Eigenmode decomposition of arbitrary field configurations

Eigenmode decomposition exploits MEEP's interconnectivity with the MPB mode solver to express an arbitrary time-harmonic field configuration as a superposition of the normal harmonic modes of your structure.

Table of Contents

Theoretical background

Consider a waveguide structure of infinite extent in the x direction with constant cross section in the transverse $[\vec{\rho} = (y, z)]$ directions. For any given angular frequency ω we may solve the time-harmonic Maxwell equations to obtain the *normal modes* of the structure---an

infinite set of vector-valued functions of the transverse coordinates $\{\mathbf{E}_n^{\pm}(\vec{\rho}), \mathbf{H}_n^{\pm}(\vec{\rho})\}$, with associated propagation constants $\{\beta_n\}$, that furnish a complete expansion basis for time-harmonic electromagnetic fields at frequency ω. That is, given any arbitrary frequency-ω field configuration of the form

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r})e^{-i\omega t}$$

$$\mathbf{H}(\mathbf{r},t) = \mathbf{H}(\mathbf{r})e^{-i\omega t}$$

we have the *exact* expansions

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}(x,\vec{\rho}) = \sum_n \left\{\alpha_n^+ \mathbf{E}_n^+(\vec{\rho})e^{+i\beta_n x} + \alpha_n^- \mathbf{E}_n^-(\vec{\rho})e^{-i\beta_n x}\right\} \qquad (1\mathbf{a})$$

$$\mathbf{H}(\mathbf{r}) = \mathbf{H}(x,\vec{\rho}) = \sum_n \left\{\alpha_n^+ \mathbf{H}_n^+(\vec{\rho})e^{+i\beta_n x} + \alpha_n^- \mathbf{H}_n^-(\vec{\rho})e^{-i\beta_n x}\right\} \qquad (1\mathbf{b})$$

where (as discussed further below) the expansion coefficients $\{\alpha_n^{\pm}\}$ may be extracted from knowledge of the time-harmonic fields $\mathbf{E}, \mathbf{H}$ on any cross-sectional surface S transverse to the waveguide.

The idea of mode expansion in MEEP is to compute the $\{\alpha_n^{\pm}\}$ coefficients above for any *arbitrary* time-harmonic field distribution resulting from a MEEP calculation. In calculations of this sort,

- the $\{\mathbf{E}, \mathbf{H}\}$ fields on the RHS of equations (1a,b) above will be frequency-domain fields stored in a `dft_flux` object in a MEEP run, where you will have arranged this `dft_flux` object to live on a cross-sectional surface S transverse to the waveguide;
- the $\{\mathbf{E}_n^{\pm}, \mathbf{H}_n^{\pm}\}$ eigenmodes and $\{\beta_n\}$ propagation constants are computed automatically under the hood by MPB as normal modes of an infinitely extended waveguide with the same cross-sectional material distribution that your structure has on the transverse slice S, and
- the $\alpha_n^{\pm}$ coefficients for as many bands as you like are computed by calling `get_eigenmode_coefficients()`, as discussed below.

C++ function prototype

The basic routine here is

```
std::vector<cdouble>
 fields::get_eigenmode_coefficients(dft_flux *flux,
                                    direction d,
                                    const volume &where,
                                    std::vector<int> ban
                                    kpoint_func k_func=0
                                    void *user_data=0);
```

where

- `flux` is a `dft_flux` object pre-populated with frequency-domain field data resulting from a time-domain MEEP calculation you have run to tabulate fields on a cross-sectional slice perpendicular to your waveguide
- `d` is the direction of power flow in the waveguide
- `where` is a `volume` describing the cross-sectional surface S
- `bands` is an array of integers that you populate with the indices of the modes for which you want expansion coefficients
- `user_func` is an *optional* function you supply to provide initial estimates of the wavevector of a mode with given frequency and band index; its prototype is

```
vec (*kpoint_func)(void user_data, double freq, int ban
```

which returns a `vec` giving your best guess for the wavevector of the `band` th mode at frequency `freq` .

The return value of `get_mode_coefficients` is an array of type `cdouble` (short for `std::complex<double>`), of length `num_freqs * num_bands` , where `num_freqs` is the number of frequencies stored in your `flux` object (equal to `flux->Nfreq`) and `num_bands` is the length of your `bands` input array. The expansion coefficient for the mode with frequency `nf` and band index `nb` is stored in the `nb*num_freqs + nf` slot of this array.

Sample application: tapering between waveguides

As a demonstration of mode expansion, we'll consider the problem of *tapering* between waveguides of different sizes. More specifically, we'll suppose we have incoming power, carried by a single mode (typically the fundamental mode) of a first waveguide (waveguide A)

that we wish to route into a single mode (typically the same mode) of a second, larger, waveguide (waveguide B), losing as little power as possible to reflections or inter-mode scattering in the process. Simply jamming the ends of the two waveguides together will result in significant losses due to the abrupt "impedance" mismatch at the interface, so instead we will consider gradually morphing ("tapering") the waveguide cross section from that of waveguide A to that of waveguide B over a finite length *L*---with a taper profile of smoothness index p---and study the dependence of the mode-to-mode power transfer on L and p.

The calculations described below are implemented by a python code called `wvg-taper.py`, which we will dissect as we proceed through the example. A C++ version of the same calculation is `wvg-taper.cpp`.

First calculation: 2D geometry

As a first example of relatively modest computational cost, we'll consider a 2D (z-invariant) problem in which the smaller and larger waveguides are simply finite-thickness slabs of dielectric material suspended in vacuum. More specifically, power travels in the *x* direction with the fields confined by the dielectric in the *y* direction; the smaller and larger waveguides have thicknesses h_A and $h_B \geq h_A$ and are connected by a taper region of length L, so the slab thickness as a function of x reads

$$h(x) = \begin{cases} h_A, & x < -\frac{L}{2} \\ T_p(x), & x \in \left[-\frac{L}{2}, +\frac{L}{2}\right] \\ h_B, & x > +\frac{L}{2} \end{cases} \qquad (1)$$

where the taper function $T_p(x)$ is a C^p function, i.e. p is the index of its first discontinuous derivative. For the cases $p = 0$ (simple linear taper) and $p = 1$, the taper functions are

$$T_p(x) = \begin{cases} h_0 + \Delta\left(\frac{x}{L}\right), & p = 0 \\ h_0 + \Delta\left[\frac{3}{2}\left(\frac{x}{L}\right) - 2\left(\frac{x}{L}\right)^3\right], & p = 1 \end{cases}$$

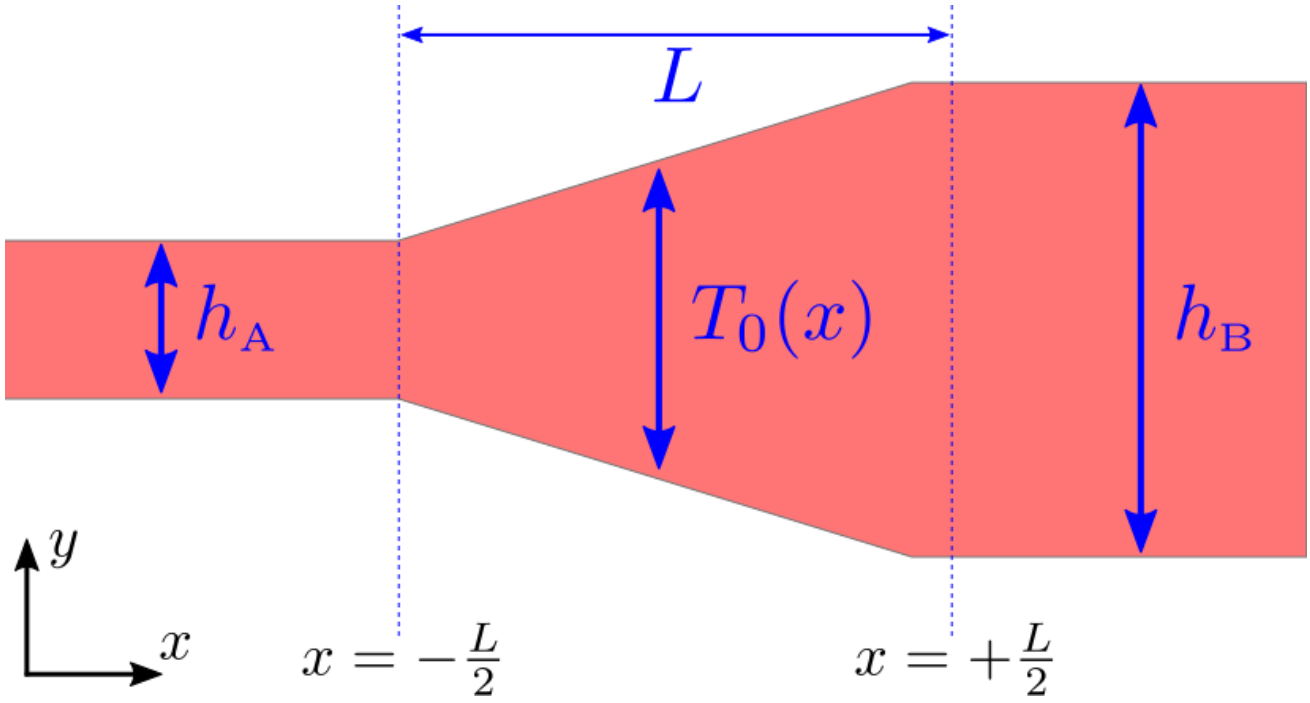
where

$$h_0 \equiv \frac{h_A + h_B}{2}, \qquad \Delta = h_B - h_A$$

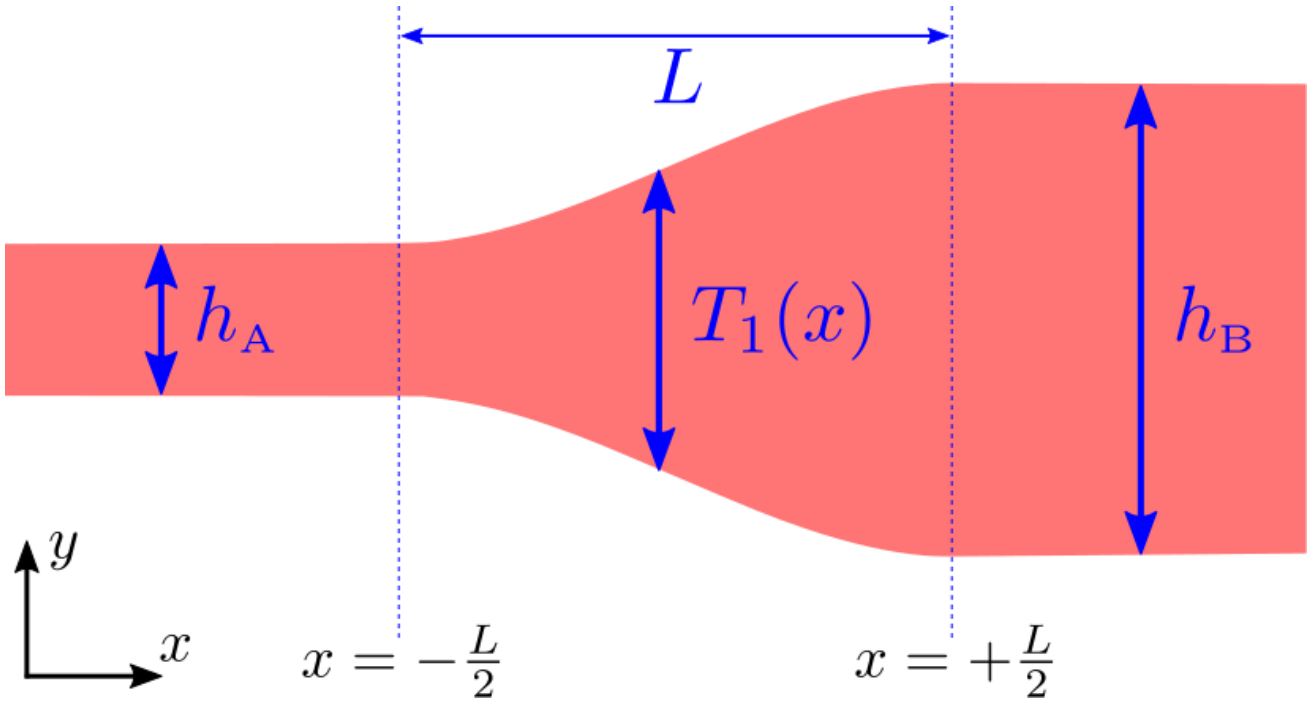
are the average and difference of the smaller and larger waveguide thicknesses.

Here are cartoons of the $p = 0$ and $p = 1$ taper geometries:

***p*=0 Taper**



p=1 Taper



Defining material functions

Because the material geometries we will be studying here are too complicated to be described as assemblies of the usual geometric primitives like blocks and cylinders, we will instead write our own user-defined material function, which inputs the coordinates of a point in space and fills in a medium structure for the material properties at that point. Actually, since the material geometry in this case involves a spatially-varying but otherwise simple (isotropic, linear, lossless) dielectric function, we can get away with the slightly simpler user-defined epsilon function, for which we need only furnish a function of position that returns a scalar relative

permittivity. This is implemented by the `my_eps_func()` routine in `wvg-taper.py`; note that it invokes a subroutine `h_func` that evaluates equation (1) above to compute the x-dependent waveguide width $h(x)$.

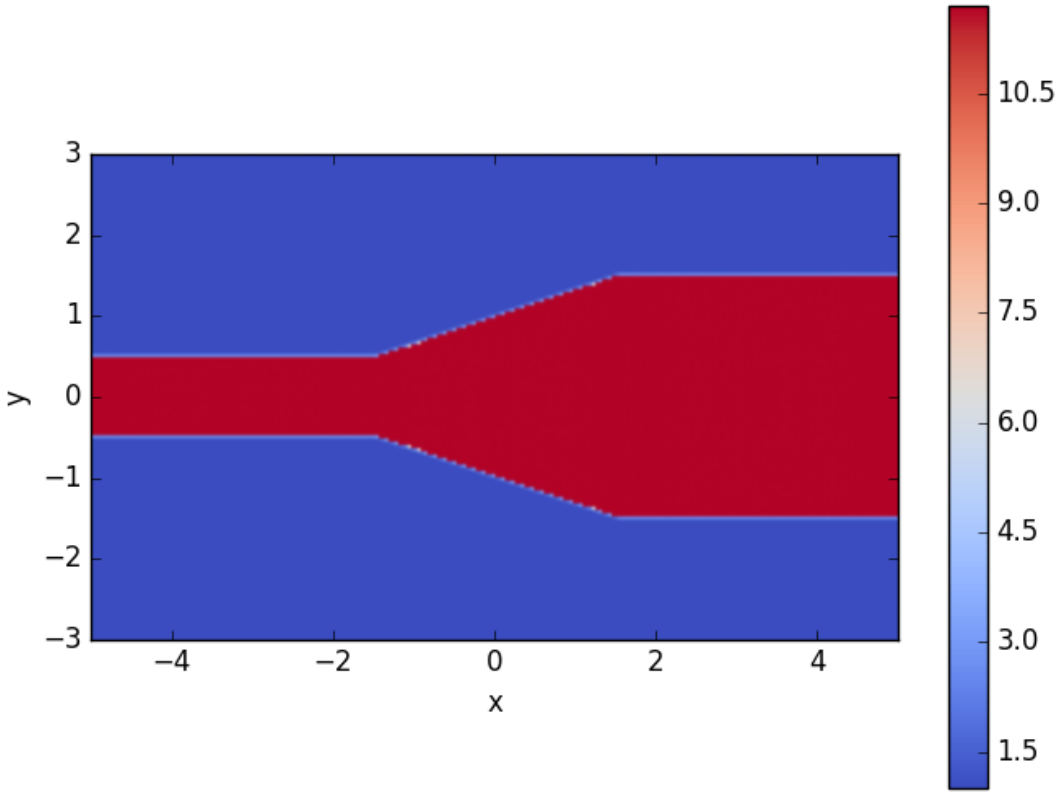
```
##################################################
# x-dependent width of waveguide
##################################################
def h_func(x, L, p, hA, hB):
  x0=x/L
  if (x0 < -0.5):
    return hA;
  if (x0 > +0.5):
    return hB;
  if (p==0):
    return 0.5*(hA+hB) + (hB-hA)*x0;
  else: # if (p==1):
    return 0.5*(hA+hB) + (hB-hA)*x0*(1.5 - 2.0*x0*x0);

##################################################
# user-defined function for position-dependent material
##################################################
def my_eps_func(loc, L, p, hA, hB, eps_out, eps_in):

    if ( abs(loc.y) > 0.5*h_func(loc.x, L, p, hA, hB) ):
     return eps_out;    # outside waveguide
    else:
     return eps_in;     # inside waveguide
```

We can pass `my_eps_func` as the value of the `epsilon_func` keyword argument to the `Simulation` class constructor; however, because this expects a function of just a single argument (the spatial point), we use a `lambda` construction to package the remaining arguments, i.e. something like

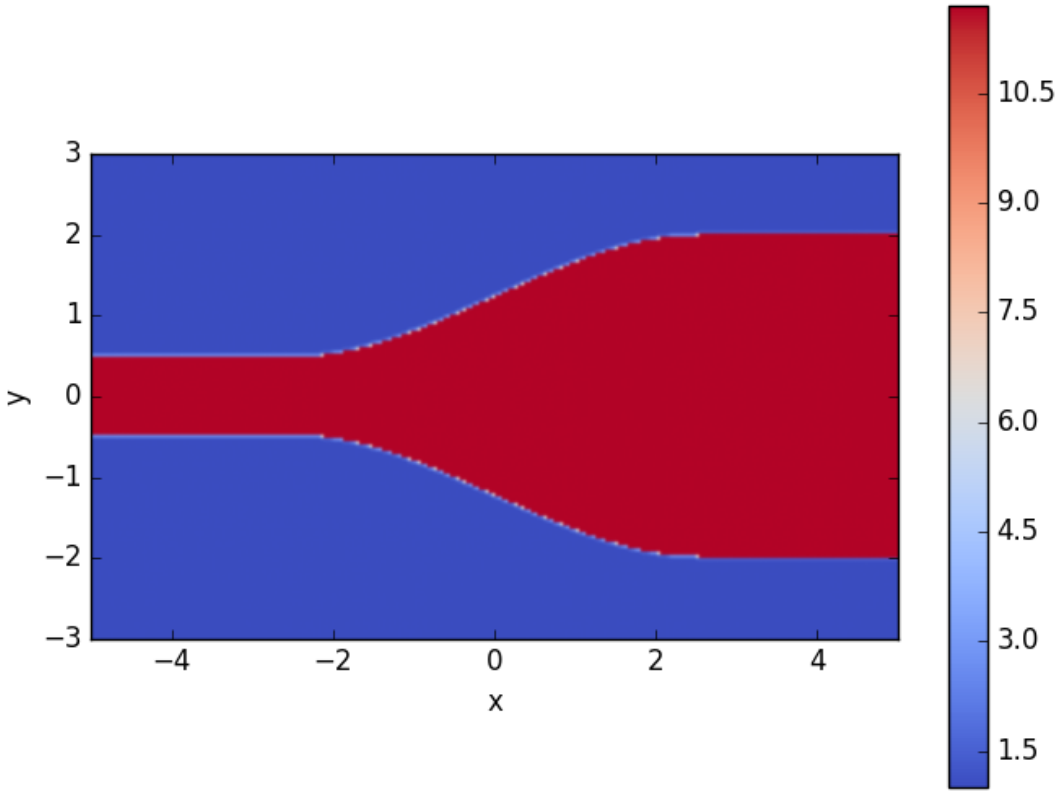
```
eps_func = lambda loc: my_eps_func(loc, L, p, hA, hB,
                                   eps_ambient, eps_wave

sim=mp.Simulation( cell_size=mp.Vector3(2*LX, 2*LY),
                   resolution=resolution,
                   boundary_layers=[mp.PML(DPML)],
                   epsilon_func = eps_func
                 )
```

The `wvg-taper.py` code defines a class called `wvg-taper` that accepts keyword arguments for various geometric parameters and instantiates a `Simulation` object as in the code snippet above. For example, here are a couple of examples involving waveguides and tapers of various geometries:

```
>>> execfile("wvg-taper.py");
>>> wt=wvg_taper(hA=1, hB=3, L=3, p=0);
Initializing structure...
...
time for set_epsilon = 0.242381 s
>>> wt.plot_eps();
```




```
>>> wt=wvg_taper(hA=1, hB=4, L=5, p=1);
Initializing structure...
...
time for set_epsilon = 0.242381 s
>>> wt.plot_eps();
```



Incidentally, the `plot_eps()` class method that produces these plots just calls `Simulation.get_array` to get a `numpy` array of ε values at the grid points, then plots it using the `imshow` routine in matplotlib:

```
def plot_eps(self):

 eps=self.sim.get_array(center    = mp.Vector3(0,0),
                        size      = self.sim.cell_si
                        component = mp.Dielectric)
 plt.figure()
 plt.imshow(eps.transpose())
 plt.show(block=False)
```

Visualizing eigenmode profiles

Next, before doing any timestepping let's take a look at the field profiles of some waveguide modes, for both the smaller and larger waveguides. For this purpose we'll use the `get_eigenmode()` routine to solve for individual eigenmodes, then call `output_mode_fields()`

to write the eigenmode field patterns to HDF5 files, after which we can make plots in matplotlib. This is done in the `plot_modes` method of the `wvg_taper` class:

Insert python code and mode diagrams here

Adding an eigenmode source and timestepping

The next step is to add an eigenmode source inside the smaller waveguide (i.e. a collection of MEEP point sources on a cross-sectional surface whose radiated fields reproduce the fields of a waveguide eigenmode carrying power in the positive X direction), then timestep to accumulate Fourier-domain fields on a cross-sectional plane within the larger waveguide. This entire procedure is carried out by the `get_flux()` method in the `wvg_taper` class, which accepts some optional arguments to fine-tune the source configuration you want.

```
##################################################
# add an eigenmode-source excitation for the #band_n
# of the smaller waveguide, then timestep to accumul
# flux in the larger waveguide.
# if frame_interval>0, a movie is created showing
# the fields on the xy plane with one frame
# every frame_interval time units (in meep time)
##################################################
def get_flux(self, fcen=0.15, df=0.075, nfreq=1, ban
             frame_interval=0):

   #--------------------------------------------------
   # add eigenmode source at midpoint of smaller wav
   #--------------------------------------------------
   f=self.sim.fields;
   res=1.0*self.sim.resolution;
   LX=0.5*self.sim.cell_size.x;
   LY=0.5*self.sim.cell_size.y;
   xA=-0.5*LX;
   xB=+0.5*LX;
   vA=mp.volume( mp.vec(xA, -LY), mp.vec(xA,+LY) )
   vB=mp.volume( mp.vec(xB, -LY), mp.vec(xB,+LY) )
   vC=mp.volume( mp.vec(-LX, -LY), mp.vec(LX,LY) )
   src=mp.GaussianSource(fcen, fwidth=df);
   kpoint=mp.vec(0.426302,0);
   parity=0;
   match_frequency=True;
   tol=1.0e-4;
   amp=1.0;
   f.add_eigenmode_source(mp.Dielectric, src, mp.X,
                          band_num, kpoint, match_fr
                          parity, res, tol, amp);

   #--------------------------------------------------
   # add DFT flux region at midpoint of larger waveg
   #--------------------------------------------------
   fluxB=f.add_dft_flux_plane(vB, fcen-0.5*df, fcen+

   #--------------------------------------------------
   # for DFT flux region for moviemaking if requeste
   #--------------------------------------------------
   fluxC=0
   if frame_interval>0:
     fluxC=f.add_dft_flux_plane(vC, fcen-0.5*df, fce

   #--------------------------------------------------
   # timestep until Poynting flux through larger wav
```

```
        # decayed to 0.1% its max value
        #--------------------------------------------
        pvInterval=1.0; # check PV decay every 1.0 meep t
        nextPVTime=f.round_time() + pvInterval;
        nextFrameTime=f.round_time();
        MaxPV=0.0;
        Stop=False;
        while Stop==False:

          f.step();

          # check for poynting-flux decay at regular inte
          FieldsDecayed=False;
          if f.round_time() > nextPVTime:
              nextPVTime += pvInterval;
              ThisPV=f.flux_in_box(mp.X,vB)
              if (ThisPV > MaxPV):
                 MaxPV = ThisPV;
              elif (ThisPV < 0.001*MaxPV):
                 FieldsDecayed=True;

          # output movie frames at regular intervals if r
          # TODO implement me

          SourcesFinished = f.round_time() > f.last_sourc
          Stop = (SourcesFinished and FieldsDecayed);

        print("finished timestepping at {}".format(f.roun
        return fluxB
```

The return value of `get_flux()` is a `flux` object that may be postprocessed to yield visualization files and/or extract eigenmode expansion coefficients.

Visualizing DFT fields

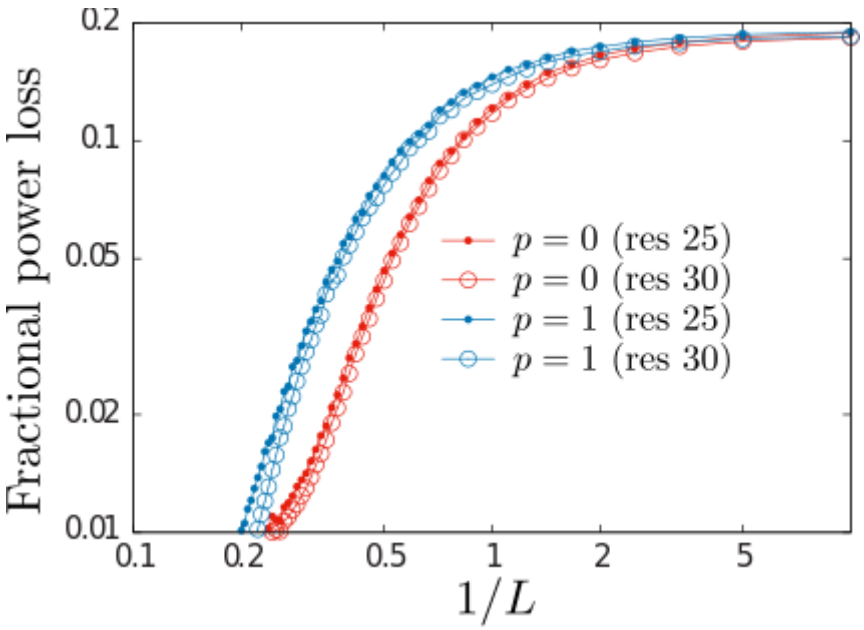
Extracting mode-expansion coefficients

Finally, we call `get_mode_coefficients` to compute the inner product of the MEEP DFT fields in the larger waveguide with each of a user-specified list of eigenmodes of the larger waveguide to compute the fraction of the power carried by each mode.

Insert python code here

Intra-modal scattering losses vs. taper length and smoothness

Repeating this calculation for many taper lengths L and smoothness indices $p = 0, 1$ yields the following plots showing the rate of decay of inter-mode scattering losses as the taper length $L \to \infty$.



Second calculation: Silicon-on-insulator strip waveguide (3D geometry)

Next we consider a setup similar to the one we just studied, but now involving a 3D geometry---a taper between *strip waveguides* defined by patterned silicon strips atop an oxide layer. The geometry is almost identical to that considered in this MPB calculation, but with the distinction that the width w of the silicon strip is no longer constant, but varies from a smaller to a larger width via a length-L taper just as in the 2D calculation we considered above.

FINISH THIS SECTION

Under the hood: How mode expansion works

The theoretical basis of the mode-expansion algorithm is the orthogonality relation satisfied by the normal modes:

$$\langle \mathbf{E}_m^\sigma | \, \mathbf{H}_n^\tau \rangle = C_m \delta_{mn} \delta_{\sigma\tau} \qquad \Big(\{\sigma, \tau\} \in \{+, -\} \Big)$$

where the inner product involves an integration over transverse coordinates:

$$\langle \mathbf{f} | \, \mathbf{g} \rangle \equiv \int_S \left[\mathbf{f}^*(\vec{\rho}) \times \mathbf{g}(\vec{\rho}) \right] \cdot \hat{\mathbf{n}} \, dA \qquad (*)$$

where S is any surface transverse to the direction of propagation and $\hat{\mathbf{n}}$ is the unit normal vector to S (i.e. just $\hat{\mathbf{z}}$ in the case considered above).

FINISH THIS SECTION

Related computational routines

Besides `get_eigenmode_coefficients`, there are a few computational routines in `libmeep` that you may find useful for problems like those considered above.

Routine for computing MPB eigenmodes (in `mpb.cpp`)

```
void *fields::get_eigenmode(double &omega,
                            direction d, const volume
                            const volume &eig_vol,
                            int band_num,
                            const vec &kpoint, bool ma
                            int parity,
                            double resolution,
                            double eigensolver_tol);
```

Calls MPB to compute the `band_num` th eigenmode at frequency `omega` for the portion of your geometry lying in `where` (typically a cross-sectional slice of a waveguide). `kpoint` is an initial starting guess for what the propagation vector of the waveguide mode will be.

Routines for working with MPB eigenmodes (in `mpb.cpp`)

The return value of `get_eigenmode` is an opaque pointer to a data structure storing information about the computed eigenmode, which may be passed to the following routines:

```
// get a single component of the eigenmode field at a gi
std::complex<double> eigenmode_amplitude(const vec &p, v

// get the group velocity of the eigenmode
double get_group_velocity(void *vedata);

// free all memory associated with the eigenmode
void destroy_eigenmode_data(void *vedata);
```

Routines for exporting frequency-domain fields (in `dft.cpp`)

```
void output_flux_fields(dft_flux *flux, const volume w
                        const char *HDF5FileName);

void output_mode_fields(void *mode_data, dft_flux *flu
                        const volume where,
                        const char *HDF5FileName);
```

`output_flux_fields` exports the components of the (frequency-domain) fields stored in `flux` to an HDF5 file with the given file name. `where` is the `volume` passed to the `flux` constructor. In general, `flux` will store data for fields at multiple frequencies, each of which will

`output_mode_fields` is similar, but instead exports the components of the eigenmode described by `mode_data` (which should be the return value of a call to `get_eigenmode`).

Routines for computing overlap integrals (in `dft.cpp`)

```
std::complex<double> get_mode_flux_overlap(void *mode_
                                           dft_flux *f
                                           int num_fre
                                           const volum

std::complex<double> get_mode_mode_overlap(void *mode1
                                           void *mode2
                                           dft_flux *f
                                           const volum
```

`get_mode_flux_overlap` computes the overlap integral (defined by equation (*) above) between the eigenmode described by `mode_data` and the fields stored in `flux` (for the `num_freq` th stored frequency, where `num_freq` ranges from 0 to `flux->Nfreq-1` .) `mode_data` should be the return value of a previous call to `get_eigenmode`.

`get_mode_mode_overlap` is similar, but computes the overlap integral between two eigenmodes. (`mode1_data` and `mode2_data` may be identical, in which case you get the inner product of the mode with itself; by the normalization convention used in MPB, this should equal the group velocity of the mode.)