
    ***** Something is broken in assigning material properties at the central grid point.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 3000
unitcell_y = unitcell_x
inc_a_x = 800
inc_b_x = 500
inc_shape = 'onion2'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 20
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate...

→ calculation

 print('\n\nCommencing NumBAT tutorial 11a - fast mode')
  prefix_str = 'ftut_11a-'
  refine_fac=1
```

```
else:
  print('\n\nCommencing NumBAT tutorial 11a')
  prefix_str = 'tut_11a-'
  refine_fac=5
# Use of a more refined mesh to produce field plots.
wguide = objects.Structure(unitcell_x,inc_a_x,inc_shape=inc_shape,
                        inc_b_x=inc_b_x,
                        unitcell_y=unitcell_y,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("Si_2016_Smith"),
                        material_b=materials.make_material("SiO2_2016_Smith"),
                        lc_bkg=.1, lc_refine_1=2.0*refine_fac, lc_refine_2=2*refine_fac)
wguide.check_mesh()
# Expected effective index of fundamental guided mode.
n_eff = wguide.get_material('a').refindex_n-0.1
new_calcs=True
# Calculate Electromagnetic modes.
if new_calcs:
  sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff, calc_EM_mode_
→energy=True)
  sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
  sim_EM_pump.save_simulation('tut_11_pump')
  sim_EM_Stokes.save_simulation('tut_11_stokes')
else:
  sim_EM_pump = mode_calcs.load_simulation('tut_11_pump')
  sim_EM_Stokes = mode_calcs.load_simulation('tut_11_stokes')
print('EM modes:\n')
kz_EM_mu =np.real(sim_EM_pump.kz_EM_all())*1e-6
neff_EM =sim_EM_pump.neff_all()
ng_EM =sim_EM_pump.ngroup_EM_all()
print('m
          | k_z [1/micron] | neff | ng')
for m in range(num_modes_EM_pump):
 print('{0:4d} {1:12.6f} {2:12.6f} {3:12.6f}'.format(m, kz_EM_mu[m], neff_EM[m], ng_
\hookrightarrowEM[m]))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff", np.round(n_eff_sim, 4))
# # Plot the E fields of the EM modes fields - specified with EM_AC='EM_E'.
# # Zoom in on the central region (of big unitcell) with xlim_, ylim_ args.
# # Only plot fields of fundamental (ival = 0) mode.
#npzfile = np.load('wguide_data.npz', allow_pickle=True)
#npzfile = np.load('wguide_data2.npz', allow_pickle=True)
#sim_EM_Stokes = npzfile['sim_EM_Stokes'].tolist()
```

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```
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.3, xlim_max=0.3, ylim_min=0.3,
                         ylim_max=0.3, ivals=range(10), contours=True, EM_AC='EM_E',
                         prefix_str=prefix_str, ticks=True, quiver_points=20)
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.3, xlim_max=0.3, ylim_min=0.3,
                         ylim_max=0.3, ivals=range(10), contours=True, EM_AC='EM_H',
                         prefix_str=prefix_str, ticks=True, quiver_points=20)
# Acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
# Calculate Acoustic modes.
if new_calcs:
  sim_AC = wquide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, calc_AC_mode_
→power=True)
  sim_AC.save_simulation('tut_11_acoustic')
else:
  sim_AC = mode_calcs.load_simulation('tut_11_acoustic')
print('AC mode properties (GHz) \n')
nu_AC = np.real(sim_AC.nu_AC_all())*1e-9
vp_AC = np.real(sim_AC.vp_AC_all())
vg_AC = np.real(sim_AC.vg_AC_all())
               nu [GHz] | vp [m/s] | vg [m/s]')
print('m
          for m in range(num_modes_AC):
 print('{0:4d} {1:12.6f} {2:12.2f} {3:12.2f}'.format(m, nu_AC[m], vp_AC[m], vg_
\rightarrow AC[m])
sim_AC.calc_acoustic_losses()
plotting.plot_mode_fields(sim_AC, EM_AC='AC', pdf_png='png', contours=False,
                         prefix_str=prefix_str, ticks=True, ivals=[0], quiver_points=20)
# Calculate the acoustic loss from our fields.
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, EM_ival_pump=EM_ival_pump,
   EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = np.real(sim_AC.nu_AC_all()[0])*1e-9 - 2 # GHz
freq_max = np.real(sim_AC.nu_AC_all()[-1])*1e-9 + 2 # GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str)
end = time.time()
print("\nSimulation time: {0:10.3f} (secs.)".format(end - start))
print('\n\n')
```

4.1.13 Tutorial 12 - SMF-28 fibre

This tutorial, contained in, tutorials/simo-tut_12-smf28.py models backward SBS in the standard SMF28 fibre using the onion2 template.

```
""" Example showing how the 'onion2' geometry template can be used
    to simulate a circular Si waveguide clad in SiO2 surrounded by air.
   Uses the two-layer onion structure which with vacuum surrounds makes a three.
→material structure.
    ***** Something is broken in assigning material properties at the central grid point.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 3000
unitcell_y = unitcell_x
inc_a_x = 800
inc_b_x = 500
inc_shape = 'onion2'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 20
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
if len(sys.argv)>1 and sys.argv[1]=='fast=1': # choose between faster or more accurate...

→ calculation

 print('\n\nCommencing NumBAT tutorial 11a - fast mode')
  prefix_str = 'ftut_11a-'
  refine_fac=1
```

```
else:
  print('\n\nCommencing NumBAT tutorial 11a')
  prefix_str = 'tut_11a-'
  refine_fac=5
# Use of a more refined mesh to produce field plots.
wguide = objects.Structure(unitcell_x,inc_a_x,inc_shape=inc_shape,
                        inc_b_x=inc_b_x,
                        unitcell_y=unitcell_y,
                        material_bkg=materials.make_material("Vacuum"),
                        material_a=materials.make_material("Si_2016_Smith"),
                        material_b=materials.make_material("SiO2_2016_Smith"),
                        lc_bkg=.1, lc_refine_1=2.0*refine_fac, lc_refine_2=2*refine_fac)
wguide.check_mesh()
# Expected effective index of fundamental guided mode.
n_eff = wguide.get_material('a').refindex_n-0.1
new_calcs=True
# Calculate Electromagnetic modes.
if new_calcs:
  sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff, calc_EM_mode_
→energy=True)
  sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
  sim_EM_pump.save_simulation('tut_11_pump')
  sim_EM_Stokes.save_simulation('tut_11_stokes')
else:
  sim_EM_pump = mode_calcs.load_simulation('tut_11_pump')
  sim_EM_Stokes = mode_calcs.load_simulation('tut_11_stokes')
print('EM modes:\n')
kz_EM_mu =np.real(sim_EM_pump.kz_EM_all())*1e-6
neff_EM =sim_EM_pump.neff_all()
ng_EM =sim_EM_pump.ngroup_EM_all()
print('m
          | k_z [1/micron] | neff | ng')
for m in range(num_modes_EM_pump):
 print('{0:4d} {1:12.6f} {2:12.6f} {3:12.6f}'.format(m, kz_EM_mu[m], neff_EM[m], ng_
\hookrightarrowEM[m]))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff", np.round(n_eff_sim, 4))
# # Plot the E fields of the EM modes fields - specified with EM_AC='EM_E'.
# # Zoom in on the central region (of big unitcell) with xlim_, ylim_ args.
# # Only plot fields of fundamental (ival = 0) mode.
#npzfile = np.load('wguide_data.npz', allow_pickle=True)
#npzfile = np.load('wguide_data2.npz', allow_pickle=True)
#sim_EM_Stokes = npzfile['sim_EM_Stokes'].tolist()
```

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```
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.3, xlim_max=0.3, ylim_min=0.3,
                         ylim_max=0.3, ivals=range(10), contours=True, EM_AC='EM_E',
                         prefix_str=prefix_str, ticks=True, quiver_points=20)
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.3, xlim_max=0.3, ylim_min=0.3,
                         ylim_max=0.3, ivals=range(10), contours=True, EM_AC='EM_H',
                         prefix_str=prefix_str, ticks=True, quiver_points=20)
# Acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
# Calculate Acoustic modes.
if new_calcs:
  sim_AC = wquide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, calc_AC_mode_
→power=True)
  sim_AC.save_simulation('tut_11_acoustic')
else:
  sim_AC = mode_calcs.load_simulation('tut_11_acoustic')
print('AC mode properties (GHz) \n')
nu_AC = np.real(sim_AC.nu_AC_all())*1e-9
vp_AC = np.real(sim_AC.vp_AC_all())
vg_AC = np.real(sim_AC.vg_AC_all())
               nu [GHz] | vp [m/s] | vg [m/s]')
print('m
           for m in range(num_modes_AC):
 print('{0:4d} {1:12.6f} {2:12.2f} {3:12.2f}'.format(m, nu_AC[m], vp_AC[m], vg_
\rightarrow AC[m])
sim_AC.calc_acoustic_losses()
plotting.plot_mode_fields(sim_AC, EM_AC='AC', pdf_png='png', contours=False,
                         prefix_str=prefix_str, ticks=True, ivals=[0], quiver_points=20)
# Calculate the acoustic loss from our fields.
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, EM_ival_pump=EM_ival_pump,
   EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = np.real(sim_AC.nu_AC_all()[0])*1e-9 - 2 # GHz
freq_max = np.real(sim_AC.nu_AC_all()[-1])*1e-9 + 2 # GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str)
end = time.time()
print("\nSimulation time: {0:10.3f} (secs.)".format(end - start))
print('\n\n')
```

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4.2 JOSA B Tutorial

Mike Smith et al. have used NumBAT throughout their 2021 SBS tutorial paper, published in J. Opt. Soc. Am. B. .. (see .. M. Smith et al, FIXME .. Generation of phonons from electrostriction in small-core optical waveguides .., *JOSA B* 3, 042109 (2021). ..) This tutorial works through backward, forward, and intermodal forward SBS. The simulation scripts and resultant mode fields are shown below.

4.2.1 BSBS - Circular Waveguide - Silica

```
print("\n Simulation time (sec.)", (end - start))
Script to evaluate backward Brillouin scattering in a cylindrical SiO2 waveguide
# Import the necessary packages
import time
import datetime
import numpy as np
import sys
import math
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k AC: acoustic wavevector
start = time.time()
# Specify Geometric Parameters - all in [nm].
wl_nm = 1550 # Wavelength of EM wave in vacuum.
# Unit cell dimensions must be sufficiently large to ensure fields are zero at outermost.
→boundary.
unitcell_x = 4.01*wl_nm # be careful to ensure not whole integer multiples
unitcell_y = unitcell_x
inc_a_x = 1000 # Waveguide widths.
inc_a_v = inc_a_x
inc_shape = 'circular' # Shape of the waveguide.
# Specify number of electromagnetic modes and acoustic modes involved in the
# calculation for BSBS
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 100
# The EM pump mode number for which to calculate interaction with AC modes. Typically 0 \!\!\! \!\!
```

```
\rightarrow for BSBS.
EM_ival_pump = 1
# The EM Stokes mode number for which to calculate interaction with AC modes. Typically...
\rightarrow 0 for BSBS.
EM_ival_Stokes = EM_ival_pump
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
# Output files are generated in a folder with the following prefix
prefix_str = 'bsbs-josab-01-1umSiO2'
# Use all specified parameters to create a waveguide object
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=materials.get_material("SiO2_2021_Poulton"),
                        lc_bkg=0.05, # mesh coarseness in background, larger lc_bkg =_
→coarser along horizontal outer edge
                        lc_refine_1=20.0, # mesh refinement factor near the interface of_
→waveguide, larger lc2 = finer along horizontal interface
                        lc_refine_2=30.0, # mesh refinement factor near the origin/
→centre of waveguide
                        plt_mesh=False, # creates png file of geometry and mesh in_
→backend/fortran/msh/
                        check_mesh=False) # note requires x-windows configuration to_
\hookrightarrow work
# Print information on material data in terminal
print('\nUsing %s material data from' % wguide.material_a.chemical)
print('Author:', wguide.material_a.author)
print('Year:', wguide.material_a.date)
print('Ref:', wguide.material_a.doi)
# Initial guess for the EM effective index of the waveguide
n_eff = wguide.material_a.n-0.1
# Calculate the Electromagnetic modes of the pump field.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print(\{0:3d\} {1:.4e}'.format(i, np.real(kz)))
# A computation interruption if needed
# sys.exit("We interrupt your regularly scheduled computation to bring you ... for now")
# Calculate the Electromagnetic modes of the Stokes field.
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
print("Plotting EM fields ")
plotting.plot_mode_fields(sim_EM_pump,
```

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```
ivals=[EM_ival_pump],
                         EM_AC='EM_E', num_ticks=3,xlim_min=0.2, xlim_max=0.2, ylim_
\rightarrowmin=0.2, ylim_max=0.2,
                         prefix_str=prefix_str, pdf_png='png', ticks=True, quiver_
\rightarrow points=40.
                         comps=['Et', 'Eabs'], n_points=1000, colorbar=True)
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("\n Fundamental optical mode ")
print(" n_eff = ", np.round(n_eff_sim, 4))
# Calculate the acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
print('\n AC wavenumber (1/m) = ', np.round(k_AC, 4))
# Calculate Acoustic modes, using the mesh from the EM calculation.
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
AC_freqs_GHz=sim_AC.nu_AC_all()*1e-9
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('{0:3d} {1:.4e}'.format(i, np.real(AC_freqs_GHz)))
# Calculate total SBS gain, photoelastic and moving boundary contributions, as
# well as other important quantities
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, EM_ival_pump=EM_ival_pump,
   EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Mask negligible gain values to improve clarity of print out.
threshold = -1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Display these in terminal
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
#determining the location of the maximum gain
maxGainloc=np.argmax(abs(masked.data));
print("Plotting acoustic mode corresponding to maximum")
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, ivals=[maxGainloc],
                         num_ticks=3, quiver_points=40, pdf_png='png',ticks=True, comps=[
→'ut','uabs'], colorbar=True)
# Displaying results for the maximum found in the selection
print("----")
print("Displaying results for maximum gain value found:")
print("Greatest SBS_gain [1/(Wm)] total \n", masked.data[maxGainloc])
```

```
print("displaying corresponding acoustic mode number (i.e., AC_field_#) for reference \n
→",maxGainloc )
print("EM Pump Power [Watts] \n", sim_EM_pump.EM_mode_power[EM_ival_pump] )
print("EM Stokes Power [Watts] \n", sim_EM_Stokes.EM_mode_power[EM_ival_Stokes] )
print("EM angular frequency [THz] \n", sim_EM_pump.omega_EM/1e12 )
print("AC Energy Density [J*m^{-1}] \n", sim_AC.AC_mode_energy[maxGainloc])
print("AC loss alpha [1/s] \n", alpha[maxGainloc] )
print("AC frequency [GHz] \n", sim_AC.Omega_AC[maxGainloc]/(1e9*2*math.pi) )
print("AC linewidth [MHz] \n", linewidth_Hz[maxGainloc]/1e6)
#since the overlap is not returned directly we'll have to deduce it
absQtot2 = (alpha[maxGainloc]*sim_EM_pump.EM_mode_power[EM_ival_pump]*sim_EM_Stokes.EM_
-mode_power[EM_ival_Stokes]*sim_AC.AC_mode_energy[maxGainloc]*masked.data[maxGainloc])/
absQtot = pow(absQtot2, 1/2)
print("Total coupling |Qtot| [W*m^{-1}*s] \n", absQtot )
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

../../JOSAB_tutorial/bsbs-josab-01-1umSiO2fields/EM_E_field_1

Fig. 4.17: Fundamental optical mode fields.

../../JOSAB_tutorial/bsbs-josab-01-1umSiO2fields/EM_E_field_1

Fig. 4.18: Fundamental optical mode fields.

../../JOSAB_tutorial/bsbs-josab-01-1umSiO2fields/EM_E_field_1

Fig. 4.19: Fundamental optical mode fields.

../../JOSAB_tutorial/bsbs-josab-01-1umSiO2fields/AC_field_28.

Fig. 4.20: Fundamental acoustic mode fields.

../../JOSAB_tutorial/bsbs-josab-01-1umSiO2fields/AC_field_28_u

Fig. 4.21: Fundamental acoustic mode fields.

../../JOSAB_tutorial/bsbs-josab-01-1umSiO2fields/AC_field_28_u

Fig. 4.22: Fundamental acoustic mode fields.

4.2.2 BSBS - Rectangular Waveguide - Silicon

```
print("\n Simulation time (sec.)", (end - start))
Script to evaluate backward Brillouin scattering in a rectangular Si waveguide
# Import the necessary packages
import time
import datetime
import numpy as np
import sys
import math
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
from matplotlib import pyplot as plt
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k_AC: acoustic wavevector
start = time.time()
# Specify Geometric Parameters - all in [nm].
wl_nm = 1550 # Wavelength of EM wave in vacuum.
inc_a_x = 450 # Waveguide widths.
inc_a_y = 200
# Unit cell dimensions must be sufficiently large to ensure fields are zero at outermost.
→boundary.
unitcell_x = 3.01*wl_nm
unitcell_y = unitcell_x #be careful to ensure not whole integer multiples
inc_shape = 'rectangular' # Shape of the waveguide.
# Specify number of electromagnetic modes and acoustic modes involved in the
# calculation for BSBS
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 100
# The mode number for the optical field. Typically 0 for BSBS.
EM ival pump = 0
# The EM Stokes mode number for which to calculate interaction with AC modes. Typically.
\rightarrow 0 for BSBS.
EM_ival_Stokes = EM_ival_pump
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
# Output files are generated in a folder with the following prefix
prefix_str = 'bsbs-josab-02-450x200nmSi'
```

(continues on next page)

```
# Use all specified parameters to create a waveguide object
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=materials.get_material("Si_2021_Poulton"),
                        lc_bkg=0.05, # mesh coarseness in background, larger lc_bkg =_
→coarser along horizontal outer edge
                        lc_refine_1=20.0, # mesh refinement factor near the interface of_
→waveguide, larger = finer along horizontal interface
                        lc_refine_2=30.0, # mesh refinement factor near the origin/

→ centre of waveguide

                        plt_mesh=False, # creates png file of geometry and mesh in_
→backend/fortran/msh/
                        check_mesh=False) # note requires x-windows configuration to work
# Print information on material data in terminal
print('\nUsing %s material data from' % wguide.material_a.chemical)
print('Author:', wguide.material_a.author)
print('Year:', wguide.material_a.date)
print('Ref:', wguide.material_a.doi)
# Initial guess for the EM effective index of the waveguide
n_eff = wguide.material_a.n-0.1
# Calculate the Electromagnetic modes of the pump field.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# A computation interruption if needed
#sys.exit("We interrupt your regularly scheduled computation to bring you ... for now")
# Calculate the Electromagnetic modes of the Stokes field.
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
# Generating images for the EM modes involved in the calculation
print("Plotting EM fields ")
plotting.plot_mode_fields(sim_EM_pump,
                         EM_AC='EM_E', num_ticks=3,xlim_min=0.4, xlim_max=0.4, ylim_
\rightarrowmin=0.4, ylim_max=0.4,
                         prefix_str=prefix_str, pdf_png='png', ticks=True, quiver_
\rightarrow points=40,
                         comps=['Et','Eabs'], n_points=1000, colorbar=True)
# Calculating the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("\n Fundamental optical mode ")
print(" n_eff = ", np.round(n_eff_sim, 4))
```

```
# Calculating the acoustic wavevector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
print('\n AC wavenumber (1/m) = ', np.round(k_AC, 4))
# Calculating Acoustic modes, using the mesh from the EM calculation.
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
# Print the frequencies of AC modes.
AC_fregs_GHz=sim_AC.nu_AC_all()*1e-9
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(AC_freqs_GHz): print('{0:3d} {1:.4e}'.format(i, np.real(nu)))
# Calculate total SBS gain, photoelastic and moving boundary contributions, as
# well as other important quantities
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
   sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, EM_ival_pump=EM_ival_pump,
   EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Mask negligible gain values to improve clarity of print out.
threshold = -1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Display these in terminal
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
#determining the location of the maximum gain
maxGainloc=np.argmax(abs(masked.data));
print("Plotting acoustic mode corresponding to maximum")
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, ivals=[maxGainloc],
                        num_ticks=3, quiver_points=40, pdf_png='png',ticks=True, comps=[
# Displaying results for the maximum found in the selection
print("----")
print("Displaying results for maximum gain value found:")
maxGainloc=np.argmax(abs(masked.data)) ;
print("Greatest SBS_gain [1/(Wm)] total \n", masked.data[maxGainloc])
print("displaying corresponding acoustic mode number (i.e., AC_field_#) for reference \n
→",maxGainloc)
print("EM Pump Power [Watts] \n", sim_EM_pump.EM_mode_power[EM_ival_pump] )
print("EM Stokes Power [Watts] \n", sim_EM_Stokes.EM_mode_power[EM_ival_Stokes] )
print("EM angular frequency [THz] \n", sim_EM_pump.omega_EM/1e12 )
print("AC Energy Density [J*m^{-1}] \n", sim_AC.AC_mode_energy[maxGainloc] )
print("AC loss alpha [1/s] \n", alpha[maxGainloc] )
print("AC frequency [GHz] \n", sim_AC.Omega_AC[maxGainloc]/(1e9*2*math.pi) )
```

(continues on next page)

../../JOSAB_tutorial/bsbs-josab-02-450x200nmSifields/EM_E_fie

Fig. 4.23: Fundamental optical mode fields.

```
../../JOSAB_tutorial/bsbs-josab-02-450x200nmSifields/EM_E_fie
```

Fig. 4.24: Fundamental optical mode fields.

```
../../JOSAB_tutorial/bsbs-josab-02-450x200nmSifields/EM_E_fie
```

Fig. 4.25: Fundamental optical mode fields.

Let's also calculate the acoustic dispersion relation for this structure.

```
print("\n Simulation time (sec.)", (end - start))
"""

Calculate dispersion diagram of the acoustic modes in a rectangular Si waveguide
"""

# Import the necessary packages
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt

sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
```

```
../../JOSAB_tutorial/bsbs-josab-02-450x200nmSifields/AC_field
```

Fig. 4.26: Fundamental acoustic mode fields.

```
../../JOSAB_tutorial/bsbs-josab-02-450x200nmSifields/AC_field
```

Fig. 4.27: Fundamental acoustic mode fields.

```
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 3.01*wl_nm
unitcell_y = unitcell_x
inc_a_x = 450 # Waveguide widths.
inc_a_y = 200
inc_shape = 'rectangular'
# Choose modes to include.
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 100
EM_ival_pump = 0
EM_ival_Stokes = EM_ival_pump
AC_ival = 'All'
# Use all specified parameters to create a waveguide object
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                       material_bkg=materials.get_material("Vacuum"),
                       material_a=materials.get_material("Si_2021_Poulton"),
                       lc_bkg=0.05, # mesh coarseness in background, larger lc_bkg =_
→coarser along horizontal outer edge
                        lc_refine_1=20.0, # mesh refinement factor near the interface of_
→waveguide, larger = finer along horizontal interface
                       lc_refine_2=30.0, # mesh refinement factor near the origin/
plt_mesh=False, # creates png file of geometry and mesh in_
→backend/fortran/msh/
```

(continues on next page)

```
../../JOSAB_tutorial/bsbs-josab-02-450x200nmSifields/AC_field
```

Fig. 4.28: Fundamental acoustic mode fields.

```
check_mesh=False) # note requires x-windows configuration to work
# Expected effective index of fundamental guided mode.
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic modes.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
# Print EM mode info
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
n_eff_sim = np.real(sim_EM_pump.neff(EM_ival_pump))
print("\n Fundamental optical mode ")
print(" n_eff = ", np.round(n_eff_sim, 4))
  k AC of backward SBS.
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
# Number of wavevectors steps.
nu_ks = 50
plt.clf()
plt.figure(figsize=(10,6))
ax = plt.subplot(1,1,1)
for i_ac, q_ac in enumerate(np.linspace(0.0,k_AC,nu_ks)):
    sim_AC = wquide.calc_AC_modes(num_modes_AC, g_ac, EM_sim=sim_EM_pump)
   prop_AC_modes = np.array([np.real(x) for x in sim_AC.Eig_values if abs(np.real(x)) >__
\rightarrowabs(np.imag(x))])
    sym_list = integration.symmetries(sim_AC)
    for i in range(len(prop_AC_modes)):
        Om = prop_AC_modes[i]*1e-9
        if sym_list[i][0] == 1 and sym_list[i][1] == 1 and sym_list[i][2] == 1:
            sym_A, = plt.plot(np.real(q_ac/k_AC), Om, 'or')
        if sym_list[i][0] == -1 and sym_list[i][1] == 1 and sym_list[i][2] == -1:
            sym_B1, = plt.plot(np.real(q_ac/k_AC), Om, 'vc')
        if sym_list[i][0] == 1 and sym_list[i][1] == -1 and sym_list[i][2] == -1:
            sym_B2, = plt.plot(np.real(q_ac/k_AC), Om, 'sb')
        if sym_list[i][0] == -1 and sym_list[i][1] == -1 and sym_list[i][2] == 1:
            sym_B3, = plt.plot(np.real(q_ac/k_AC), Om, '^g')
   print("Wavevector loop", i_ac+1, "/", nu_ks)
ax.set_ylim(0,15)
ax.set_xlim(0,1)
plt.legend([sym_A, sym_B1, sym_B2, sym_B3],['A',r'B$_1$',r'B$_2$',r'B$_3$'], loc='lower_
→right')
plt.xlabel(r'Axial wavevector (normalised)')
plt.ylabel(r'Frequency (GHz)')
plt.savefig('dispersioncurves_classified.png', bbox_inches='tight')
plt.close()
```

(continued from previous page) print("\n Simulation time (sec.)", (end - start))

../../DSAB_tutorial/dispersioncurves_classified.png

Fig. 4.29: Acoustic dispersion diagram with modes categorised by symmetry as in Table 1 of "Formal selection rules for Brillouin scattering in integrated waveguides and structured fibers" by C. Wolff, M. J. Steel, and C. G. Poulton https://doi.org/10.1364/0E.22.032489

end = time.time()

4.2.3 FSBS - Circular Waveguide - Silica

```
print("\n Simulation time (sec.)", (end - start))
Script to evaluate forward Brillouin scattering in a cylindrical SiO2 waveguide
# Import the necessary packages
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
import copy
import math
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k AC: acoustic wavenumber
start = time.time()
# Specify Geometric Parameters - all in [nm].
wl_nm = 1550 # Wavelength of EM wave in vacuum.
# Unit cell dimensions must be sufficiently large to ensure fields are zero at outermost.
→boundary.
unitcell_x = 4.01*wl_nm #be careful to ensure not whole integer multiples
unitcell_y = unitcell_x
inc_a_x = 1000 # Waveguide widths.
inc_a_y = inc_a_x
inc_shape = 'circular' # Shape of the waveguide.
# Specify number of electromagnetic modes and acoustic modes involved in the
# calculation for FSBS
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num modes AC = 100
# The EM pump mode(s) for which to calculate interaction with AC modes. Typically 0 for
\hookrightarrow FSBS.
EM_ival_pump = 1
# The EM Stokes mode(s) for which to calculate interaction with AC modes. Typically 0.
\rightarrow for FSBS.
EM_ival_Stokes = EM_ival_pump
```

```
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
# Output files are generated in a folder with the following prefix
prefix_str = 'fsbs-josab-03-1umSiO2'
# Use all specified parameters to create a waveguide object
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                       material_bkg=materials.get_material("Vacuum"),
                       material_a=materials.get_material("SiO2_2021_Poulton"),
                       lc_bkg=0.05, # mesh coarseness in background, larger lc_bkg =_
→coarser along horizontal outer edge
                        lc_refine_1=20.0, # mesh refinement factor near the interface of_
→waveguide, larger lc2 = finer along horizontal interface
                       lc_refine_2=30.0, # mesh refinement factor near the origin/
plt_mesh=False, # creates png file of geometry and mesh in_
→backend/fortran/msh/
                       check_mesh=False) # note requires x-windows configuration to work
# Explicitly remind ourselves what data we're using.
print('\nUsing %s material data from' % wguide.material_a.chemical)
print('Author:', wguide.material_a.author)
print('Year:', wguide.material_a.date)
print('Ref:', wguide.material_a.doi)
# Initial guess for the EM effective index of the waveguide
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic Modes
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff = ", np.round(n_eff_sim, 4))
# A computation interruption if needed
# sys.exit("We interrupt your regularly scheduled computation to bring you something.
→ completely different... for now")
#calculate the EM modes for the Stokes
sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
# Generate images for the EM modes involved in the calculation
# note: use EM_AC='EM_H' for magnetic H field
print("Plotting EM fields ")
```

(continues on next page)

```
plotting.plot_mode_fields(sim_EM_pump,
                         ivals=[EM_ival_pump],
                         EM_AC='EM_E', num_ticks=3,xlim_min=0.2, xlim_max=0.2, ylim_
\rightarrowmin=0.2, ylim_max=0.2,
                         prefix_str=prefix_str, pdf_png='png', ticks=True, quiver_
\rightarrow points=40,
                         comps=['Et','Eabs'], n_points=1000, colorbar=True)
# Specify an acoustic wavevector that is sufficiently close to zero and print
k_AC = 5
print('\n AC wavenumber (1/m) = ', np.round(k_AC, 4))
# Calculate Acoustic Modes
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
# Print the frequencies of AC modes.
AC_freqs_GHz=sim_AC.nu_AC_all()*1e-9
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('{0:3d} {1:.4e}'.format(i, np.real(AC_freqs_GHz)))
# Calculate total SBS gain, photoelastic and moving boundary contributions, as
# well as other important quantities
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Display these in terminal
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
#determining the location of the maximum gain
maxGainloc=7; #note sometimes its necessary to manually specify as certain values are.
→NOT possible by symmetry arguments
print("Plotting acoustic modes")
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, ivals=[maxGainloc],
                         num_ticks=3, quiver_points=40, pdf_png='png',ticks=True, comps=[
→'ut','uabs'], colorbar=True)
# Displaying results for the maximum found in the selection
print("----")
print("Displaying results for maximum (physically realisable) \"gain\" value found:")
print("Greatest SBS_gain [1/(Wm)] total \n", masked.data[maxGainloc])
```

```
print("displaying corresponding acoustic mode number (i.e., AC_field_#) for reference \n
→",maxGainloc )
print("EM Pump Power [Watts] \n", sim_EM_pump.EM_mode_power[EM_ival_pump] )
print("EM Stokes Power [Watts] \n", sim_EM_Stokes.EM_mode_power[EM_ival_Stokes] )
print("EM angular frequency [THz] \n", sim_EM_pump.omega_EM/1e12 )
print("AC Energy Density [J*m^{-1}] \n", sim_AC.AC_mode_energy[maxGainloc])
print("AC loss alpha [1/s] \n", alpha[maxGainloc] )
print("AC frequency [GHz] \n", sim_AC.Omega_AC[maxGainloc]/(1e9*2*math.pi) )
print("AC linewidth [MHz] \n", linewidth_Hz[maxGainloc]/1e6)
#since the overlap is not returned directly we'll have to deduce it
absQtot2 = (alpha[maxGainloc]*sim_EM_pump.EM_mode_power[EM_ival_pump]*sim_EM_Stokes.EM_
-mode_power[EM_ival_Stokes]*sim_AC.AC_mode_energy[maxGainloc]*masked.data[maxGainloc])/
absQtot = pow(absQtot2, 1/2)
print("Total coupling |Qtot| [W*m^{-1}*s] \n", absQtot )
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

../../JOSAB_tutorial/fsbs-josab-03-1umSiO2fields/EM_E_field_1

Fig. 4.30: Fundamental optical mode fields.

../../JOSAB_tutorial/fsbs-josab-03-1umSiO2fields/EM_E_field_1

Fig. 4.31: Fundamental optical mode fields.

../../JOSAB_tutorial/fsbs-josab-03-1umSiO2fields/EM_E_field_1

Fig. 4.32: Fundamental optical mode fields.

../../JOSAB_tutorial/fsbs-josab-03-1umSiO2fields/AC_field_7.pr

Fig. 4.33: Fundamental acoustic mode fields.

../../JOSAB_tutorial/fsbs-josab-03-1umSiO2fields/AC_field_7_ua

Fig. 4.34: Fundamental acoustic mode fields.

../../JOSAB_tutorial/fsbs-josab-03-1umSiO2fields/AC_field_7_u

Fig. 4.35: Fundamental acoustic mode fields.

4.2.4 FSBS - Rectangular Waveguide - Silicon

```
print("\n Simulation time (sec.)", (end - start))
Script to evaluate forward Brillouin scattering in a rectangular Si waveguide
# Import the necessary packages
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
import copy
import math
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k AC: acoustic wavenumber
start = time.time()
# Specify Geometric Parameters - all in [nm].
wl_nm = 1550
unitcell_x = 3.01*wl_nm
unitcell_y = unitcell_x
inc_a_x = 450 # Waveguide widths.
inc_a_y = 200
inc_shape = 'rectangular'
# Specify number of electromagnetic modes and acoustic modes involved in the
# calculation for FSBS
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num modes AC = 100
# The EM pump mode(s) for which to calculate interaction with AC modes. Typically 0 for
\hookrightarrow FSBS.
EM_ival_pump = 0
# The EM Stokes mode(s) for which to calculate interaction with AC modes. Typically 0_{\sf u}
\rightarrow for FSBS.
EM_ival_Stokes = EM_ival_pump
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
```

(continues on next page)

```
# Output files are generated in a folder with the following prefix
prefix_str = 'fsbs-josab-04-450x200nmSi'
# Use all specified parameters to create a waveguide object
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                       material_bkg=materials.get_material("Vacuum"),
                       material_a=materials.get_material("Si_2021_Poulton"),
                       lc_bkg=0.05, # mesh coarseness in background, larger lc_bkg =_
→coarser along horizontal outer edge
                       lc_refine_1=20.0, # mesh refinement factor near the interface of_
→waveguide, larger = finer along horizontal interface
                       lc_refine_2=30.0, # mesh refinement factor near the origin/
plt_mesh=False, # creates png file of geometry and mesh in_
→backend/fortran/msh/
                       check_mesh=False) # note requires x-windows configuration to work
# Explicitly remind ourselves what data we're using.
print('\nUsing %s material data from' % wguide.material_a.chemical)
print('Author:', wguide.material_a.author)
print('Year:', wguide.material_a.date)
print('Ref:', wguide.material_a.doi)
# Initial guess for the EM effective index of the waveguide
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic Modes
sim_EM_pump = wquide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff = ", np.round(n_eff_sim, 4))
# A computation interruption if needed
# sys.exit("We interrupt your regularly scheduled computation to bring you something.
→ completely different... for now")
#calculate the EM modes for the Stokes
sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
# Generate images for the EM modes involved in the calculation
# note: use EM_AC='EM_H' for magnetic H field
print("Plotting EM fields ")
plotting.plot_mode_fields(sim_EM_pump,
                        ivals=[EM_ival_pump],
                        EM_AC='EM_E', num_ticks=3,xlim_min=0.4, xlim_max=0.4, ylim_
```

```
\rightarrowmin=0.4, ylim_max=0.4,
                        prefix_str=prefix_str, pdf_png='png', ticks=True, quiver_
\rightarrow points=40,
                        comps=['Et', 'Eabs'], n_points=1000, colorbar=True)
# Specify an acoustic wavevector that is sufficiently close to zero and print
print('\n AC wavenumber (1/m) = ', np.round(k_AC, 4))
# Calculate Acoustic Modes
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
# Print the frequencies of AC modes.
AC_freqs_GHz=sim_AC.nu_AC_all()*1e-9
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('{0:3d} {1:.4e}'.format(i, np.real(AC_freqs_GHz)))
# Calculate total SBS gain, photoelastic and moving boundary contributions etc
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Display these in terminal
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
#determining the location of the maximum gain
maxGainloc=6; #note sometimes its necessary to manually specify as certain values are.
→NOT possible by symmetry arguments
print("Plotting acoustic modes")
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, ivals=[maxGainloc],
                        num_ticks=3, quiver_points=40, pdf_png='png',ticks=True, comps=[
# Displaying results for the maximum found in the selection
print("----")
print("Displaying results for maximum (physically realisable) \"gain\" value found:")
print("Greatest SBS_gain [1/(Wm)] total \n", masked.data[maxGainloc])
print("displaying corresponding acoustic mode number (i.e., AC_field_#) for reference \n
→".maxGainloc )
print("EM Pump Power [Watts] \n", sim_EM_pump.EM_mode_power[EM_ival_pump] )
print("EM Stokes Power [Watts] \n", sim_EM_Stokes.EM_mode_power[EM_ival_Stokes] )
```

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../../JOSAB_tutorial/fsbs-josab-04-450x200nmSifields/EM_E_fie

Fig. 4.36: Fundamental optical mode fields.

../../JOSAB_tutorial/fsbs-josab-04-450x200nmSifields/EM_E_fie

Fig. 4.37: Fundamental optical mode fields.

../../JOSAB_tutorial/fsbs-josab-04-450x200nmSifields/EM_E_fie

Fig. 4.38: Fundamental optical mode fields.

../../JOSAB_tutorial/fsbs-josab-04-450x200nmSifields/AC_field

Fig. 4.39: Fundamental acoustic mode fields.

../../JOSAB_tutorial/fsbs-josab-04-450x200nmSifields/AC_field_

Fig. 4.40: Fundamental acoustic mode fields.

../../JOSAB_tutorial/fsbs-josab-04-450x200nmSifields/AC_field

Fig. 4.41: Fundamental acoustic mode fields.

4.2.5 IFSBS - Circular Waveguide - Silica

```
print("\n Simulation time (sec.)", (end - start))
Script to evaluate intermodal forward Brillouin scattering in a cylindrical SiO2.
→wavequide
# Import the necessary packages
import time
import datetime
import numpy as np
import sys
import copy
from matplotlib.ticker import AutoMinorLocator
import math
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k AC: acoustic wavenumber
start = time.time()
# Specify Geometric Parameters - all in [nm].
wl_nm = 1550 # Wavelength of EM wave in vacuum.
# Unit cell dimensions must be sufficiently large to ensure fields are zero at outermost.
→boundary.
unitcell_x = 4.01*wl_nm #be careful to ensure not whole integer multiples
unitcell_y = unitcell_x
inc_a_x = 1000 # Waveguide width.
inc_a_y = inc_a_x
inc_shape = 'circular' # Shape of the waveguide.
# Specify number of electromagnetic modes, acoustic modes, and which EM indices
# are involved in the calculation for intermodal FSBS
num_modes_EM_pump = 20
num modes EM Stokes = num modes EM pump
num_modes_AC = 100 # Number of acoustic modes to solve for.
# The EM pump mode(s) for which to calculate interaction with AC modes.
# Can specify a mode number (zero has lowest propagation constant) or 'All'.
EM_ival_pump = 1
# The EM Stokes mode(s) for which to calculate interaction with AC modes.
EM ival Stokes = 0
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
```

```
# Output files are generated in a folder with the following prefix
prefix_str = 'ifsbs-josab-05-1umSi02'
# Use all specified parameters to create a waveguide object
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                       material_bkg=materials.get_material("Vacuum"),
                        material_a=materials.get_material("SiO2_2021_Poulton"),
                        lc_bkg=0.05, # mesh coarseness in background, larger lc_bkg =_
→coarser along horizontal outer edge
                        lc_refine_1=20.0, # mesh refinement factor near the interface of_
→waveguide, larger lc2 = finer along horizontal interface
                        lc_refine_2=30.0, # mesh refinement factor near the origin/
plt_mesh=False, # creates png file of geometry and mesh in_
→backend/fortran/msh/
                        check_mesh=False) # note requires x-windows configuration to work
# Initial guess for the EM effective index of the waveguide
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic Modes
print("Starting EM pump modes")
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff, debug=False)
print("Starting EM Stokes modes")
sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
# Generate images for the EM modes involved in the calculation
print("Starting EM field plotting ")
plotting.plot_mode_fields(sim_EM_pump,
                         ivals=[EM_ival_pump,EM_ival_Stokes],
                         EM_AC='EM_E', num_ticks=3,xlim_min=0.2, xlim_max=0.2, ylim_
\rightarrowmin=0.2, ylim_max=0.2,
                         prefix_str=prefix_str, pdf_png='png', ticks=True, quiver_
\rightarrow points=40,
                         comps=['Et','Eabs'], n_points=1000, colorbar=True)
# A computation interruption if needed
# sys.exit("We interrupt your regularly scheduled computation to bring you something.
→completely different... for now")
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('{0:3d} {1:.4e}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff = ", np.round(n_eff_sim, 4))
```

(continues on next page)

```
# Calculate and print the acoustic wave vector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
print('Intermode q_AC (Hz) \n', k_AC)
# Calculate Acoustic Modes
print("Starting acoustic modes")
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, debug=False)
# Print the frequencies of AC modes.
AC_fregs_GHz=sim_AC.nu_AC_all()*1e-9
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('{0:3d} {1:.4e}'.format(i, np.real(AC_freqs_GHz)))
# Calculate total SBS gain, photoelastic and moving boundary contributions, as
# well as other important quantities
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
   sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Display these in terminal
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
# determining the location of the maximum gain
maxGainloc=6; #note sometimes its necessary to manually specify as certain values are
→NOT possible by symmetry arguments
print("Plotting acoustic mode corresponding to maximum")
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, ivals=[maxGainloc],
                         num_ticks=3, quiver_points=40, pdf_png='png',ticks=True,_
# Displaying results for the maximum found in the selection
print("----")
print("Displaying results for maximum gain value found:")
print("Greatest SBS_gain [1/(Wm)] total \n", masked.data[maxGainloc])
print("displaying corresponding acoustic mode number (i.e., AC_field_#) for reference \n
→",maxGainloc)
print("EM Pump Power [Watts] \n", sim_EM_pump.EM_mode_power[EM_ival_pump] )
print("EM Stokes Power [Watts] \n", sim_EM_Stokes.EM_mode_power[EM_ival_Stokes] )
print("EM angular frequency [THz] \n", sim_EM_pump.omega_EM/1e12 )
print("AC Energy Density [J*m^{-1}] \n", sim_AC.AC_mode_energy[maxGainloc] )
print("AC loss alpha [1/s] \n", alpha[maxGainloc] )
print("AC frequency [GHz] \n", sim_AC.Omega_AC[maxGainloc]/(1e9*2*math.pi) )
```

../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/EM_E_field_0

Fig. 4.42: Fundamental optical mode fields.

```
../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/EM_E_field_0
```

Fig. 4.43: Fundamental optical mode fields.

../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/EM_E_field_0

Fig. 4.44: Fundamental optical mode fields.

```
../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/EM_E_field_
```

Fig. 4.45: Second order optical mode fields.

../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/EM_E_field_

Fig. 4.46: Second order optical mode fields.

../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/EM_E_field_

Fig. 4.47: Second order optical mode fields.

../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/AC_field_6.

Fig. 4.48: Fundamental acoustic mode fields.

../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/AC_field_6_u

Fig. 4.49: Fundamental acoustic mode fields.

../../JOSAB_tutorial/ifsbs-josab-05-1umSiO2fields/AC_field_6_u

Fig. 4.50: Fundamental acoustic mode fields.

4.2.6 IFSBS - Rectangular Waveguide - Silicon

```
print("\n Simulation time (sec.)", (end - start))
Script to evaluate intermodal forward Brillouin scattering in a rectangular Si waveguide
# Import the necessary packages
import time
import datetime
import numpy as np
import sys
import copy
from matplotlib.ticker import AutoMinorLocator
import math
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k_AC: acoustic wavenumber
start = time.time()
# Specify Geometric Parameters - all in [nm].
wl_nm = 1550
unitcell_x = 3.01*wl_nm
unitcell_y = unitcell_x
inc_a_x = 450 # Waveguide widths.
inc_a_y = 200
inc_shape = 'rectangular'
# Specify number of electromagnetic modes, acoustic modes, and which EM indices
# are involved in the calculation for intermodal FSBS
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num_modes_AC = 100 # Number of acoustic modes to solve for.
# The EM pump mode(s) for which to calculate interaction with AC modes.
# Can specify a mode number (zero has lowest propagation constant) or 'All'.
EM_ival_pump = 0
# The EM Stokes mode(s) for which to calculate interaction with AC modes.
EM_ival_Stokes = 1
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
# Output files are generated in a folder with the following prefix
prefix_str = 'ifsbs-josab-06-450x200nmSi'
```

(continues on next page)

```
# Use all specified parameters to create a waveguide object
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=materials.get_material("Si_2021_Poulton"),
                        lc_bkg=0.05, # mesh coarseness in background, larger lc_bkg =_
→coarser along horizontal outer edge
                        lc_refine_1=20.0, # mesh refinement factor near the interface of_
→waveguide, larger = finer along horizontal interface
                        lc_refine_2=30.0, # mesh refinement factor near the origin/

→ centre of waveguide

                        plt_mesh=False, # creates png file of geometry and mesh in_
→backend/fortran/msh/
                        check_mesh=False) # note requires x-windows configuration to_
\rightarrowwork
# Initial guess for the EM effective index of the waveguide
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic Modes
print("Starting EM pump modes")
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff, debug=False)
print("Starting EM Stokes modes")
sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
# Generate images for the EM modes involved in the calculation
print("Plotting EM fields ")
# print("no plotting")
plotting.plot_mode_fields(sim_EM_pump,
                         ivals=[EM_ival_pump,EM_ival_Stokes],
                         EM_AC='EM_E', num_ticks=3,xlim_min=0.4, xlim_max=0.4, ylim_
\rightarrowmin=0.4, ylim_max=0.4,
                         prefix_str=prefix_str, pdf_png='png', ticks=True, quiver_
\rightarrow points=40,
                         comps=['Et','Eabs'], n_points=1000, colorbar=True)
# A computation interruption if needed
# sys.exit("We interrupt your regularly scheduled computation to bring you something.
→ completely different... for now")
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("n_eff = ", np.round(n_eff_sim, 4))
```

```
# Calculate and print the acoustic wave vector
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
print('Intermode q_AC (Hz) \n', k_AC)
# Calculate Acoustic Modes
print("starting acoustic modes")
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, debug=False)
# Print the frequencies of AC modes.
AC_fregs_GHz=sim_AC.nu_AC_all()*1e-9
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('{0:3d} {1:.4e}'.format(i, np.real(AC_freqs_GHz)))
# Calculate total SBS gain, photoelastic and moving boundary contributions, as
# well as other important quantities
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Display these in terminal
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
#determining the location of the maximum gain
maxGainloc=np.argmax(abs(masked.data));
print("Plotting acoustic mode corresponding to maximum")
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, ivals=[maxGainloc],
                        num_ticks=3, quiver_points=40, pdf_png='png',ticks=True, comps=[
→ 'ut', 'uabs'], colorbar=True)
# Displaying results for the maximum found in the selection
print("----")
print("Displaying results for maximum gain value found:")
maxGainloc=np.argmax(abs(masked.data));
print("Greatest SBS_gain [1/(Wm)] total \n", masked.data[maxGainloc])
print("displaying corresponding acoustic mode number (i.e., AC_field_#) for reference \n
→",maxGainloc )
print("EM Pump Power [Watts] \n", sim_EM_pump.EM_mode_power[EM_ival_pump] )
print("EM Stokes Power [Watts] \n", sim_EM_Stokes.EM_mode_power[EM_ival_Stokes] )
print("EM angular frequency [THz] \n", sim_EM_pump.omega_EM/1e12 )
print("AC Energy Density [J*m^{-1}] \n", sim_AC.AC_mode_energy[maxGainloc] )
```

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../../JOSAB_tutorial/ifsbs-josab-06-450x200nmSifields/EM_E_fic

Fig. 4.51: Fundamental optical mode fields.

../../JOSAB_tutorial/ifsbs-josab-06-450x200nmSifields/EM_E_fic

Fig. 4.52: Fundamental optical mode fields.

../../JOSAB_tutorial/ifsbs-josab-06-450x200nmSifields/EM_E_fic

Fig. 4.53: Fundamental optical mode fields.

Fig. 4.54: Second order optical mode fields.

Fig. 4.55: Second order optical mode fields.

Fig. 4.56: Second order optical mode fields.

Fig. 4.57: Fundamental acoustic mode fields.

```
../../JOSAB_tutorial/ifsbs-josab-06-450x200nmSifields/AC_field
```

Fig. 4.58: Fundamental acoustic mode fields.

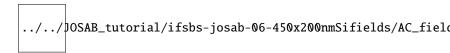


Fig. 4.59: Fundamental acoustic mode fields.

4.3 Literature Examples

Having become somewhat familiar with NumBAT, we now set out to replicate a number of examples from the recent literature located in the lit_examples directory. The examples are presented in chronological order. We note the particular importance of examples 5-8 which include experimental and numerical results that are in good agreement.

4.3.1 LitEx 1 – Laude and Beugnot, *AIP Advances* (2013): BSBS in a silica rectangular waveguide

This example simo-lit_01-Laude-AIPAdv_2013-silica.py is based on the calculation of backward SBS in a small rectangular silica waveguide described in V. Laude and J.-C. Beugnot, Generation of phonons from electrostriction in small-core optical waveguides, *AIP Advances* **3**, 042109 (2013).

Observe the use of a material named materials.materials_dict["Si02_2013_Laude"] specifically modelled on the parameters in this paper. This technique allows users to easily compare exactly to other authors without changing their preferred material values for their own samples and experiments.

```
""" Replicating the results of
    Generation of phonons from electrostriction in
    small-core optical waveguides
    Laude et al.
   http://dx.doi.org/10.1063/1.4801936
    Replicating silica example.
.....
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl nm = 1550
unitcell_x = 7*wl_nm
unitcell_y = unitcell_x
inc_a_x = 1500
inc_a_y = 1000
```

```
inc_shape = 'rectangular'
# Optical Parameters
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 120
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
prefix_str = 'lit_01-'
# Use all specified parameters to create a waveguide object.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=materials.get_material("Si02_2013_Laude"),
                        lc_bkg=1, lc_refine_1=400.0, lc_refine_2=50.0)
# Expected effective index of fundamental guided mode.
n_eff = 1.3
# Calculate Electromagnetic modes.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.4, xlim_max=0.4, ivals=[EM_ival_pump],
                         ylim_min=0.4, ylim_max=0.4, EM_AC='EM_E',
                         prefix_str=prefix_str, pdf_png='png')
# Print the wavevectors of EM modes.
print('k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values), 4))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.Eig_values*((wl_nm*1e-9)/(2.*np.pi)))
print("n_eff = ", np.round(n_eff_sim, 4))
k_AC = np.real(sim_EM_pump.Eig_values[EM_ival_pump] - sim_EM_Stokes.Eig_values[EM_ival_
→Stokes])
shift_Hz = 8e9
# Calculate Acoustic modes.
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_Hz)
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, pdf_png='png')
# Print the frequencies of AC modes.
print('Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
```

```
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 4 # GHz
freq_max = 13 # GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
    semilogy=True, prefix_str=prefix_str, pdf_png='png')
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 9.5 # GHz
freq_max = 10 # GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='_zoom', pdf_png='png')
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

../../lit_examples/lit_01-fields/EM_E_field_0.png

Fig. 4.60: Fundamental optical mode fields.

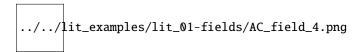


Fig. 4.61: High gain acoustic mode, marked as C in paper.

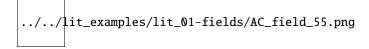


Fig. 4.62: High gain acoustic mode, marked as D in paper.

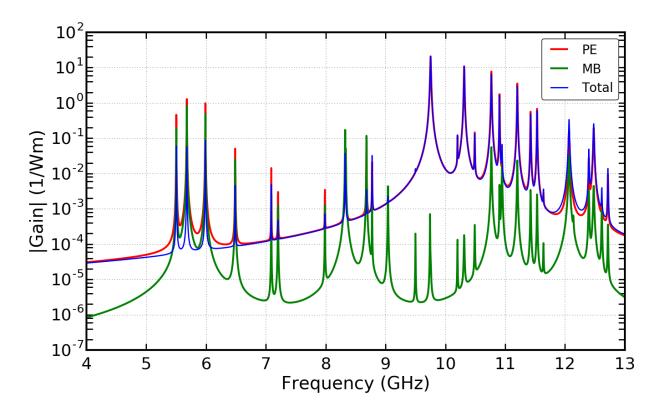


Fig. 4.63: Gain spectra on semilogy axis.

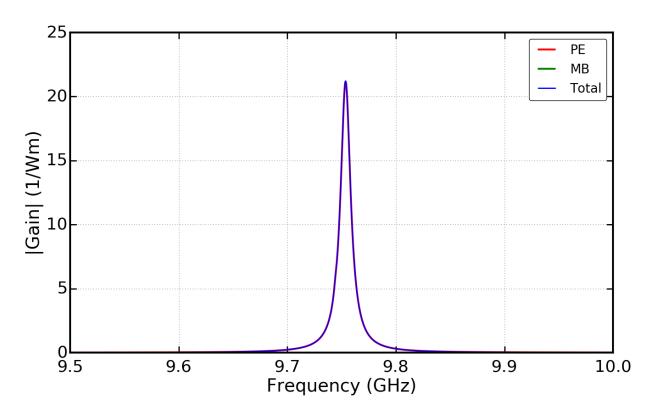


Fig. 4.64: Gain spectra zoomed in on mode D.

4.3.2 LitEx 2 – Laude and Beungot, *AIP Advances* (2013): BSBS in a rectangular silicon waveguide

This example in simo-lit_02-Laude-AIPAdv_2013-silicon.py again follows the paper of V. Laude and J.-C. Beugnot, Generation of phonons from electrostriction in small-core optical waveguides, *AIP Advances* **3**, 042109 (2013), but this time looks at the *silicon* waveguide case.

```
""" Replicating the results of
    Generation of phonons from electrostriction in
    small-core optical waveguides
   Laude et al.
   http://dx.doi.org/10.1063/1.4801936
   Replicating silicon example.
    Note requirement for lots of modes and therefore lots of memory.
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 4*wl_nm
unitcell_y = unitcell_x*2/3
inc a x = 1500
inc_a_y = 1000
inc_shape = 'rectangular'
# Optical Parameters
num_modes_EM_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num_modes_AC = 800
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
```

```
prefix_str = 'lit_02-'
# Use all specified parameters to create a waveguide object.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=materials.get_material("Si_2013_Laude"),
                        lc_bkg=1, lc_refine_1=400.0, lc_refine_2=50.0)
# Expected effective index of fundamental guided mode.
n_eff = 3.4
# Calculate Electromagnetic modes.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.2, xlim_max=0.2, ivals=[EM_ival_pump],
                         ylim_min=0.2, ylim_max=0.2, EM_AC='EM_E',
                         prefix_str=prefix_str, pdf_png='png')
# Print the wavevectors of EM modes.
print('k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values), 4))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.Eig_values*((wl_nm*1e-9)/(2.*np.pi)))
print("n_eff = ", np.round(n_eff_sim, 4))
k_AC = np.real(sim_EM_pump.Eig_values[EM_ival_pump] - sim_EM_Stokes.Eig_values[EM_ival_
→Stokes])
shift_Hz = 31e9
# Calculate Acoustic modes.
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_Hz)
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, pdf_png='png')
# Print the frequencies of AC modes.
print('Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 20 # GHz
freq_max = 45 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
    EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
    semilogy=True, prefix_str=prefix_str, pdf_png='png')
```

```
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

../../lit_examples/lit_02-fields/AC_field_4.png

Fig. 4.65: High gain acoustic mode, marked as G in paper.

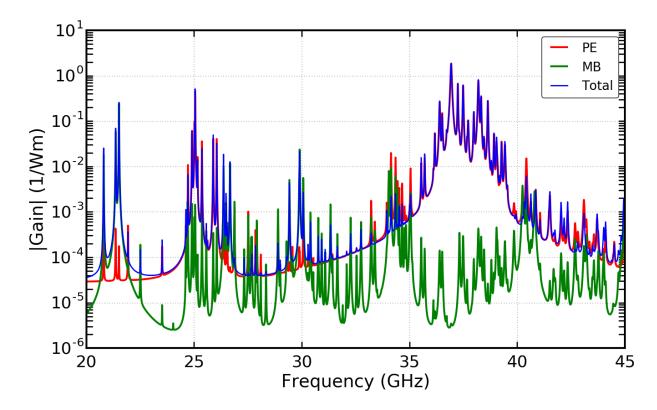


Fig. 4.66: Gain spectra on semilogy axis.

4.3.3 LitEx 3 – Beugnot *et al*, *Nature Communications* (2014): BSBS in a tapered fibre - scanning widths

This example, in simo-lit_03-Beugnot-NatComm_2014.py, is based on the calculation of backward SBS in a micron scale optical fibre described in J.-C. Beugnot *et al.*, Brillouin light scattering from surface acoustic waves in a subwavelength-diameter optical fibre, *Nature Communications* **5**, 5242 (2014).

```
""" Replicating the results of
   Brillouin light scattering from surface acoustic
    waves in a subwavelength-diameter optical fibre
   Beugnot et al.
   http://dx.doi.org/10.1038/ncomms6242
import time
import datetime
import numpy as np
import sys
from multiprocessing import Pool
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Select the number of CPUs to use in simulation.
num cores = 5
# Geometric Parameters - all in nm.
wl nm = 1550
unitcell_x = 4*wl_nm
unitcell_y = unitcell_x
inc_shape = 'circular'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 80
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
# Expected effective index of fundamental guided mode.
n_{eff} = 1.18
```

```
freq_min = 4
freq_max = 12
width_min = 600
width_max = 1200
num_widths = 301
inc_a_x_range = np.linspace(width_min, width_max, num_widths)
num_interp_pts = 2000
def modes_n_gain(inc_a_x):
    inc_a_y = inc_a_x
    # Use all specified parameters to create a waveguide object.
   wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                            material_bkg=materials.get_material("Vacuum"),
                            material_a=materials.get_material("SiO2_2016_Smith"),
                            lc_bkg=1, lc_refine_1=400.0, lc_refine_2=50.0)
   sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
    sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
   k_AC = np.real(sim_EM_pump.Eig_values[EM_ival_pump] - sim_EM_Stokes.Eig_values[EM_
→ival_Stokes])
    shift_Hz = 4e9
    sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_
→Hz)
   set_q_factor = 600.
    SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.

    gain_and_qs(
        sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
        EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival)#,__

    fixed_Q=set_q_factor)
    interp_values = plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB,__
→linewidth_Hz, k_AC,
        EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min, freq_max, num_interp_pts=num_
→interp_pts.
        save_fig=False, suffix_str='%i' %int(inc_a_x))
    # Clear memory
   wguide = sim_EM_pump = sim_EM_Stokes = sim_AC = None
   SBS_gain = SBS_gain_PE = SBS_gain_MB = linewidth_Hz = Q_factors = alpha = None
   return interp_values
# Run widths in parallel across num_cores CPUs using multiprocessing package.
pool = Pool(num_cores)
width_objs = pool_map(modes_n_gain, inc_a_x_range)
# Note pool.map() doesn't pass errors back from fortran routines very well.
# It's good practise to run the extrema of your simulation range through map()
# before launcing full multicore simulation.
```

```
gain_array = np.zeros((num_interp_pts, num_widths))
for w, width_interp in enumerate(width_objs):
   gain_array[:,w] = width_interp[::-1]
# np.savez('gain_array_data', gain_array=gain_array)
# npzfile = np.load('gain_array_data.npz')
# gain_array = npzfile['gain_array'].tolist()
fig = plt.figure()
ax1 = fig.add\_subplot(1,1,1)
im = ax1.imshow(np.abs(gain_array), aspect='auto', interpolation='none',
                vmin=0, vmax=np.max(np.abs(gain_array)))#, cmap='jet')
num_xticks = 5
num_yticks = 5
ax1.xaxis.set_ticks_position('bottom')
ax1.set_xticks(np.linspace(0,(num_widths-1),num_xticks))
ax1.set_yticks(np.linspace((num_interp_pts-1),0,num_yticks))
ax1.set_xticklabels(["%4.0f" % i for i in np.linspace(width_min,width_max,num_xticks)])
ax1.set_yticklabels(["%4.0f" % i for i in np.linspace(freq_min,freq_max,num_yticks)])
plt.xlabel(r'Width (nm)')
plt.ylabel('Frequency (GHz)')
plt.savefig('lit_03-gain-width_scan.pdf')
plt.savefig('lit_03-gain-width_scan.png')
plt.close()
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

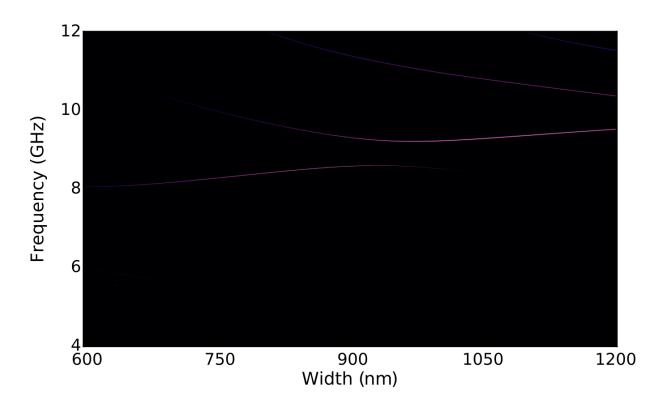


Fig. 4.67: Full acoustic wave spectrum for silica microwire, as per Fig. 4a in paper.

4.3.4 LitEx 4 – Van Laer *et al*, *Nature Photonics* (2015): FSBF in a waveguide on a pedestal

This example, in simo-lit_04-pillar-Van_Laer-NatPhot_2015.py, is based on the calculation of forward SBS in a pedestal silicon waveguide described in R. Van Laer *et al.*, Interaction between light and highly confined hypersound in a silicon photonic nanowire, *Nature Photonics* **9**, 199 (2015).

Note that the absence of an absorptive boundary in the acoustic model causes a problem where the slab layer significantly distorting acoustic modes. Adding this feature is a priority for a future release of NumBAT. The following example shows an approximate way to avoid the problem for now.

```
""" Replicating the results of
    Interaction between light and highly confined
   hypersound in a silicon photonic nanowire
    Van Laer et al.
   http://dx.doi.org/10.1038/nphoton.2015.11
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
import copy
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl nm = 1550
unitcell_x = 4*wl_nm
unitcell_y = 0.5*unitcell_x
inc_a_x = 450
inc_a_y = 230
inc_shape = 'pedestal'
pillar_x = 15
pillar_y = 300
slab_a_x = 2000
slab_a_y = 800
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 60
```

```
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
prefix_str = 'lit_04-pillar-'
# Rotate crystal axis of Si from <100> to <110>, starting with same Si_2016_Smith data.
Si_110 = copy.deepcopy(materials.materials_dict["Si_2015_Van_Laer"])
Si_110.rotate_axis(np.pi/4,'y-axis', save_rotated_tensors=True)
# Use all specified parameters to create a waveguide object.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        slab_a_x=slab_a_x, slab_a_y=slab_a_y,
                        pillar_x=pillar_x, pillar_y=pillar_y,
                        material_bkg=materials.materials_dict["Vacuum"],
                                                                                     #_
→background
                        material_a=Si_110,
                                                                   # rih
                        material_b=materials.materials_dict["Si02_2015_Van_Laer"],
∽slab
                        material_c=materials.materials_dict["Si02_2015_Van_Laer"], #_
→pillar
                        lc_bkg=1, lc_refine_1=800.0, lc_refine_2=500.0)
# Expected effective index of fundamental guided mode.
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic Modes
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
plotting.plot_mode_fields(sim_EM_pump, ivals=[EM_ival_pump],
                         xlim_min=0.4, xlim_max=0.4, ylim_min=0.4, ylim_max=0.2,
                         EM_AC='EM_E', prefix_str=prefix_str, pdf_png='png')
# Print the wavevectors of EM modes.
print('k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values), 4))
# Calculate the EM effective index of the waveguide.
n_{eff\_sim} = np.real(sim_EM_pump.Eig\_values[0]*((wl_nm*1e-9)/(2.*np.pi)))
k AC = 5
shift_Hz = 8e9
# Calculate Acoustic Modes
sim_AC = wquide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_Hz)
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, pdf_png='png')
set_q_factor = 306
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
```

../../lit_examples/lit_04-pillar-fields/EM_E_field_0.png

Fig. 4.68: Fundamental optical mode fields.

../../lit_examples/lit_04-pillar-fields/AC_field_38.png

Fig. 4.69: Dominant high gain acoustic mode. Note how the absence of an absorptive boundary on the SiO2 slab causes this layer to significantly distorted the acoustic modes.

We may also choose to study the simplified situation where the pedestal is removed.

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
    Interaction between light and highly confined
    hypersound in a silicon photonic nanowire
    Van Laer et al.
    http://dx.doi.org/10.1038/nphoton.2015.11

    Making simplification of ignoring the pedestal.
"""

import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
import copy
```

```
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from plotting import Decorator
from fortran import NumBAT
# use this class to add or alter features to the final plots
class EMDecorator(Decorator):
 def __init__(self):
    super().__init__()
 def extra_axes_commands(self, ax):
   ax.tick_params(axis='x',color='gray', which='both')
    ax.tick_params(axis='y',color='gray', which='both')
   if self.is_single_plot():
      ax.tick_params(axis='x',length=20)
      ax.tick_params(axis='y',length=20)
      ax.tick_params(axis='x',width=2)
      ax.tick_params(axis='y',width=2)
      ax.tick_params(axis='x',length=10,which='minor')
      ax.tick_params(axis='y',length=10,which='minor')
      ax.tick_params(axis='x',width=2, which='minor')
      ax.tick_params(axis='y',width=2, which='minor')
emdecorate=EMDecorator()
#acdecorate=ACDecorator()
start = time.time()
# Geometric Parameters - all in nm.
w1 nm = 1550
unitcell_x = 5*wl_nm
unitcell_y = 0.5*unitcell_x
inc_a_x = 485
inc_a_y = 230
inc_shape = 'rectangular'
num_modes_EM_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 60
EM_ival_pump = 0
EM ival Stokes = 0
AC_ival = 'All'
```

```
prefix_str = 'fig6-'
# Rotate crystal axis of Si from <100> to <110>, starting with same Si_2016_Smith data.
Si_110 = copy.deepcopy(materials.get_material("Si_2016_Smith")
# Si_110 = copy.deepcopy(materials.materials_dict["Si_2015_Van_Laer"])
Si_110.rotate_axis(np.pi/4, 'z-axis', save_rotated_tensors=True)
# Use all specified parameters to create a waveguide object.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=Si_110, symmetry_flag=False,
                        lc_bkg=.25, lc_refine_1=200.0, lc_refine_2=200.0)
# Expected effective index of fundamental guided mode.
n_eff = wguide.material_a.n-0.1
doem=True
doac=True
new_calcs=False
if doem:
  # Calculate Electromagnetic Modes
  if new_calcs:
    sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
   np.savez(prefix_str+'wguide_data', sim_EM_pump=sim_EM_pump)
   npzfile = np.load(prefix_str+'wguide_data.npz', allow_pickle=True)
   sim_EM_pump = npzfile['sim_EM_pump'].tolist()
  sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
  np.savez(prefix_str+'wguide_data2', sim_EM_Stokes=sim_EM_Stokes)
  #npzfile = np.load(prefix_str+'wquide_data2.npz', allow_pickle=True)
  #sim_EM_Stokes = npzfile['sim_EM_Stokes'].tolist()
 plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.43, xlim_max=0.43, ivals=[EM_ival_
\rightarrow pump],
                           ylim_min=0.43, ylim_max=0.43, EM_AC='EM_E',
                           n_points=2000, quiver_points=10, prefix_str=prefix_str, pdf_
→png='png',
                           ticks=True, comps=('Ex', 'Eabs', 'Et'), decorator=emdecorate)
  # Print the wavevectors of EM modes.
  print('k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values), 4))
  # Calculate the EM effective index of the waveguide.
 n_eff_sim = np.real(sim_EM_pump.Eig_values*((wl_nm*1e-9)/(2.*np.pi)))
  print("n_eff = ", np.round(n_eff_sim, 4))
if doac:
  k_AC = 5 # close but not quite zero
```

```
# Calculate Acoustic Modes
  if new_calcs:
    sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
   np.savez(prefix_str+'wguide_data_AC', sim_AC=sim_AC)
   npzfile = np.load(prefix_str+'wguide_data_AC.npz', allow_pickle=True)
    sim_AC = npzfile['sim_AC'].tolist()
  # Print the frequencies of AC modes.
  print('Freq of AC modes (GHz) \n', np.round((sim_AC.Eig_values)*1e-9, 4))
  #print('Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
  plotting.plot_mode_fields(sim_AC, ivals=(7,), EM_AC='AC', prefix_str=prefix_str,
                           pdf_png='png', comps=('ux','uy','ut','uabs'), ticks=True,
                           xlim_min=-0.05, ylim_min=-.05, xlim_max=-0.05, ylim_max=-.05)
set_q_factor = 306
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC, EM_ival_pump=EM_ival_pump,
   EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_Q=set_q_factor)
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 9.1 \# GHz
freq_max = 9.3 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='', pdf_png='png')
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

Which gives good agreement for the gain spectrum.

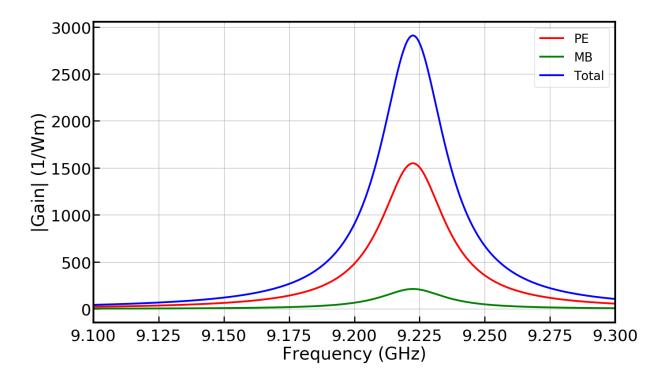


Fig. 4.70: Gain spectrum for the simplified case of a waveguide surrounded by vacuum.

4.3.5 LitEx 5 – 2015 - Van Laer *et al*, *New Journal of Physics* (2015): FSBF in a waveguide without a pedestal

This example, in simo-lit_05-Van_Laer-NJP_2015.py, continues the study of forward SBS in a pedestal silicon waveguide described in R. Van Laer *et al.*, Interaction between light and highly confined hypersound in a silicon photonic nanowire, *Nature Photonics* **9**, 199 (2015).

In this case, we simply remove the pedestal and model the main rectangular waveguide. This makes the acoustic loss calculation incorrect but avoids the problem of acoustic energy being excessively concentrated in the substrate.

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
   Net on-chip Brillouin gain based on suspended
    silicon nanowires
    Van Laer et al.
   http://dx.doi.org/10.1088/1367-2630/17/11/115005
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
import copy
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 5*wl_nm
unitcell_y = 0.5*unitcell_x
inc_a_x = 450
inc_a_y = 230
inc_shape = 'rectangular'
num_modes_EM_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 60
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
prefix_str = 'lit_05-'
```

```
# Rotate crystal axis of Si from <100> to <110>, starting with same Si_2016_Smith data.
Si_110 = copy.deepcopy(materials.get_material("Si_2016_Smith")
Si_110.rotate_axis(np.pi/4,'y-axis', save_rotated_tensors=True)
# Use all specified parameters to create a waveguide object.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=Si_110, symmetry_flag=False,
                        lc_bkg=1, lc_refine_1=1200.0, lc_refine_2=800.0)
# Expected effective index of fundamental guided mode.
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic Modes
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
# np.savez('wguide_data', sim_EM_pump=sim_EM_pump)
# npzfile = np.load('wguide_data.npz')
# sim_EM_pump = npzfile['sim_EM_pump'].tolist()
sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
# np.savez('wguide_data2', sim_EM_Stokes=sim_EM_Stokes)
# npzfile = np.load('wguide_data2.npz')
# sim_EM_Stokes = npzfile['sim_EM_Stokes'].tolist()
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.45, xlim_max=0.45,
                         ivals=[EM_ival_pump], ylim_min=0.45, ylim_max=0.45,
                         EM_AC='EM_E', n_points=1500,
                         prefix_str=prefix_str, pdf_png='png')
# Print the wavevectors of EM modes.
print('k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values), 4))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.Eig_values*((wl_nm*1e-9)/(2.*np.pi)))
print("n_eff = ", np.round(n_eff_sim, 4))
k_AC = 5 # close but not quite zero
# Calculate Acoustic Modes
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump)
# np.savez('wguide_data_AC', sim_AC=sim_AC)
# npzfile = np.load('wguide_data_AC.npz')
# sim_AC = npzfile['sim_AC'].tolist()
# Print the frequencies of AC modes.
print('Freq of AC modes (GHz) \n', np.round((sim_AC.Eig_values)*1e-9, 4))
print('Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, pdf_png='png')
set_q_factor = 230 # NJP
```

```
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_

    Q=set_q_factor)

# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 9.1 # GHz
freq_max = 9.4 \# GHz
plotting gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='', pdf_png='png')
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

```
../../lit_examples/lit_05-fields/EM_E_field_0.png
```

Fig. 4.71: Fundamental optical mode fields.

```
../../lit_examples/lit_05-fields/AC_field_6.png
```

Fig. 4.72: Dominant high gain acoustic mode.

4.3.6 LitEx 6 – Florez et al, Nature Communications (2016): BSBS self-cancellation in a tapered fibre ($d=550~\mathrm{nm}$)

This example, in simo-lit_06_1-Florez-NatComm_2016-d550nm.py, looks at the phenomenon of Brillouin "self-cancellation" due to the electrostrictive and radiation pressure effects acting with opposite sign. This was described in O. Florez *et al.*, Brillouin self-cancellation, *Nature Communications* 7, 11759 (2016).

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
   Brillouin scattering self-cancellation
   Florez et al.
   http://dx.doi.org/10.1038/ncomms11759
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from plotting import Decorator
from fortran import NumBAT
# use this class to add or alter features to the final plots
class EMDecorator(Decorator):
  def __init__(self):
    super().__init__()
    #title font=24
    #self._multi_sizes= {'title':title_font-2, 'subplot_title':title_font-5, 'cbar_tick
→':title_font-10, 'ax_tick':title_font-10, 'ax_label':title_font-10 }
    #self._single_sizes= {'ax_label':80, 'subplot_title':80, 'cbar_tick':60, 'ax_tick':70}
    ##self._single_sizes= {'ax_label':60, 'subplot_title':60, 'cbar_tick':40, 'ax_tick':40}
   #self._is_single=True
  def extra_axes_commands(self, ax):
    circle1 = plt.Circle((0, 0), 0.275, color='black', fill=False)
    ax.add_artist(circle1)
class ACDecorator(Decorator):
  def __init__(self):
   super().__init__()
    #title_font=24
    #self._multi_sizes= {'title':title_font-2, 'subplot_title':title_font-5, 'cbar_tick
```

```
self._single_sizes= {'ax_label':30, 'subplot_title':40, 'cbar_tick':20, 'ax_tick':30,
→'title_pad':20}
    self._single_sizes= {'ax_label':80, 'subplot_title':80, 'cbar_tick':60, 'ax_tick':70,
→'title_pad':25}
   self._is_single=True
 def extra_axes_commands(self, ax):
   circle1 = plt.Circle((0, 0), 0.275, color='black', fill=False)
   ax.add_artist(circle1)
emdecorate=EMDecorator()
acdecorate=ACDecorator()
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 2*wl_nm
unitcell_y = unitcell_x
inc_a_x = 550 # Diameter
inc_a_y = inc_a_x
inc_shape = 'circular'
num_modes_EM_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 40
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
prefix_str = 'fig10-'
# Use all specified parameters to create a waveguide object.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                       material_bkg=materials.get_material("Vacuum"),
                       material_a=materials.get_material("SiO2_2013_Laude"),
                       lc_bkg=.25, lc_refine_1=170.0, lc_refine_2=85.0)
# Expected effective index of fundamental guided mode.
n_{eff} = 1.4
doem=True
doac=True
new_calcs=False
if doem:
 # Calculate Electromagnetic Modes
 if new_calcs:
   sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
```

```
np.savez('wguide_data_florez', sim_EM_pump=sim_EM_pump)
  else:
   npzfile = np.load('wguide_data_florez.npz', allow_pickle=True)
    sim_EM_pump = npzfile['sim_EM_pump'].tolist()
  sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
 plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.3, xlim_max=0.3, ivals=[EM_ival_
\rightarrow pump],
                           ylim_min=0.3, ylim_max=0.3, EM_AC='EM_E',
                           prefix_str=prefix_str, pdf_png='png', ticks=True,
                           decorator=emdecorate, quiver_points=20)
  # Print the wavevectors of EM modes.
  print('k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values), 4))
  # Calculate the EM effective index of the waveguide.
 n_eff_sim = np.real(sim_EM_pump.Eig_values*((wl_nm*1e-9)/(2.*np.pi)))
  print("n_eff = ", np.round(n_eff_sim, 4))
if not doac: sys.exit(0)
k_AC = np.real(sim_EM_pump.Eig_values[EM_ival_pump] - sim_EM_Stokes.Eig_values[EM_ival_
→Stokes])
shift_Hz = 4e9
# Calculate Acoustic Modes
if new calcs:
  sim_AC = wquide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_
 np.savez('wguide_data_florez_AC', sim_AC=sim_AC)
else:
 npzfile = np.load('wguide_data_florez_AC.npz', allow_pickle=True)
  sim_AC = npzfile['sim_AC'].tolist()
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, suffix_str='',
ticks=True, ivals=[4,5], comps=('ut', 'uabs'),
xlim_min=-.1, ylim_min=-.1, xlim_max=-.1, ylim_max=-.1,
decorator=acdecorate, quiver_points=20, pdf_png='png',colorbar=True)
# Print the frequencies of AC modes.
print('Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
set_q_factor = 1000.
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_

    Q=set_q_factor)
```

```
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 5 # GHz
freq_max = 12 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
    EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, pdf_png='png')
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 5.86 \# GHz
freq_max = 5.9 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='-5', pdf_png='png')
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 6.28 \# GHz
freq_max = 6.32 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='-6', pdf_png='png')
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 8.09 \# GHz
freq_max = 8.13 \# GHz
plotting gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
    EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='-8', pdf_png='png')
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 11.65 # GHz
freq_max = 11.69 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='-11', pdf_png='png')
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

```
../../lit_examples/lit_06_1-fields/AC_field_4.png
```

Fig. 4.73: TR_{21} acoustic mode fields of a nanowire with diameter 550 nm.

```
../../lit_examples/lit_06_1-fields/AC_field_5.png
```

Fig. 4.74: R_{01} acoustic mode fields of a nanowire with diameter 550 nm.

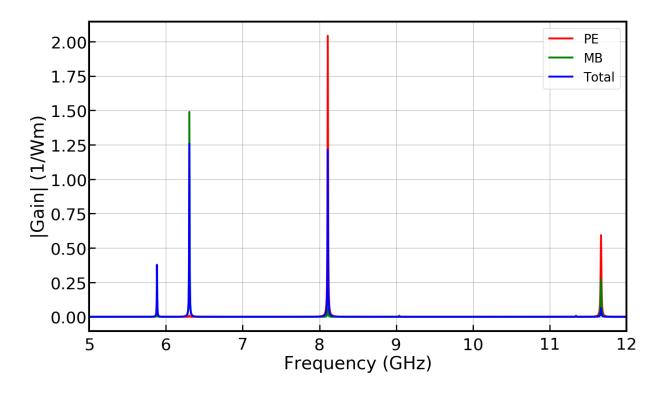
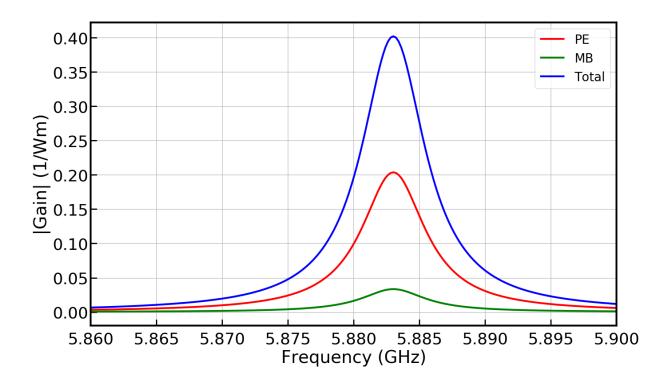
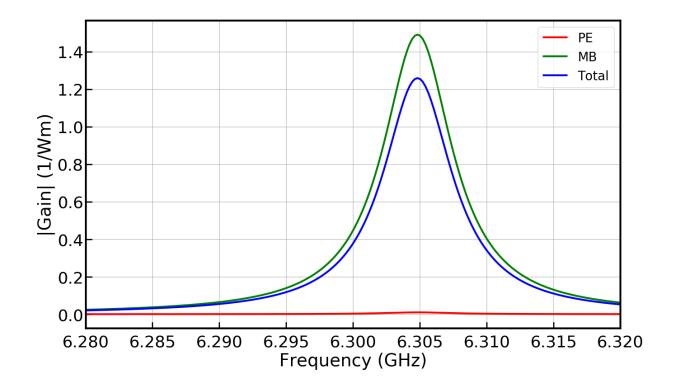
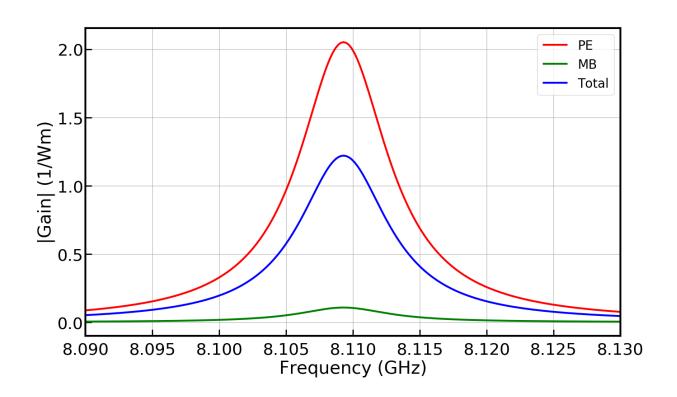


Fig. 4.75: Gain spectra of a nanowire with diameter 550 nm, matching blue curve of Fig. 3b in paper.







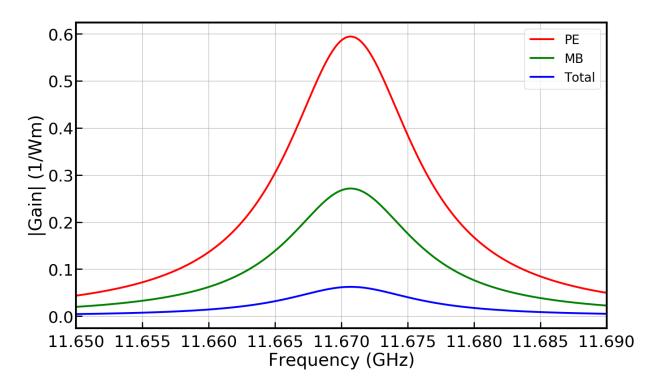


Fig. 4.76: Zoomed in gain spectra around gaint peaks of 550 nm diameter NW.

4.3.7 LitEx 6b – Florez et al, Nature Communications (2016): BSBS self-cancellation in a tapered fibre ($d=1160~\mathrm{nm}$)

This example, in simo-lit_06_2-Florez-NatComm_2016-1160nm.py, again looks at the paper O. Florez *et al.*, Brillouin self-cancellation, *Nature Communications* **7**, 11759 (2016), but now for a wider core.

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
    Brillouin scattering self-cancellation
   Florez et al.
   http://dx.doi.org/10.1038/ncomms11759
import time
import datetime
import numpy as np
import sys
import matplotlib
matplotlib.use('pdf')
import matplotlib.pyplot as plt
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550
unitcell_x = 3*wl_nm
unitcell_y = unitcell_x
inc_a_x = 1160 # Diameter
inc_a_y = inc_a_x
inc_shape = 'circular'
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
num\_modes\_AC = 40
EM_ival_pump = 0
EM_ival_Stokes = 0
AC_ival = 'All'
prefix_str = 'lit_06_2-'
# Use all specified parameters to create a waveguide object.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=materials.get_material("Si02_2013_Laude"),
```

```
#lc_bkg=1, lc_refine_1=600.0, lc_refine_2=300.0)
                        lc_bkg=.1, lc_refine_1=15.0, lc_refine_2=10.0)
wquide.check_mesh()
# Expected effective index of fundamental guided mode.
n_eff = 1.4
# Calculate Electromagnetic Modes
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.3, xlim_max=0.3, ivals=[EM_ival_pump],
                         ylim_min=0.3, ylim_max=0.3, EM_AC='EM_E',
                         prefix_str=prefix_str, pdf_png='png')
# Print the wavevectors of EM modes.
print('k_z \text{ of EM modes } n', np.round(np.real(sim_EM_pump.Eig_values), 4))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.Eig_values*((wl_nm*1e-9)/(2.*np.pi)))
print("n_eff = ", np.round(n_eff_sim, 4))
k_AC = np.real(sim_EM_pump.Eig_values[EM_ival_pump] - sim_EM_Stokes.Eig_values[EM_ival_
→Stokes])
shift_Hz = 4e9
# Calculate Acoustic Modes
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_Hz)
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str)
# Print the frequencies of AC modes.
print('Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
set_q_factor = 1000.
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_
→Q=set_q_factor)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 5 # GHZ
freq_max = 12 # GHz
plotting gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, pdf_png='pdf')
```

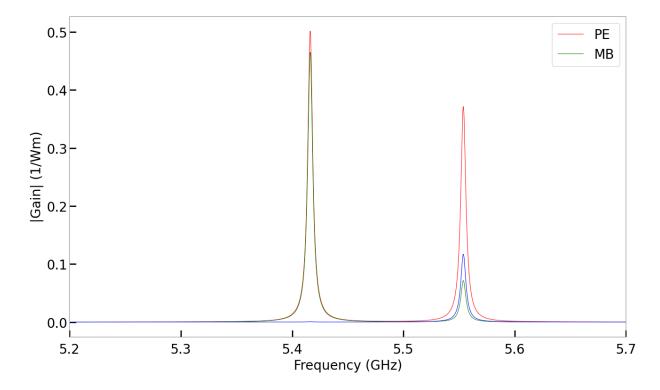


Fig. 4.77: Gain spectra of a nanowire with diameter 1160 nm, as in Fig. 4 of Florez, showing near perfect cancellation at 5.4 GHz.

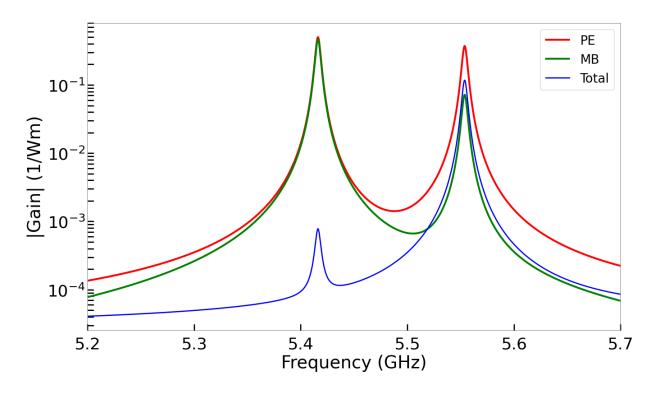


Fig. 4.78: Gain spectra of a nanowire with diameter 1160 nm, as in Fig. 4 of paper, showing near perfect cancellation at 5.4 GHz.

4.3.8 LitEx 7 – Kittlaus et al, Nature Photonics (2016), FSBF in a silicon rib waveguide

This example, in ../../lit_examples/simo-lit_07-Kittlaus-NatPhot_2016.py, explores a first geometry showing large forward SBS in silicon as described in E. Kittlaus *et al.*, Large Brillouin amplification in silicon, *Nature Photonics* **10**, 463 (2016).

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
   Large Brillouin amplification in silicon
   Kittlaus et al.
   http://dx.doi.org/10.1038/nphoton.2016.112
import time
import datetime
import numpy as np
import sys
import copy
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k_AC: acoustic wavenumber
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550 # Wavelength of EM wave in vacuum.
# Unit cell must be large to ensure fields are zero at boundary.
unitcell_x = 6*wl_nm
unitcell_y = 0.4*unitcell_x
# Waveguide widths.
inc a x = 1000
inc_a_y = 80
# Shape of the waveguide.
inc_shape = 'rib'
slab_a_x = 3000
slab_a_y = 130
# Number of electromagnetic modes to solve for.
num_modes_EM_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
# Number of acoustic modes to solve for.
```

```
num modes AC = 40
# The EM pump mode(s) for which to calculate interaction with AC modes.
# Can specify a mode number (zero has lowest propagation constant) or 'All'.
EM_ival_pump = 0
# The EM Stokes mode(s) for which to calculate interaction with AC modes.
EM_ival_Stokes = 0
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
# Si_110 = copy.deepcopy(materials.materials_dict["Si_2015_Van_Laer"])
Si_110 = copy.deepcopy(materials.get_material("Si_2016_Smith")
Si_110.rotate_axis(np.pi/4,'y-axis', save_rotated_tensors=True)
prefix_str = 'lit_07-'
# Use specified parameters to create a waveguide object.
# Note use of rough mesh for demonstration purposes.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        slab_a_x=slab_a_x, slab_a_y=slab_a_y,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=Si_110,
                        material_b=Si_110, symmetry_flag=False,
                        lc_bkg=1, lc_refine_1=2000.0, lc_refine_2=1000.0)
# Expected effective index of fundamental guided mode.
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic Modes
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff)
# np.savez('wguide_data', sim_EM_pump=sim_EM_pump)
# npzfile = np.load('wguide_data.npz')
# sim_EM_pump = npzfile['sim_EM_pump'].tolist()
sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.4, xlim_max=0.4, ivals=[EM_ival_pump],
                         ylim_min=0.3, ylim_max=0.3, EM_AC='EM_E', num_ticks=3,
                         prefix_str=prefix_str, pdf_png='png')
# Print the wavevectors of EM modes.
print('k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values), 4))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.Eig_values*((wl_nm*1e-9)/(2.*np.pi)))
print("n_eff = ", np.round(n_eff_sim, 4))
k_AC = 5
shift_Hz = 2e9
# Calculate Acoustic Modes
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_Hz)
# np.savez('wguide_data_AC', sim_AC=sim_AC)
```

```
# npzfile = np.load('wguide_data_AC.npz')
# sim_AC = npzfile['sim_AC'].tolist()
# Print the frequencies of AC modes.
print('Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str,
                         ivals=[0,1,2,3,4,5,6,7,8,9],
                         num_ticks=3, xlim_min=0.1, xlim_max=0.1, pdf_png='png')
set_q_factor = 680.
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
    EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_
→Q=set_q_factor)
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 4.2 # GHz
freq_max = 4.3 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
    EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, suffix_str='', pdf_png='png')
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

```
../../lit_examples/lit_07-fields/EM_E_field_0.png
```

Fig. 4.79: Fundamental optical mode fields.

```
../../lit_examples/lit_07-fields/AC_field_19.png
```

Fig. 4.80: Dominant high gain acoustic mode.

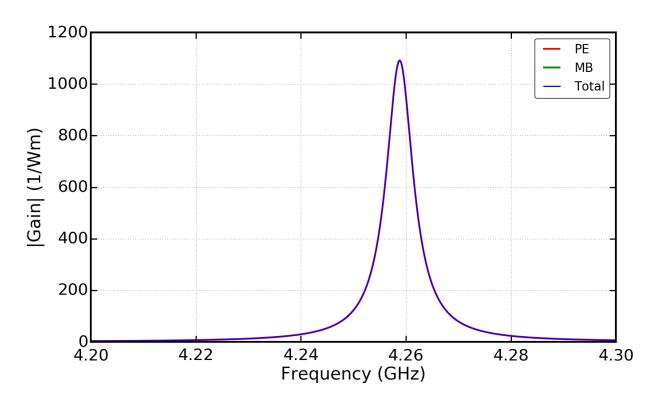


Fig. 4.81: Gain spectra showing gain due to photoelastic effect, gain due to moving boundary effect, and total gain.

4.3.9 LitEx 8 – Kittlaus *et al*, *Nature Communications* (2017): Intermodal FSBF in a silicon wavequide

This example (simo-lit_08-Kittlaus-NatComm_2017.py), also from the Yale group, examines intermode forward Brillouin scattering in silicon.

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
    On-chip inter-modal Brillouin scattering
   Kittlaus et al.
   http://dx.doi.org/10.1038/ncomms15819
import time
import datetime
import numpy as np
import sys
import copy
from matplotlib.ticker import AutoMinorLocator
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from plotting import Decorator
from fortran import NumBAT
class EMDecorator(Decorator):
  def __init__(self):
   super().__init__()
  def extra_axes_commands(self, ax):
   ax.tick_params(axis='x',color='gray', which='both')
    ax.tick_params(axis='y',color='gray', which='both')
   if self._is_single:
      ax.tick_params(axis='x',length=20)
      ax.tick_params(axis='y',length=20)
      ax.tick_params(axis='x',width=2)
      ax.tick_params(axis='y',width=2)
      ax.tick_params(axis='x',length=10,which='minor')
      ax.tick_params(axis='y',length=10,which='minor')
      ax.tick_params(axis='x',width=2, which='minor')
      ax.tick_params(axis='y',width=2, which='minor')
      ax.set_xticks(np.arange(-1.00, 1.01, .1), minor=True)
      ax.set_yticks([-.3,0,.3])
      ax.set_yticks([-.5,-.4,-.2,-.1,.1,.2,.4,.5], minor=True)
    ax.set_aspect('equal')
```

```
emdecorate=EMDecorator()
class ACDecorator(plotting.Decorator):
  def __init__(self):
    super().__init__()
    self.set_singleplot_fontsize('ax_label',30)
   self.set_singleplot_fontsize('subplot_title',30)
    self.set_singleplot_fontsize('cbar_tick',20)
    self.set_singleplot_fontsize('ax_tick',30)
   self.set_singleplot_axes_property('cbar_pad','-30%') # compensate for call to set_
→aspect() below
    self.set_multiplot_axes_property('cbar_pad','-30%')
                                                          # compensate for call to set_
→aspect() below
    self.set_singleplot_axes_property('cbar_size','2%')
                                                          # compensate for call to set_
→aspect() below
    self.set_multiplot_axes_property('cbar_size','2%')
                                                          # compensate for call to set_
→aspect() below
 def extra_axes_commands(self, ax):
   ax.set_aspect(3)
   pass
acdecorate=ACDecorator()
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k_AC: acoustic wavenumber
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550 # Wavelength of EM wave in vacuum.
# Unit cell must be large to ensure fields are zero at boundary.
unitcell_x = 7*wl_nm
unitcell_y = 0.7*unitcell_x
# Waveguide widths.
inc_a_x = 1500
inc_a_y = 80
# Shape of the waveguide.
# Use double coated geometry to control meshing around rib waveguide.
inc_shape = 'rib_double_coated'
slab_a_x = 2850
slab_a_y = 135
# areas included purely
slab_b_y = 500
coat_x = 50
coat_y = 100
```

```
coat2 x = 100
coat2_y = 200
#original old gmsh set that works
lc_bkg = 4 # background
lc_refine_1 = 8000 # edge of rib
lc_refine_2 = 3000 # edge of slab_a
lc_refine_3 = 50  # edge of coat
lc_refine_4 = 20  # edge of slab_b
lc_refine_5 = 4  # edge of coat2
# ##working set
# 1c_bkg = .5 # background
# lc_refine_1 = 1000 # edge of rib
# lc_refine_2 = 400  # edge of slab_a
# lc_refine_3 = 10  # edge of coat
# lc_refine_4 = 5 # edge of slab_b
# 1c_refine_5 = 1 # edge of coat2
# #scaled working set: doesn't work
# lc_bkg = 1 # background
# lc_refine_1 = 2000 # edge of rib
# 1c_refine_2 = 600  # edge of slab_a
# lc_refine_3 = 10  # edge of coat
# lc_refine_4 = 4  # edge of slab_b
# lc_refine_5 = 1 # edge of coat2
##scaled working set: doesn't work
#lc_bkg = .1 # background
#lc_refine_1 = 200 # edge of rib
#lc_refine_2 = 75 # edge of slab_a
#lc_refine_3 = 50  # edge of coat
\#c5 = 50 \# edge \ of \ slab\_b
#lc_refine_5 = 50 # edge of coat2
# Number of electromagnetic modes to solve for.
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
# Number of acoustic modes to solve for.
num modes AC = 35
# The EM pump mode(s) for which to calculate interaction with AC modes.
# Can specify a mode number (zero has lowest propagation constant) or 'All'.
EM_ival_pump = 0
# The EM Stokes mode(s) for which to calculate interaction with AC modes.
EM ival Stokes = 1 # INTERMODE SBS TEO to TE1
# The AC mode(s) for which to calculate interaction with EM modes.
AC ival = 'All'
```

```
# Si_110 = copy.deepcopy(materials.get_material("Si_2015_Van_Laer")
Si_110 = copy.deepcopy(materials.get_material("Si_2016_Smith")
Si_110.rotate_axis(np.pi/4, 'z-axis', save_rotated_tensors=True)
prefix_str = 'fig16-'
# Use specified parameters to create a waveguide object.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        slab_a_x=slab_a_x, slab_a_y=slab_a_y, slab_b_y=slab_b_y,
                        coat_x=coat_x, coat_y=coat_y, coat2_x=coat2_x, coat2_y=coat2_y,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=Si_110, #plt_mesh=True,
                        material_b=Si_110, material_c=materials.get_material(["Vacuum"),
                        material_d=materials.get_material(["Vacuum"), material_
→e=materials.get_material("Vacuum"),
                        symmetry_flag=False,
                        lc_bkg=lc_bkg, lc_refine_1=lc_refine_1, lc_refine_2=lc_refine_2,
                        lc_refine_3=lc_refine_3, lc_refine_4=lc_refine_4, lc_refine_5=lc_
→refine_5)
# Expected effective index of fundamental guided mode.
n_eff = wguide.material_a.n-0.1
# Calculate Electromagnetic Modes
print("starting EM pump modes")
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff=n_eff, debug=True)
#np.savez('wquide_data', sim_EM_pump=sim_EM_pump)
# npzfile = np.load('wguide_data.npz', allow_pickle=True)
# sim_EM_pump = npzfile['sim_EM_pump'].tolist()
print("starting EM Stokes modes")
sim_EM_Stokes = mode_calcs.fwd_Stokes_modes(sim_EM_pump)
# np.savez('wguide_data2', sim_EM_Stokes=sim_EM_Stokes)
# npzfile = np.load('wguide_data2.npz', allow_pickle=True)
# sim_EM_Stokes = npzfile['sim_EM_Stokes'].tolist()
print("starting EM field plotting ")
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.4, xlim_max=0.4,
                         ivals=[EM_ival_pump,EM_ival_Stokes],
                         ylim_min=0.435, ylim_max=0.435, EM_AC='EM_E', num_ticks=3,
                         prefix_str=prefix_str, pdf_png='png', ticks=True,
                         decorator=emdecorate, quiver_points=20,
                         comps=('Ex','Ey', 'Ez','Eabs','Et'), n_points=2000,_
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.4, xlim_max=0.4,
                         ivals=[EM_ival_pump,EM_ival_Stokes],
                         ylim_min=0.435, ylim_max=0.435, EM_AC='EM_H', num_ticks=3,
                         prefix_str=prefix_str, pdf_png='png', ticks=True,
                         decorator=emdecorate, quiver_points=20,
                         comps=('Hx','Hy', 'Hz','Habs','Ht'), n_points=2000,_

¬colorbar=True)
```

```
# Print the wavevectors of EM modes.
print('k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values), 4))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.Eig_values*((wl_nm*1e-9)/(2.*np.pi)))
print("n_eff = ", np.round(n_eff_sim, 4))
k_AC = np.real(sim_EM_pump.Eig_values[EM_ival_pump] - sim_EM_Stokes.Eig_values[EM_ival_
→Stokes])
print('Intermode q_AC (Hz) \n', k_AC)
shift_Hz = 2e9
# Calculate Acoustic Modes
print("starting acoustic modes")
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_Hz,__
→debug=True)
# np.savez('wguide_data_AC', sim_AC=sim_AC)
# npzfile = np.load('wguide_data_AC.npz', allow_pickle=True)
# sim_AC = npzfile['sim_AC'].tolist()
# Print the frequencies of AC modes.
print('Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
selected_AC_modes = [7, 13, 23]
print("AC modes selected for field plotting", selected_AC_modes)
print("plotting acoustic modes")
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str, ivals=selected_AC_
→modes,
                         num_ticks=3, xlim_min=-.05, xlim_max=-0.05, ylim_min=-.1, ylim_
\rightarrow max=-0.1,
                         quiver_points=20, pdf_png='png',ticks=True, comps=('ux','ut','uz
→', 'uabs'),
                         decorator=acdecorate, colorbar=True)
set_q_factor = 460.
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_
→Q=set_q_factor)
# Mask negligible gain values to improve clarity of print out.
threshold = 1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
```

../../lit_examples/lit_08-fields/EM_E_field_0.png

Fig. 4.82: Fundamental (symmetric TE-like) optical mode fields.

../../lit_examples/lit_08-fields/EM_E_field_1.png

Fig. 4.83: 2nd lowest order (anti-symmetric TE-like) optical mode fields.

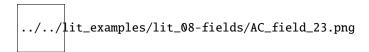


Fig. 4.84: Dominant high gain acoustic mode.

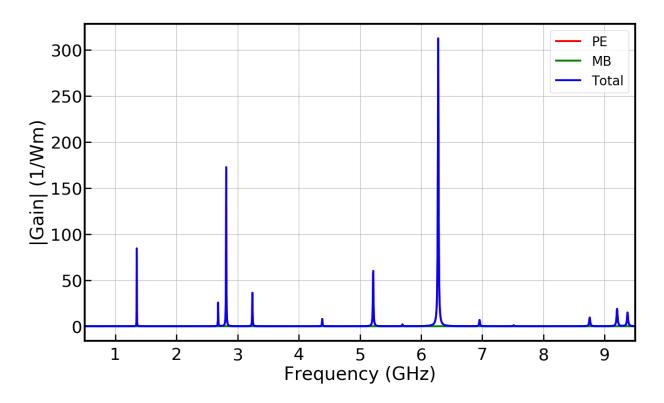


Fig. 4.85: Gain spectra showing gain due to photoelastic effect, gain due to moving boundary effect, and total gain.

4.3.10 LitEx 9 – Morrison et al, Optica (2017): BSBS in a chalcogenide rib waveguide

This example, in simo-lit_09-Morrison-Optica_2017.py, from the Sydney group examines backward SBS in a chalcogenide rib waveguide.

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
    Compact Brillouin devices through hybrid
    integration on Silicon
   Morrison et al.
   https://doi.org/10.1364/OPTICA.4.000847
import time
import datetime
import numpy as np
import sys
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k AC: acoustic wavenumber
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 1550 # Wavelength of EM wave in vacuum.
# Unit cell must be large to ensure fields are zero at boundary.
unitcell_x = 6*wl_nm
unitcell_y = 0.75*unitcell_x
# Waveguide widths.
inc_a_x = 1900
inc_a_y = 680
# Shape of the waveguide.
inc_shape = 'rib_coated'
slab_a_x = 4000
slab_a_y = 1000
coat_x = 200
coat_y = 1000
# Number of electromagnetic modes to solve for.
num\_modes\_EM\_pump = 20
```

```
num_modes_EM_Stokes = num_modes_EM_pump
# Number of acoustic modes to solve for.
num\_modes\_AC = 100
# The EM pump mode(s) for which to calculate interaction with AC modes.
# Can specify a mode number (zero has lowest propagation constant) or 'All'.
EM_ival_pump = 0
# The EM Stokes mode(s) for which to calculate interaction with AC modes.
EM_ival_Stokes = 0
# The AC mode(s) for which to calculate interaction with EM modes.
AC_ival = 'All'
prefix_str = 'lit_09-'
# Use specified parameters to create a waveguide object.
# Note use of rough mesh for demonstration purposes.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        slab_a_x=slab_a_x, slab_a_y=slab_a_y, coat_x=coat_x, coat_y=coat_
∽y ,
                        material_bkg=materials.get_material("Vacuum"),
                        material_a=materials.get_material("As2S3_2017_Morrison"), #_
→waveguide
                        material_b=materials.get_material("Si02_2016_Smith"),
                                                                                   # slab
                        material_c=materials.get_material("SiO2_2016_Smith"),
#lc_bkg=1, lc_refine_1=800.0, lc_refine_2=400.0)
                        lc_bkg=.1, lc_refine_1=10.0, lc_refine_2=10.0)
# Expected effective index of fundamental guided mode.
n_eff = wguide.material_a.n-0.1
# Calculate the Electromagnetic modes of the pump field.
sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
# # np.savez('wguide_data', sim_EM_pump=sim_EM_pump)
# npzfile = np.load('wguide_data.npz')
# sim_EM_pump = npzfile['sim_EM_pump'].tolist()
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.4, xlim_max=0.4, ivals=[EM_ival_pump],
                         ylim_min=0.3, ylim_max=0.3, EM_AC='EM_E', num_ticks=3,
                         prefix_str=prefix_str, pdf_png='png')
# Calculate the Electromagnetic modes of the Stokes field.
sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
# np.savez('wguide_data2', sim_EM_Stokes=sim_EM_Stokes)
# npzfile = np.load('wguide_data2.npz')
# sim_EM_Stokes = npzfile['sim_EM_Stokes'].tolist()
# Print the wavevectors of EM modes.
print('\n k_z of EM modes \n', np.round(np.real(sim_EM_pump.Eig_values),4))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.Eig_values[0]*((wl_nm*1e-9)/(2.*np.pi)))
print("\n n_eff = ", np.round(n_eff_sim, 4))
```

```
k_AC = np.real(sim_EM_pump.Eig_values[EM_ival_pump] - sim_EM_Stokes.Eig_values[EM_ival_
→Stokes])
print('\n AC wavenumber (1/m) = ', np.round(k_AC, 4))
k AC= 2.*9173922.1698
# Calculate Acoustic modes.
shift_Hz = 7.5*1e9 # select the lowest frequency to start FEM search from.
sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_Hz)
# # np.savez('wguide_data_AC', sim_AC=sim_AC)
# npzfile = np.load('wguide_data_AC.npz')
# sim_AC = npzfile['sim_AC'].tolist()
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str,
     num_ticks=3, xlim_min=0.1, xlim_max=0.1, pdf_png='png')
# Print the frequencies of AC modes.
print('\n Freq of AC modes (GHz) \n', np.round(np.real(sim_AC.Eig_values)*1e-9, 4))
set_Q_factor = 190 # set the mechanic Q manually
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB. Also calculate acoustic loss alpha.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival, fixed_
→Q=set_Q_factor)
# Mask negligible gain values to improve clarity of print out.
threshold = -1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Print the Backward SBS gain of the AC modes.
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 7.2 # GHz
freq_max = 8.1 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str, pdf_png='png')
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

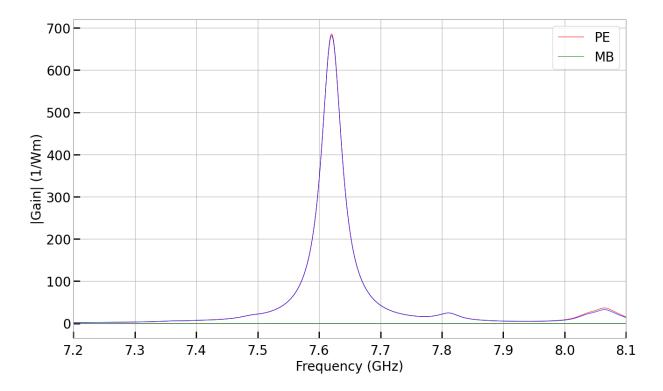


Fig. 4.86: Gain spectra showing gain due to photoelastic effect, gain due to moving boundary effect, and total gain.

4.3.11 LitEx 10 - Wolff et al, Optics Express (2014): SBS in the mid-infrared

This example, in simo-lit_10-Wolff-OptExpress-2014.py and simo-lit_10a-Wolff-OptExpress-2014.py, by C. Wolff and collaborators examines backward SBS in the mid-infrared using germanium as the core material in a rectangular waveguide with a silicon nitride cladding.

The second of these two files illustrates the rotation of the core material from the [100] orientation to the [110] orientation. The second file prints out the full elastic properties of the germanium material in both orientations which are seen to match the values in the paper by Wolff et al.

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
    Germanium as a material for stimulated Brillouin scattering in the mid-infrared
    Wolff et al.
    https://doi.org/10.1364/0E.22.030735
"""

import time
import datetime
import numpy as np
import sys

sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
```

```
import plotting
from fortran import NumBAT
from nbtypes import PointGroup
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k_AC: acoustic wavenumber
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 4000 # Wavelength of EM wave in vacuum.
# Unit cell must be large to ensure fields are zero at boundary.
unitcell_x = 1.5*wl_nm
unitcell_y = 0.75*unitcell_x
# Waveguide widths.
inc a x = 1200
inc_a_y = 550
# Shape of the waveguide.
inc_shape = 'rectangular'
# Number of electromagnetic modes to solve for.
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
# Number of acoustic modes to solve for.
num modes AC = 25
# The EM pump mode(s) for which to calculate interaction with AC modes.
# Can specify a mode number (zero has lowest propagation constant) or 'All'.
EM_ival_pump = 0
# The EM Stokes mode(s) for which to calculate interaction with AC modes.
EM ival Stokes = 0
# The AC mode(s) for which to calculate interaction with EM modes.
AC ival = 'All'
prefix_str = 'lit_10-'
#reuse fields=True  # use saved data
reuse_fields=False # calculate from scratch
# Use specified parameters to create a waveguide object.
# Note use of rough mesh for demonstration purposes.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
#slab_a_x=slab_a_x, slab_a_y=slab_a_y,
#coat_x=coat_x, coat_y=coat_y,
                        material_bkg=materials.get_material("Si3N4_2014_Wolff"),
                        material_a=materials.get_material("Ge_cubic_2014_Wolff"), #_
→waveguide
                        lc_bkg=1, lc_refine_1=50.0, lc_refine_2=50.0)
# Expected effective index of fundamental guided mode.
```

```
n_eff = wguide.material_a.n-0.1
# Calculate the Electromagnetic modes of the pump field.
if not reuse_fields:
  sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
  np.savez('wguide_data', sim_EM_pump=sim_EM_pump)
else:
 npzfile = np.load('wguide_data.npz', allow_pickle=True)
  sim_EM_pump = npzfile['sim_EM_pump'].tolist()
sim_EM_pump.analyse_symmetries(PointGroup.C2V)
sim_EM_pump.set_r0_offset(3.0e-6, -2.250e-6)
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.2, xlim_max=0.2, ivals=[EM_ival_pump],
                         ylim_min=0.2, ylim_max=0.2, EM_AC='EM_E', num_ticks=3,_
→ticks=True.
                         prefix_str=prefix_str)
if not reuse_fields:
  sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
  np.savez('wguide_data2', sim_EM_Stokes=sim_EM_Stokes)
else:
 npzfile = np.load('wguide_data2.npz', allow_pickle=True)
  sim_EM_Stokes = npzfile['sim_EM_Stokes'].tolist()
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print('\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("\n n_eff = ", np.round(n_eff_sim, 4))
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
print('\n AC wavenumber (1/m) = ', np.round(k_AC, 4))
# Calculate Acoustic modes.
shift_Hz = 5.5*1e9 # select the lowest frequency to start FEM search from.
if not reuse_fields:
  sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_
 np.savez('wguide_data_AC', sim_AC=sim_AC)
 npzfile = np.load('wguide_data_AC.npz', allow_pickle=True)
  sim_AC = npzfile['sim_AC'].tolist()
sim_AC.analyse_symmetries(PointGroup.C2V)
sim_AC.set_r0_offset(3.0e-6, -2.250e-6)
```

```
# Print the frequencies of AC modes.
v_nu=sim_AC.nu_AC_all()
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('\{0:3d\} {1:.4e}'.format(i, np.real(nu)*1e-9))
#set_Q_factor = 190 # set the mechanic Q manually
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB. Also calculate acoustic loss alpha.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival #, fixed_
→Q=set_Q_factor
   )
# Mask negligible gain values to improve clarity of print out.
threshold = -1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Print the Backward SBS gain of the AC modes.
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str,
     num_ticks=3, xlim_min=0.1, xlim_max=0.1,
     modal_gains_PE=SBS_gain_PE[EM_ival_pump, EM_ival_Stokes,:],
     modal_gains_MB=SBS_gain_MB[EM_ival_pump, EM_ival_Stokes,:],
     modal_gains=SBS_gain[EM_ival_pump, EM_ival_Stokes,:])
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 5.0 # GHz
freq_max = 11.0 \# GHz
plotting gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
   EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
   prefix_str=prefix_str)
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

```
print("\n Simulation time (sec.)", (end - start))
""" Replicating the results of
    Germanium as a material for stimulated Brillouin scattering in the mid-infrared
    Wolff et al.
    https://doi.org/10.1364/OE.22.030735
"""
import time
```

```
import datetime
import numpy as np
import sys
import copy
sys.path.append("../backend/")
import materials
import objects
import mode_calcs
import integration
import plotting
from fortran import NumBAT
from nbtypes import PointGroup
# Naming conventions
# AC: acoustic
# EM: electromagnetic
# k AC: acoustic wavenumber
start = time.time()
# Geometric Parameters - all in nm.
wl_nm = 4000 # Wavelength of EM wave in vacuum.
# Unit cell must be large to ensure fields are zero at boundary.
unitcell_x = 1.5*wl_nm
unitcell_y = 0.75*unitcell_x
# Waveguide widths.
inc_a_x = 1020
inc_a_y = 700
# Shape of the waveguide.
inc_shape = 'rectangular'
# Number of electromagnetic modes to solve for.
num\_modes\_EM\_pump = 20
num_modes_EM_Stokes = num_modes_EM_pump
# Number of acoustic modes to solve for.
num\_modes\_AC = 100
# The EM pump mode(s) for which to calculate interaction with AC modes.
# Can specify a mode number (zero has lowest propagation constant) or 'All'.
EM_ival_pump = 0
# The EM Stokes mode(s) for which to calculate interaction with AC modes.
EM_ival_Stokes = 0
# The AC mode(s) for which to calculate interaction with EM modes.
AC ival = 'All'
prefix_str = 'lit_10b-'
#reuse_fields=True # use saved data
reuse fields=False # calculate from scratch
Ge_110 = copy.deepcopy(materials.get_material("Ge_cubic_2014_Wolff"))
```

```
print('Initial Ge_100:', Ge_110.full_str())
Ge_110.rotate_axis(np.pi/4., 'y-axis', save_rotated_tensors=True)
print('Rotated Ge_110:', Ge_110.full_str())
# Use specified parameters to create a waveguide object.
# Note use of rough mesh for demonstration purposes.
wguide = objects.Struct(unitcell_x,inc_a_x,unitcell_y,inc_a_y,inc_shape,
                        material_bkg=materials.get_material("Si3N4_2014_Wolff"),
                        material_a=Ge_110,
                        lc_bkg=1, lc_refine_1=50.0, lc_refine_2=50.0)
# Expected effective index of fundamental guided mode.
n_eff = wguide.material_a.n-0.1
# Calculate the Electromagnetic modes of the pump field.
if not reuse_fields:
  sim_EM_pump = wguide.calc_EM_modes(num_modes_EM_pump, wl_nm, n_eff)
 np.savez('wguide_data', sim_EM_pump=sim_EM_pump)
  npzfile = np.load('wguide_data.npz', allow_pickle=True)
  sim_EM_pump = npzfile['sim_EM_pump'].tolist()
sim_EM_pump.analyse_symmetries(PointGroup.C2V)
sim_EM_pump.set_r0_offset(3.0e-6, -2.250e-6)
plotting.plot_mode_fields(sim_EM_pump, xlim_min=0.2, xlim_max=0.2, ivals=[EM_ival_pump],
                         ylim_min=0.2, ylim_max=0.2, EM_AC='EM_E', num_ticks=3,_
→ticks=True,
                         prefix_str=prefix_str)
if not reuse_fields:
  sim_EM_Stokes = mode_calcs.bkwd_Stokes_modes(sim_EM_pump)
 np.savez('wguide_data2', sim_EM_Stokes=sim_EM_Stokes)
  npzfile = np.load('wguide_data2.npz', allow_pickle=True)
  sim_EM_Stokes = npzfile['sim_EM_Stokes'].tolist()
# Print the wavevectors of EM modes.
v_kz=sim_EM_pump.kz_EM_all()
print('\n k_z of EM modes [1/m]:')
for (i, kz) in enumerate(v_kz): print(\{0:3d\} \{1:.4e\}'.format(i, np.real(kz)))
# Calculate the EM effective index of the waveguide.
n_eff_sim = np.real(sim_EM_pump.neff(0))
print("\n n_eff = ", np.round(n_eff_sim, 4))
k_AC = np.real(sim_EM_pump.kz_EM(EM_ival_pump) - sim_EM_Stokes.kz_EM(EM_ival_Stokes))
print('\n AC wavenumber (1/m) = ', np.round(k_AC, 4))
```

```
# Calculate Acoustic modes.
shift_Hz = 5.5*1e9 # select the lowest frequency to start FEM search from.
if not reuse_fields:
  sim_AC = wguide.calc_AC_modes(num_modes_AC, k_AC, EM_sim=sim_EM_pump, shift_Hz=shift_
 np.savez('wguide_data_AC', sim_AC=sim_AC)
else:
 npzfile = np.load('wguide_data_AC.npz', allow_pickle=True)
  sim_AC = npzfile['sim_AC'].tolist()
sim_AC.analyse_symmetries(PointGroup.C2V)
sim_AC.set_r0_offset(3.0e-6, -2.250e-6)
# Print the frequencies of AC modes.
v_nu=sim_AC.nu_AC_all()
print('\n Freq of AC modes (GHz):')
for (i, nu) in enumerate(v_nu): print('\{0:3d\} {1:.4e}'.format(i, np.real(nu)*1e-9))
#set_Q_factor = 190 # set the mechanic Q manually
# Calculate interaction integrals and SBS gain for PE and MB effects combined,
# as well as just for PE, and just for MB. Also calculate acoustic loss alpha.
SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, Q_factors, alpha = integration.gain_
→and_qs(
    sim_EM_pump, sim_EM_Stokes, sim_AC, k_AC,
   EM_ival_pump=EM_ival_pump, EM_ival_Stokes=EM_ival_Stokes, AC_ival=AC_ival #, fixed_
→ Q=set_Q_factor
   )
# Mask negligible gain values to improve clarity of print out.
threshold = -1e-3
masked_PE = np.ma.masked_inside(SBS_gain_PE[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked_MB = np.ma.masked_inside(SBS_gain_MB[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
masked = np.ma.masked_inside(SBS_gain[EM_ival_pump,EM_ival_Stokes,:], 0, threshold)
# Print the Backward SBS gain of the AC modes.
print("\n Displaying results with negligible components masked out")
print("SBS_gain [1/(Wm)] PE contribution \n", masked_PE)
print("SBS_gain [1/(Wm)] MB contribution \n", masked_MB)
print("SBS_gain [1/(Wm)] total \n", masked)
plotting.plot_mode_fields(sim_AC, EM_AC='AC', prefix_str=prefix_str,
     num_ticks=3, xlim_min=0.1, xlim_max=0.1,
     modal_gains_PE=SBS_gain_PE[EM_ival_pump, EM_ival_Stokes,:],
     modal_gains_MB=SBS_gain_MB[EM_ival_pump, EM_ival_Stokes,:],
     modal_gains=SBS_gain[EM_ival_pump, EM_ival_Stokes,:])
# Construct the SBS gain spectrum, built from Lorentzian peaks of the individual modes.
freq_min = 5.0 # GHz
freq_max = 11.0 \# GHz
plotting.gain_spectra(sim_AC, SBS_gain, SBS_gain_PE, SBS_gain_MB, linewidth_Hz, k_AC,
    EM_ival_pump, EM_ival_Stokes, AC_ival, freq_min=freq_min, freq_max=freq_max,
```

```
prefix_str=prefix_str)
end = time.time()
print("\n Simulation time (sec.)", (end - start))
```

../../lit_examples/lit_10-gain_spectra-MB_PE_comps.png

../../lit_examples/lit_10b-gain_spectra-MB_PE_comps.png

CHAPTER

FIVE

PYTHON INTERFACE

This chapter provides a technical auto-generated summary of the NumBAT Python API.

The API consists of five core modules:

- materials, for defining waveguide materials and their properties;
- objects, for constructing waveguides from materials;
- mode_calcs, for the core calculation of electromagnetic and acoustic modes;
- integration, for performing calculations relating to SBS gain;
- plotting, for creating output plots of modes and gain functions.

5.1 materials module

The materials module provides functions for specifying all relevant optical and elastic properties of waveguide materials.

The primary class is materials.Material however users will rarely use this class directly. Instead, we generally specify material properties by writing new .json files stored in the folder backend/materials_data. Materials are then loaded to build waveguide structures using the function materials.get_material().

5.2 objects module

The objects module provides functions for defining and constructing waveguides.

5.3 mode_calcs module

The mode_calcs module is responsible for the core engine to construct and solve the optical and elastic finite-element problems.

5.4 integration module

The integration module is responsible for calculating gain and loss information from existing mode data.

5.5 plotting module

The plotting module is responsible for generating all standard graphs.

CHAPTER

SIX

FORTRAN BACKEND

The intention of NumBAT is that the Fortran FEM routines are essentially black boxes. They are called from mode_calcs.py and return the modal fields. However, there are a few important things to know about the workings of these routines.

6.1 FEM Mode Solvers

6.1.1 Making New Mesh

At some point you may well wish to study a structure that is not described by an existing NumBAT mesh template. In this section we provide an example of how to create a new mesh. In this case we will create a rib waveguide that is has a coating surrounding the guiding region.

Creating a mesh is typically a three step process: first we define the points that define the outline of the structures, then we define the lines connecting the points and the surfaces formed out of the lines. The first step is best done in a text editor in direct code, while the second can be done using the open source program gmsh GUI. The third step involves adding some lines to the NumBAT backend.

To start we are going to make a copy of NumBAT/backend/fortran/msh/empty_msh_template.geo

```
$ cd NumBAT/backend/fortran/msh/
$ cp empty_msh_template.geo rib_coated_msh_template.geo
```

Step 1

Opening the new file in a text editor you see it contains points defining the unit cell. The points are defined as

```
Point(1) = {x, y, z, meshing_value}
```

We start by adding the two points that define the top of the substrate (the bottom will be the bottom edge of the unit cell at $\{0, -h\}$ and $\{d, -h\}$). We use a placeholder slab thickness of 100 nm, which is normalised by the width of the unit cell.

```
slab1 = 100;
s1 = slab1/d_in_nm;
Point(5) = {0, -h+s1, 0, lc};
Point(6) = {d, -h+s1, 0, lc};
```

We then add a further layer on top of the bottom slab, this time using a placeholder thickness of 50 nm. Note that each point must be labeled by a unique number.:

```
slab2 = 50;
s2 = slab2/d_in_nm;
Point(7) = {0, -h+s1+s2, 0, lc};
Point(8) = {d, -h+s1+s2, 0, lc};
```

We next define the peak of the rib, which involves a width and a height,

```
ribx = 200;
riby = 30;
rx = ribx/d_in_nm;
ry = riby/d_in_nm;
Point(9) = {d/2-rx/2, -h+s1+s2, 0, lc_refine_1};
Point(10) = {d/2+rx/2, -h+s1+s2, 0, lc_refine_1};
Point(11) = {d/2-rx/2, -h+s1+s2+ry, 0, lc_refine_1};
Point(12) = {d/2+rx/2, -h+s1+s2+ry, 0, lc_refine_1};
```

Lastly we coat the whole structure with a conformal layer.

```
coatx = 20;
coaty = 20;
cx = coatx/d_in_nm;
cy = coaty/d_in_nm;
Point(13) = {0, -h+s1+s2+cy, 0, 1c};
Point(14) = {d, -h+s1+s2+cy, 0, 1c};
Point(15) = {d/2-rx/2-cx, -h+s1+s2+cy, 0, 1c};
Point(16) = {d/2+rx/2+cx, -h+s1+s2+cy, 0, 1c};
Point(17) = {d/2-rx/2-cx, -h+s1+s2+2*cy+ry, 0, 1c};
Point(18) = {d/2+rx/2+cx, -h+s1+s2+2*cy+ry, 0, 1c};
```

Step 2

To create the lines that connect the points, and the mesh surfaces it is easiest to use gmsh (although it can also be written directly in code). Open your geometry file in gmsh:

```
NumBAT/backend/fortran/msh$ gmsh rib_coated_msh_template.geo
```

Navigate through the side menu to Modules/Geometry/Elementary entities/Add and click "Straight line". Now click consecutively on the point you wish to connect.

Navigate through the side menu to Modules/Geometry/Elementary entities/Add and click "Plane surface". Now click on the boundary of each enclosed area. Remember to separate out your inclusion from the background by highlighting it when asked for "hole boundaries". If the inclusion is complicated it is best to carve up the background area into smaller simpler areas that don't have any inclusions ("holes"), for example see slot coated.

Navigate through the side menu to Modules/Geometry/Physical groups/Add and click "Line". Now click on the lines that make up each side of the unit cell boundary, pressing the "e" key to end your selection once the each side is fully highlighted.

Navigate through the side menu to Modules/Geometry/Physical groups/Add and click "Surface". Now click on all the surfaces of a given material type (in this example there is only one surface per material). It is crucial to remember the order you defined the physical surfaces in. Now open the .geo file in your favorite text editor, scroll to the bottom, and change the numbering of the physical surfaces to start at 1, and to increase by one per surface type. Eg. by tradition 1 is the background material, 2 is the waveguide, 3 is the bottom substrate, and 4 is the cladding.

```
Physical Surface(1) = {24};
Physical Surface(2) = {28};
Physical Surface(3) = {30};
Physical Surface(4) = {26};
```

The important thing is to make a note of the chosen labeling! This is best done by taking a screen-shot of the geometry in gmsh, labeling this with material types and physical dimensions, and then adding this file to the Num-BAT/docs/msh_type_lib folder.

Step 3

The last step is to add your geometry to the make_mesh function in NumBAT/backend/objects.py.

This involves adding a new elif statement for the inc_shape, in this case 'rib_coated', and then adding lines that define how the final mesh will be created based on the template. This involves giving the mesh a name, specifying the number of element types, and modifying the template geometric parameters. See objects.py for details.

One last thing, if the geometry contains only rectangular shapes, and all elements are therefore linear (rather than curvilinear), you should also add the inc_shape name to the self.linear_element_shapes list in objects.py. This will ensure that the most efficient semi-analytic integration routines are used. If NumBAT is not told that the mesh is linear it will default to using numerical quadrature.

6.1.2 FEM Errors

There are 2 main errors that can be easily triggered within the Fortran FEM routines. These cause them to simulation to abort and the terminal to be unresponsive (until you kill python or the screen session).

The first of these is

```
VALPR_64: info_32 != 0 :

VALPR_64: iparam_32(5) =

VALPR_64: number of converged values =

py_calc_modes.f: convergence problem with valpr_64

py_calc_modes.f: You should probably increase resolution of mesh!

py_calc_modes.f: n_conv != nval :
```

Long story short, this indicates that the FEM mesh is too coarse for solutions for higher order Bloch modes (Eigenvaules) to converge. This error is easily fixed by increasing the mesh resolution. Decrease 'lc_bkg' and/or increase 'lc_refine_1' etc.

The second error is

```
Error with _naupd, info_32 = -8
Check the documentation in _naupd.
Aborting...
```

This is the opposite problem, when the mesh is so fine that the simulation is overloading the memory of the machine. More accurately the memory depends on the number of Eigenvalues being calculated as well as the number of FEM mesh points. The best solution to this is to increase 'lc_bkg' and/or decrease 'lc_refine_1' etc.

CHAPTER

SEVEN

INDICES AND TABLES

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