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.

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Theoretical background¹

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 timeharmonic 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

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

$$\mathbf{H}(\mathbf{r}) = \mathbf{H}(x,ec{
ho}) = \sum_n \left\{ lpha_n^+ \mathbf{H}_n^+(ec{
ho}) e^{+ieta_n x} + lpha_n^- \mathbf{H}_n^-(ec{
ho}) e^{-ieta_n x}
ight\}$$

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 {E, 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 {E_n[±], H_n[±]} eigenmodes and {β_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 α_n^{\pm} coefficients for as many bands as you like are computed by calling get_eigenmode_coefficients(), as discussed below.

Main function prototype

The highest-level interface to the mode-expansion implementation in Meep is the libmeep function meep::fields::get_eigenmode_coefficients, callable from C++ or python. This routine makes use of several lower-level libmeep functions that you may also find useful; these are documented below and their use is illustrated in the tutorial that follows.

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 2 * 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 coefficients $\{\alpha^+, \alpha^-\}$ for the mode with frequency nf and band index nb are stored sequentially starting at slot 2*nb*num_freqs + nf of this array:

```
std::vector<cdouble> coeffs=f.get eigenmode coefficient
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);
int num bands = bands.size();
int num freqs = Flux->Nfreq;
for(int nb=0; nb<num bands; nb++)</pre>
 for(int nf=0; nf<num freqs++; nf++)</pre>
  {
    // get coefficients of forward- and backward-travel
    // waves in eigenmode bands[nb] at frequency #nf
    cdouble AlphaPlus = coeffs[2*nb*num freqs + nf + 0
    cdouble AlphaMinus = coeffs[2*nb*num freqs + nf + 1]
```

```
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 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 w_A and $w_B \ge w_A$ and are connected by a taper region of length L, so the slab thickness as a function of x reads

$$w(x) = egin{cases} w_A, & x < -rac{L}{2} \ T_p(x), & x \in \left[-rac{L}{2}, +rac{L}{2}
ight] \ w_B, & x > +rac{L}{2} \end{cases}$$

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 $p = \{0, 1, 2\}$, the taper functions are

$$T_p(x) = egin{cases} w_0 + \Delta\left(rac{x}{L}
ight), & p = 0 \ w_0 + \Delta\left[rac{3}{2}ig(rac{x}{L}ig) - 2ig(rac{x}{L}ig)^3ig], & p = 1, \ w_0 + \Delta\left[rac{15}{8}ig(rac{x}{L}ig) - 5ig(rac{x}{L}ig)^3 + 6ig(rac{x}{L}ig)^5ig], & p = 2 \end{cases}$$

where

$$w_0\equiv rac{w_A+w_B}{2},\qquad \Delta=w_B-w_A$$

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

Here are pictures of the p = 0, 1, 2 taper geometries for the case of a taper of length L = 4between waveguides of thickness $w_A = 1$ and $w_B = 3$. (See below for the python code that produces these plots.)

p=0 Taper



p=1 Taper







In these figures, the dashed lines at $x = x_{A,B}$ indicate the locations of cross-sectional planes that we will use in our calculation: the plane at $x = x_A$ is where we will place an eigenmode source in our Meep calculation to describe incoming power entering from the smaller waveguide, while the plane at $x = x_B$ is where we will tabulate the Fourier-domain fields in our Meep calculation and determine their overlaps with the eigenmodes of the larger waveguide to compute mode-expansion coefficients.

User-defined material function

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 w_{func} that evaluates equation (3) above to compute the x-dependent waveguide width w(x).

```
# x-dependent width of waveguide
def w func(x, L, p, wA, wB):
 if | == 0:
   return wA if x<0 else wB
 x0=x/L
 if (x_0 < -0.5):
   return wA;
 elif (x0 > +0.5):
   return wB;
 elif p==2:
   return 0.5*(wA+wB) + (wB-wA)*x0*(15.0 + x0*x0*(-40.0))
 elif p==1:
   return 0.5^{*}(wA+wB) + (wB-wA)^{*}x0^{*}(1.5 - 2.0^{*}x0^{*}x0);
 else: # default t p==0, simple linear taper
   return 0.5*(wA+wB) + (wB-wA)*x0;
# user-defined function for position-dependent material
def my eps func(loc, L, p, wA, wB, eps out, eps in):
```

```
if ( abs(loc.y) > 0.5*w_func(loc.x, L, p, wA, wB) ):
    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

.

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's how we made the pictures of the structures shown above: a couple of examples involving waveguides and tapers of various geometries:

```
>>> execfile("wvg-taper.py");
>>> wt=wvg_taper(wA=1, wB=3, L=4, p=0); wt.plot_eps();
>>> wt=wvg_taper(wA=1, wB=3, L=4, p=1); wt.plot_eps();
>>> wt=wvg_taper(wA=1, wB=3, L=4, p=2); wt.plot_eps();
```

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:

Visualizing eigenmode profiles

.

Next, before doing any timestepping let's calculate and plot the field profiles of some waveguide modes, for both the smaller and larger waveguides. This calculation is done by the plot_modes function in the wvg_taper class; you can look at the full Python code to see how it's done in full detail, but here is a synopsys:

• For the lowest-frequency (n = 1) eigenmode of the smaller waveguide, and for the first several eigenmodes of the larger waveguide, we call the meep::fields::get_eigenmode routine in libmeep. This routine inputs a frequency (fcen), an integer (nb), and a meep::volume specifying a cross-sectional slice through our geometry, then invokes MPB to determine the nb th eigenmode at frequency fcen for an *infinitely extended* waveguide with constant cross section matching that of our slice. For example, to compute the n = 1 eigenmode for an infinite waveguide whose cross section matches that of our structure at $x=x_A$, we say

nb = 1; # want first eigenmode vA = mp.volume(mp.vec(xA, -YP), mp.vec(xA,+YP)) # c modeA = f.get_eigenmode(fcen, mp.X, vA, vA, nb, k0, True

The return value of get_eigenmode is a data structure containing information on the computed eigenmode; for example, to get the group velocity or propagation vector of the mode you could say

```
vgrp = get_group_velocity(modeA);
k_vector = get_k(modeA)
```

Alternatively, you can call the $meep::fields::output_mode_fields$ routine to export the E and H components of the eigenmode (at grid points lying in the cross-sectional plane) to an HDF5 file, i.e.

f.output_mode_fields(modeA, fluxA, vA, "modeA");

where fluxA is a meep::dft_flux structure created for the cross section described by vA. This will create a file called modeA.h5 containing values of field components at grid points in vA.

 Having computed eigenmodes with get_eigenmode and written their field profiles to HDF5 files with output_mode_fields, we can read the data back in for postprocessing, such as (for example) plotting eigenmode field profiles. This is done by the plot_fields routine in wvg-taper.py; the basic flow looks something like this:

```
# open HDF5 file
file = h5py.File("modeA.h5", 'r')
# read array of Ey values on grid points
ey = file["ey" + suffix + ".r"][()] + 1j*file["ey" +
# plot real part
plt.plot(np.real(Ey))
```

The plot_modes routine in wvg-taper.py repeats this process for the lowest mode x_A (ModeA1) and the first several modes at x_B (ModeB1...B6) and plots the results:



Adding an eigenmode source and timestepping

The next step is to add an *eigenmode source* inside the smaller waveguide---that is, a collection of Meep point sources, lying on the cross-sectional surface at x_A , whose radiated fields reproduce the fields of a given waveguide eigenmode at a given frequency:

Next, we timestep to accumulate Fourier-domain fields on a cross-sectional plane within the larger waveguide. This is done by the get_flux() method in `wvg_taper.py.

The timestepping continues until the instantaneous Poynting flux through the flux plane at x_B has decayed to 0.1% of its maximum value. When the timestepping is finished, the Fourier-domain fields on the plane at x_B are stored in a dft_flux object called fluxB. and we can call meep::fields::output_flux_fields to export the fields to an HDF5 file, similar to output_mode_fields which we used above:

f.output_flux_fields(fluxB, vB, 'fluxB')

This produces a file called fluxB.h5. One slight difference from output_mode_fields is that dft_flux objects typically store field data for multiple frequencies, so the field-component datasets in the HDF5 file have names like ey_0.r, ey_1.i.

Visualizing DFT fields

Having written Fourier-transform fields to HDF5 files, we can read in the data and plot, as we did previously for mode profiles. In the $wvg_taper.py$ code this is again handled by the plot_fields routine. Here are the results of this process for a few different values of the taper length L and smoothness index p:



Take-home messages:

- For L = 0 (no taper, i.e. abrupt junction) the fields at x_B look nothing like the fields of the lowest eigenmode for the larger structure (second row of this plot); clearly there is significant contamination from higher modes.
- As we increase the taper length and the smoothness index the fields at x_B more and more closely resemble the lowest eigenmode fields, indicating that the taper is working to transfer power adiabatically from lowest mode to lowest mode.

Making movies

The get_flux() routine in the wvg_taper.py supports a keyword parameter frame_interval which, if nonzero, defines an interval (in meep time) at which images of the instantaneous Poynting flux over the entire geometry are to be written to .h5 files. The default is frame_interval=0, in which case these images will not be written.

If you specify (say) frame_interval=1 to get_flux() for a geometry with (say) taper length L = 1.2 and smoothness index p = 1, you will get approximately 100 files with names like



To assemble all these frame files into a movie using FFMPEG, go like this:

ffmpeg -i 'L1.2_p1_f%d.png' L1.2_p1.mpg

(Note that the string %d in the input filename is a wildcard that will match all integer values; it needs to be in single quotes to protect it from shell expansion.)

Here are the movies for the various cases considered above:







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.

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 $L\to\infty$.



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)

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

// 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)

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)

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. (model_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.)

Under the hood: How mode expansion works

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

$$\langle \mathbf{E}_{m}^{\sigma} | \mathbf{H}_{n}^{\tau} \rangle = C_{m} \delta_{mn} \delta_{\sigma\tau} \qquad \left(\{ \sigma, \tau \} \in \{ +, - \} \right) \tag{4}$$

where the inner product involves an integration over transverse coordinates:

$$\langle \mathbf{f} | \, \mathbf{g} \rangle \equiv \int_{S} \left[\mathbf{f}^{*}(\vec{\rho}) \times \mathbf{g}(\vec{\rho}) \right] \cdot \hat{\mathbf{n}} \, dA \tag{5}$$

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). The normalization constant C_m is a matter of convention, but in MPB it is taken to be the group velocity of the mode, v_m , times the area A_S of the cross-sectional surface S:

$$C_m = v_m A_S. (6)$$

Now consider a Meep calculation in which we have accumulated frequency-domain \mathbf{E}^{meep} and \mathbf{H}^{meep} fields on a dft-flux object located on a cross-sectional surface S. Invoking the eigenmode expansion (1) and choosing (without loss of generality) the origin of the x axis to be the position of the cross-sectional plane, the tangential components of the frequencydomain Meep fields take the form

$$\mathbf{E}_{\parallel}^{\text{meep}} = \sum_{n} (\alpha_{n}^{+} + \alpha_{n}^{-}) \mathbf{E}_{n\parallel}^{+}, \tag{7}$$

$$\mathbf{H}_{\parallel}^{\text{meep}} = \sum_{n} (\alpha_{n}^{+} - \alpha_{n}^{-}) \mathbf{H}_{n\parallel}^{+}, \qquad (8)$$

where we used the well-known relations between the tangential components of the forward-traveling and backward-traveling field modes:

$$\mathbf{E}_{n\parallel}^{+}=+\mathbf{E}_{n\parallel}^{-},\qquad \mathbf{H}_{n\parallel}^{+}=-\mathbf{H}_{n\parallel}^{-}.$$

Taking the inner product (5) of both sides of equations (7) and (8) with the ${f H}$ and ${f E}$ fields of each eigenmode and using equations (4) and (6), we find

$$egin{aligned} &\langle \mathbf{H}_m | \, \mathbf{E}^{ ext{meep}}
angle = + (lpha_n^+ + lpha_n^-) v_m A_S \ &\langle \mathbf{E}_m | \, \mathbf{H}^{ ext{meep}}
angle = - (lpha_n^+ - lpha_n^+) v_m A_S \end{aligned}$$

Thus, by evaluating the integrals on the LHS of these equations---numerically, using the MPBcomputed eigenmode fields $\{\mathbf{E}, \mathbf{H}\}_m$ and the Meep-computed fields $\{\mathbf{E}, \mathbf{H}\}^{\text{meep}}\}$ as tabulated on the computational grid---and combining the results appropriately, we can extract the coefficients $\{\alpha_m^{\pm}\}$ in the expansion (1). This calculation is carried out by the routine $\texttt{meep::fields::get_mode_flux_overlap}$. (Although simple in principle, the implementation is complicated by the fact that, in multi-processor calculations, the Meep fields needed to evaluate the integrals are generally not all present on any one processor, but are instead distributed over multiple processors, requiring some interprocess communication to evaluate the full integral.)

The Poynting flux carried by the Meep fields (7,8) may be expressed in the form

$$S_x = rac{1}{2} {
m Re} \, ig \langle {f E}^{
m meep} | \, {f H}^{
m meep} ig
angle = rac{1}{2} \sum_n \left\{ |lpha_n^+|^2 - |lpha_n^-|^2)
ight\} v_n A_S \, \, .$$

and thus the fractional power carried by any one (forward- or backward-traveling) eigenmode is given by

$$ext{fractional power carried by }\pm ext{-traveling mode }n=rac{|lpha_n^{\pm}|^2v_nA_S}{2S_x}$$

1. The theory of waveguide modes is covered in many references; one that we have found useful is Snyder and Love, *Optical Waveguide Theory* (Springer, 1983). ↔