# Meep

*MIT Electromagnetic Equation Propogation*

(this is the old and somewhat obsolete LaTeX manual)

—See http://ab-initio.mit.edu/meep/doc for the latest documentation—

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# Chapter 1

# Discretizing Maxwell's equations

Maxwell's equations in the absence of sources are:

$$\frac{d\mathbf{H}}{dt} = -c\nabla \times \mathbf{E} \tag{1.1}$$

$$\frac{d\mathbf{D}}{dt} = c\nabla \times \mathbf{H} \tag{1.2}$$

If the material is a simple isotropic dielectric, we can simply write $\mathbf{D} = \epsilon\mathbf{E}$ and get on with our lives. Alas, all too often this is not the case! We need to be able to deal with anisotropic dielectrics in which $\epsilon$ is a tensor quantity, nonlinear materials in which $\epsilon$ is a function of $\mathbf{E}$ itself, and polaritonic and polaronic materials in which $\epsilon$ is a function of frequency.

### 1.0.1 Frequency-dependent epsilon

In the case of a frequency-dependent $\epsilon$, we write

$$\mathbf{D} = \epsilon_\infty \mathbf{E} + \mathbf{P} \tag{1.3}$$

where $\mathbf{P}$ is the polarization as a function of time associated with the frequency dependence of $\epsilon$. Actually, in general there will be a set of polarizations, and we'll need a summation here. For simplicity we'll only describe the case of a single polarization in this section. The time dependence of a single polarization is given by

$$\frac{d^2\mathbf{P}}{dt^2} + \gamma\frac{d\mathbf{P}}{dt} + \omega_0^2\mathbf{P} = \Delta\epsilon\ \omega_0^2\mathbf{E} \tag{1.4}$$

where $\gamma$, $\omega_0$ and $\Delta\epsilon$ are material parameters. The energy lost due to the absorption by this resonance is simply

$$\Delta U = \mathbf{P}\frac{d\mathbf{E}}{dt} \tag{1.5}$$

In fact, if one sets $\Delta\epsilon$ to be negative, we can model gain effectively in this way, and in this case keeping track of the energy allows us to model a situation in which there is a depleteable population inversion which is causing the gain—this is the situation of gain with saturation.

### 1.0.2 Nonlinear dielectrics

In nonlinear dielectrics $\mathbf{D}$ is typically given by a cubic function of $\mathbf{E}$.

$$\mathbf{D} = \left(\epsilon + \xi \left|\mathbf{E}\right|^2\right) \mathbf{E} \tag{1.6}$$

### 1.0.3 Anisotropic dielectrics

In anisotropic dielectrics the dielectric constant is a tensor quantity rather than a scalar quantity. In this case we write (FIXME: how to do a tensor in latex?)

$$\mathbf{D} = \bar{\bar{\epsilon}}\mathbf{E} \tag{1.7}$$

$$\mathbf{E} = \bar{\bar{\epsilon}}^{-1}\mathbf{D} \tag{1.8}$$

$$\tag{1.9}$$

### 1.0.4 Putting it all together

Putting it all together, we get a simplified time stepping of something like

$$\frac{d\mathbf{H}}{dt} = -c\nabla \times \mathbf{E} \tag{1.10}$$

$$\frac{d\mathbf{E}}{dt} = \left(\bar{\bar{\epsilon}}_\infty + \mathbf{E} \cdot \bar{\bar{\xi}} \cdot \mathbf{E}\right)^{-1} \left(c\nabla \times \mathbf{H} - \sum_i \frac{d\mathbf{P}_i}{dt}\right) \tag{1.11}$$

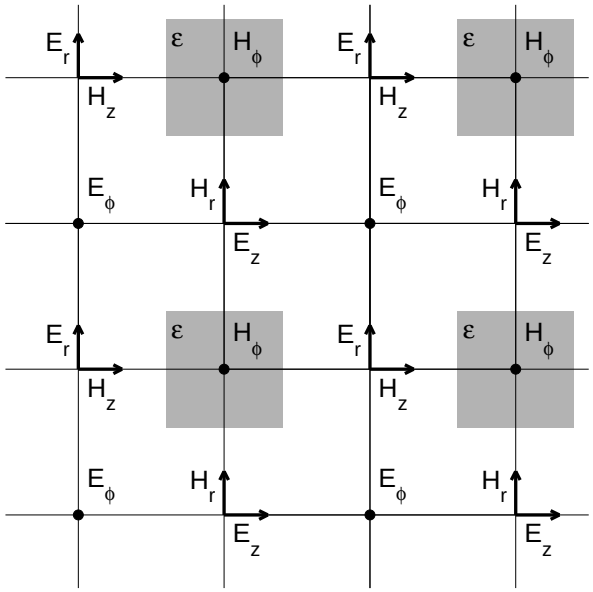
$$\frac{d^2\mathbf{P}_i}{dt^2} + \gamma_i \frac{d\mathbf{P}_i}{dt} + {\omega_0}_i^2 \mathbf{P}_i = \Delta\epsilon_i \, {\omega_0}_i^2 \mathbf{E} \tag{1.12}$$

## 1.1 The Yee lattice

In discretizing Maxwell's equations, we need to put $\mathbf{E}$ and $\mathbf{H}$ on a grid. Because we only need to calculate the curl of these quantities, we only need to know them at limited locations–this gives us the accuracy of a fine grid while only requiring as much data as a grid twice as coarse. This trick is called the Yee lattice. Figure 1.1 shows the Yee lattice in cylindrical coordinates (with $\hat{z}$ being to the right). The gray squares indicate the locations at which $\epsilon$ is stored.

The Yee lattice has the property that all the derivatives needed for $\nabla \times \mathbf{H}$ are known at the Yee lattice points of $\mathbf{E}$. For example, if you look at the $H_\phi$ location. $\frac{dH_\phi}{dt}$ depends on $\frac{dE_r}{dz}$ and $\frac{dE_z}{dr}$. This is great, because $E_r$ is known to the right and left of $H_\phi$, and $E_z$ is known above and below $H_\phi$.

Figure 1.1: Yee lattice in cylindrical coordinates.




The same principle that the Yee lattice does with space, we also do with time. **E** and **H** are known at different times, so that the time derivative of **E** is known at a **H** time and vice versa.

## 1.2 Maxwell's equations in cylindrical coordinates

Here are Maxwell's equations in cylindrical coordinates. We take the fields to be of the form:

$$\mathbf{E}(r, \phi, z) = \mathbf{E}_m(r, z)e^{im\phi}$$

Without further ado:

$$\frac{1}{c}\frac{dH_r}{dt} = \frac{dE_\phi}{dz} - \frac{im}{r}E_z \tag{1.13}$$

$$\frac{1}{c}\frac{dH_\phi}{dt} = \frac{dE_z}{dr} - \frac{dE_r}{dz} \tag{1.14}$$

$$\frac{1}{c}\frac{dH_z}{dt} = \frac{im}{r}E_r - \frac{1}{r}\frac{d(rE_\phi)}{dr} \tag{1.15}$$

$$\frac{\epsilon}{c}\frac{dE_r}{dt} = \frac{im}{r}H_z - \frac{dH_\phi}{dz} \tag{1.16}$$

$$\frac{\epsilon}{c}\frac{dE_\phi}{dt} = \frac{dH_r}{dz} - \frac{dH_z}{dr} \tag{1.17}$$

$$\frac{\epsilon}{c}\frac{dE_z}{dt} = \frac{1}{r}\frac{d(rH_\phi)}{dr} - \frac{im}{r}H_r \tag{1.18}$$

# Chapter 2

# PML

PML (Perfectly Matched Layers) is used to provide absorbing boundary conditions in either the $z$ or $r$ direction. PML consists of a material in which some of the field components are split into two fields, each of which has a conductivity associated with it, which is responsible for the absorption of the PML.

PML is a sort of material that contains a set of conductivities $\sigma_r$, $\sigma_\phi$ and $\sigma_z$. These conductivities are both **E** and **H** conductivities—yes, we have magnetic monopoles moving around in our PML. $\ddot\smile$ Each $\sigma$ causes absorption of radiation in the direction it is named after. Thus $\sigma_\phi$ is small, and almost unnecesary, and is only needed because of the curvature of the radial surface. The value of $\sigma_\phi$ at a given radius is equal to

$$\sigma_\phi(r) = \frac{1}{r}\int_0^r \sigma_r(r)dr \tag{2.1}$$

If we had a IDTD (Infinitesimal Difference Time Domain) code, PML would be perfectly absorbing, regardless of the variation of $\sigma$ with position. However, since meep is a lowly FDTD code, we have to make sure that $\sigma$ varies only slowly from one grid point to the next. We do this by making $\sigma_z$ (for example) vary as $z^2$, with a maximum value of $\sigma_{max}$ right in front of the boundary. At the edge of the PML region is a metalic boundary condition. The optimal value of $\sigma_{max}$ is determined by a tradeoff between reflection off the metallic boundary, caused by too little a $\sigma_{max}$, and reflection off the sigma itself, caused by too large a $\sigma_{max}$, which makes for a large variation of $\sigma$ from one grid point to the next.

Here are the field equations for a PML material:

$$\frac{dH_{r\phi}}{dt} = -c\frac{im}{r}E_z - \sigma_\phi H_{r\phi} \qquad \frac{dH_{rz}}{dt} = c\frac{dE_\phi}{dz} - \sigma_z H_{rz} \tag{2.2}$$

$$\frac{dH_{\phi z}}{dt} = -c\frac{dE_r}{dz} - \sigma_z H_{\phi z} \qquad \frac{dH_{\phi r}}{dt} = c\frac{dE_z}{dr} - \sigma_r H_{\phi r} \tag{2.3}$$

$$\frac{dH_{zr}}{dt} = -c\frac{1}{r}\frac{d(rE_\phi)}{dr} - \sigma_r H_{zr} \qquad \frac{dH_{z\phi}}{dt} = c\frac{im}{r}E_r - \sigma_\phi H_{z\phi} \tag{2.4}$$

$$\epsilon\frac{dE_{r\phi}}{dt} = c\frac{im}{r}H_z - \sigma_\phi E_{r\phi} \qquad \epsilon\frac{dE_{rz}}{dt} = -c\frac{dH_\phi}{dz} - \sigma_z E_{rz} \tag{2.5}$$

$$\epsilon\frac{dE_{\phi z}}{dt} = c\frac{dH_r}{dz} - \sigma_z E_{\phi z} \qquad \epsilon\frac{dE_{\phi r}}{dt} = -c\frac{dH_z}{dr} - \sigma_r E_{\phi r} \tag{2.6}$$

$$\epsilon\frac{dE_{zr}}{dt} = c\frac{1}{r}\frac{d(rH_\phi)}{dr} - \sigma_r E_{zr} \qquad \epsilon\frac{dE_{z\phi}}{dt} = -c\frac{im}{r}H_r - \sigma_\phi E_{z\phi} \tag{2.7}$$

# Chapter 3

# Of polaritons and plasmons

Most real materials, at least in some frequency range, have polarizations that are not actually instantaneously proportional to the local electric field. We model these polaritonic and plasmonic effects by introducing one or more additional polarization fields, to be propogated along with the electric and magnetic field. The polarization field, $\mathbf{P}$, is a vector field which exists on the electric field Yee lattice points.

The polarization field obeys a second order differential equation, which means that we need to keep track of the polarization at two time steps, in order to integrate it.

$$\frac{d^2\mathbf{P}}{dt^2} + \gamma\frac{d\mathbf{P}}{dt} + \omega^2\mathbf{P} = \Delta\epsilon\ \omega^2\mathbf{E} \tag{3.1}$$

To this, we need add one more term to maxwell's equation for $\mathbf{E}$:

$$c\nabla \times \mathbf{H} = \epsilon_\infty\frac{d\mathbf{E}}{dt} + \frac{d\mathbf{P}}{dt} \tag{3.2}$$

So far, the polarization is beautifully simple. However, we would love to be able to put polaritonic materials into our PML regions, and unfortunately in the PML region the electric field has been split into two components, so we need to figure out which of the two components gets the contribution from $\frac{d\mathbf{P}}{dt}$. The obvious solution to this (well, maybe not exactly obvious, but it is the solution) is to split the polarization field also into two components in the PML region, just as we split the electric and magnetic fields.

The electric field propogation equations in PML then become:

$$\epsilon\frac{dE_{r\phi}}{dt} = c\frac{im}{r}H_z - \sigma_\phi E_{r\phi} - \frac{dP_{r\phi}}{dt} \tag{3.3}$$

$$\epsilon\frac{dE_{\phi z}}{dt} = c\frac{dH_r}{dz} - \sigma_z E_{\phi z} - \frac{dP_{\phi z}}{dt} \tag{3.4}$$

$$\epsilon\frac{dE_{zr}}{dt} = c\frac{1}{r}\frac{d(rH_\phi)}{dr} - \sigma_r E_{zr} - \frac{dP_{zr}}{dt} \tag{3.5}$$

$$\epsilon \frac{dE_{rz}}{dt} = -c\frac{dH_\phi}{dz} - \sigma_z E_{rz} - \frac{dP_{rz}}{dt} \tag{3.6}$$

$$\epsilon \frac{dE_{\phi r}}{dt} = -c\frac{dH_z}{dr} - \sigma_r E_{\phi r} - \frac{dP_{\phi r}}{dt} \tag{3.7}$$

$$\epsilon \frac{dE_{z\phi}}{dt} = -c\frac{im}{r}H_r - \sigma_\phi E_{z\phi} - \frac{dP_{z\phi}}{dt} \tag{3.8}$$

# Chapter 4

# Hints for writing finite difference time domain code

(Or *Things I forgot many times, so I wrote down so maybe I won't make the same mistake again.*)

There is just one rule to remember when writing time domain code, and that is (as Lefteris has repeatedly told me) "Always know *when* each equation is evaluated." The trick, of course, lies in knowing how to apply this rule, and remembering to actually apply it (and I think the latter is perhaps harder than the former).

As an example, I'll convert a PML polariton equation into a finite difference equation taken from equation 3.8 of chapter 3.

$$\epsilon \frac{dE_{z\phi}}{dt} = -c\frac{im}{r}H_r - \sigma_\phi E_{z\phi} - \frac{dP_{z\phi}}{dt}$$

If we consider the **E** timesteps to be at times $n$, $n+1$ etc., then this equation needs to be evaluated at time $n+\frac{1}{2}$. This is no problem for most of the terms, but it means that the $\sigma_\phi E_{z\phi}$ term needs to be an average of its values at time $n$ and $n+1$. In short (taking $\Delta t$ to be unity)...

$$\epsilon(E_{z\phi}^{n+1} - E_{z\phi}^{n}) = -c\frac{im}{r}H_r^{n+\frac{1}{2}} - \sigma_\phi(E_{z\phi}^{n+1} + E_{z\phi}^{n}) - (dP_{z\phi}^{n+1} - dP_{z\phi}^{n})$$

Simplifying a tad gives

$$E_{z\phi}^{n+1} - E_{z\phi}^{n} = \frac{1}{\epsilon + \frac{1}{2}\sigma_\phi}\left(-c\frac{im}{r}H_r^{n+\frac{1}{2}} - \sigma_\phi E_{z\phi}^{n} - (dP_{z\phi}^{n+1} - dP_{z\phi}^{n})\right)$$

Basically, that is all there is to it. You now have the equation to determine $E_{z\phi}^{n+1}$ from $E_{z\phi}^{n}$, $\frac{im}{r}H_r^{n+\frac{1}{2}}$, $dP_{z\phi}^{n+1}$ and $dP_{z\phi}^{n}$.

# Chapter 5

# Tutorial

## 5.1 A simple 2D system.

This example is intended to let you quickly get started using meep to run a simple calculation. As such, it will include within it the complete code of the example itself. Meep is a C++ library, so your control file is a small C++ program.

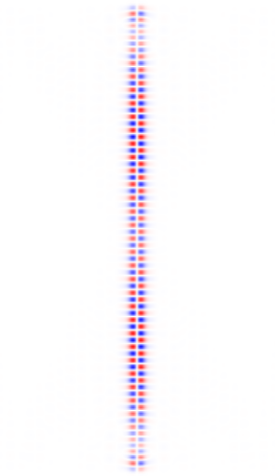
At the beginning of your control file, you have to include the "meep.h" header and use the "meep" namespace...

```
#include <meep.hpp>
using namespace meep;
```

Next we create a function to define epsilon. This function accepts a "vec" argument, and returns a double, which is the value of epsilon. For this example, we use an index-guided waveguide with some air slits cut in it. You can choose whatever units you like in which to define your structure. In this case we choose the width of the waveguide as our unit, which is also equal to 1 micron.

```
const double half_cavity_width = 0.5*0.68, air_slit_width = 0.38,
             grating_periodicity = 0.48,
             half_waveguide_width = 1.0,
             num_air_slits = 15.0,
             high_dielectric = 12.0, low_dielectric = 11.5;
const double pml_thickness = 1.0;
const double x_center = 7.7 + pml_thickness;
const double y_center = 10.5 + pml_thickness;
double eps(const vec &rr) {
  // Displacement from center of cavity is r:
  const vec r = rr - vec(x_center, y_center);
  // First the air slits:
  double dx = fabs(r.x()) - half_cavity_width;
  if (dx < num_air_slits*grating_periodicity && dx > 0.0) {
```

Figure 5.1: $E_z$



```
    while (dx > grating_periodicity) dx -= grating_periodicity;
    if (dx < air_slit_width) return 1.0;
  }
  // Now check if the y value is within the waveguide:
  if (fabs(r.y()) < half_waveguide_width) return high_dielectric;
  // Otherwise we must be in the surrounding low dielectric:
  return low_dielectric;
}
```

The main function should always start by creating an initialize object. This object is responsible for setting up MPI if we are running on multiple processors, and cleaning up properly when it is deleted (which means we are done).

```
int main(int argc, char *argv[]) {
  initialize mpi(argc, argv);
```

The "s" structure defines the contents of the unit cell. It needs a volume, which includes the size of the grid and the resolution, as well as the epsilon function we defined earlier. Here we also choose to use PML absorbing boundary conditions in all directions, since we are interested in the high Q mode in the cavity.

```
  const double amicron = 10; // a micron is this many grid points.
  const volume vol = voltwo(2*x_center, 2*y_center, amicron);
  const symmetry S = mirror(Y, vol) + rotate2(Y, vol);
  structure s(vol, eps, pml(pml_thickness), S);
```

To avoid clutter, we'll create a directory to hold the output. The function `make_output_directory` creates a directory based on the name of the example

program along with an extension. It also backs up the C++ source file if it can find it. If the directory already exists, then it reuses it, unless the C++ control file has changed, in which case it creates a new one.

```
  const char *dirname = make_output_directory(__FILE__);
  s.set_output_directory(dirname);
```

The structure only holds the epsilon. We will also need a "fields" object to hold our electric and magnetic fields. We add a point source oriented in the $E_z$ direction, located in the center of our cavity.

```
  fields f(&s);
  const double wavelength = 1.72;
  const double freq = 1.0/wavelength;
  f.add_point_source(Hy, freq, 10.0, 0.0, 5.0, vec(x_center,y_center));
```

I'm not interested in seeing the source itself, so I'll keep time stepping until the current time is greater than the last time at which the source is running.

```
  while (f.time() < f.last_source_time()) f.step();
```

Now we'll wait a bit (to let the low-Q modes die off) and then take a snapshot of the fields in HDF5 format.

```
  while (f.time() < 200.0) f.step();
  f.output_hdf5(Hx, f.total_volume());
  f.output_hdf5(Hy, f.total_volume());
  f.output_hdf5(Ez, f.total_volume());
}
```

And now we're done, although you might wonder if we've done anything worthwhile, since all we got out of this was a picture...

## 5.2 A considerably more complicated 2D example.

This example demonstrates a lot more of what you can do using meep. The system is the same as in the previous example, but this time we will calculate the quality factor of the cavity. Again, the entire control file will be included here, but I'll skip over sections that have already been explained.

```
#include <meep.hpp>
using namespace meep;

const double half_cavity_width = 0.5*0.68, air_slit_width = 0.38,
             grating_periodicity = 0.48,
             half_waveguide_width = 1.0,
             num_air_slits = 15.0,
```

```
            high_dielectric = 12.0, low_dielectric = 11.5;
const double pml_thickness = 1.0;
const double x_center = 7.7 + pml_thickness;
const double y_center = 10.5 + pml_thickness;
double eps(const vec &rr) {
  // Displacement from center of cavity is r:
  const vec r = rr - vec(x_center, y_center);
  // First the air slits:
  double dx = fabs(r.x()) - half_cavity_width;
  if (dx < num_air_slits*grating_periodicity && dx > 0.0) {
    while (dx > grating_periodicity) dx -= grating_periodicity;
    if (dx < air_slit_width) return 1.0;
  }
  // Now check if the y value is within the waveguide:
  if (fabs(r.y()) < half_waveguide_width) return high_dielectric;
  // Otherwise we must be in the surrounding low dielectric:
  return low_dielectric;
}
```

This time we use the `deal_with_ctrl_c();` function. This is a handy utility function that is useful when running your meep code interactively. It traps the SIGINT signal, so when you hit cntl-C, rather than simply exiting, the global variable `interrupt` is incremented. If you really want to exit, just hit cntl-C again, and when `interrupt` reaches 2, the program will exit.

```
int main(int argc, char *argv[]) {
  initialize mpi(argc, argv);
  deal_with_ctrl_c();
  const double amicron = 10; // a micron is this many grid points.
  const volume vol = voltwo(2*x_center, 2*y_center, amicron);
  const symmetry S = mirror(Y, vol) + rotate2(Y, vol);
  structure s(vol, eps, pml(pml_thickness), S);
  const char *dirname = make_output_directory(__FILE__);
  s.set_output_directory(dirname);
  fields f(&s);
  const double wavelength = 1.72;
  const double freq = 1.0/wavelength;
  f.add_point_source(Hy, freq, 5.0, 0.0, 5.0, vec(x_center,y_center));
```

We add an additional check below "`&&` interrupt!" so that when the user hits cntl-C we exit the loop.

```
  while (f.time() < f.last_source_time() && !interrupt) f.step();
  f.output_hdf5(Ez, f.total_volume());
  while (f.time() < 400.0 && !interrupt) f.step();
```

This time we're going to run the simulation longer, so we would like to get occasional informative messages. To do this we define a variable to hold the next time we want to print a message.

```
double next_print_time = 500.0;
```

To calculate the $Q$ of our cavity, we use a monitor point `p`. We also store the value of $H_y$ at our monitor point in a file named "hy" periodically. We create this file using `create_output_file`, which creates and opens a file for writing in the given output directory. This utility function works properly whether we are running in parallel or not.

```
monitor_point *p = NULL;
FILE *myout = create_output_file(dirname, "hy");
while (f.time() <= 2000.0 && !interrupt) {
  // Now we'll start taking data!
  f.step();
```

To get the monitor point data we use the `get_new_point` method of `fields`. This ends up creating a linked list containing the values of the field at the monitor point as a function of time, which we will later use to run harminv and get the $Q$.

```
  p = f.get_new_point(vec(x_center,y_center), p);
```

We use the `get_component` method to extract the (complex) fields from the monitor point so we can print them. We use the `master_fprintf` function because we only want to get one copy of the information even if we're running in parallel.

```
  master_fprintf(myout, "%g\t%g\t%g\n", f.time(),
                 real(p->get_component(Hy)),
                 imag(p->get_component(Hy)));
```

Every time we reach the `next_print_time` we print out a copy of the $E_z$ fields, along with a little message indicating the time and the total energy (which should be decaying at this point). The function `master_printf` is a utility function that works basically like `printf`, except that when running in parallel only one of the processors (the "master") does the printing. You should use this function rather than something like "`if (my_rank()==0) printf(...)`", since the latter can cause problems if the arguments to printf require synchronization between the processes.

```
  if (f.time() >= next_print_time) {
    f.output_hdf5(Ez, f.total_volume());
    master_printf("Energy is %g at time %g\n",
                  f.total_energy(), f.time());
    next_print_time += 500.0;
  }
}
```

Files which are opened with `create_output_file` need to be closed with `master_fclose`, which does the Right Thing when running in parallel.

Figure 5.2: Contents of "freqs" file

```
0.651297 7.26245e-07 -896801 0.00821062 -0.000426369
```

```
  master_fclose(myout);
```

Having collected all the monitor point data, we now want to run harminv[1] on it to find the $Q$ of our resonant cavity. The `harminv` method gives us the complex amplitudes, the frequencies and the decay rates. The decay rate is given in the same units as the frequency, so you could choose to view it as the imaginary part of the frequency if you like.

This harminv step is the real reason for using the ctrl-C trick, since if while running this example we get impatient and decide we have enough data we can just hit ctrl-C and get the results using what data we have. This means you can just set the code to run for an excessively long time without risking losing everything if you lose patience.

In case you're wondering about the "`\begin{verbatim}`", it's there so I can easily include the output in this manual (see Figure 5.2).

```
  complex<double> *amp, *freqs;
  int num;

  FILE *myfreqs = create_output_file(dirname, "freqs");
  master_fprintf(myfreqs, "\\begin{verbatim}\n");
  master_printf("Harminving Hy...\n");
  interrupt = 0; // Harminv even if we were interrupted.
  p->harminv(Hy, &amp, &freqs, &num, 0.8*freq, 1.2*freq, 5);
  for (int i=0;i<num;i++) {
    master_fprintf(myfreqs, "%g\t%g\t%g\t%g\t%g\n",
                   real(freqs[i]), imag(freqs[i]),
                   -real(freqs[i])/imag(freqs[i]),
                   real(amp[i]), imag(amp[i]));
  }
  master_fprintf(myfreqs, "%cend{verbatim}\n", '\\');
  master_fclose(myfreqs);
  delete[] dirname;
}
```

[1] If you don't know what harminv is, I'm not going to explain it here, so you may as well ask me in person (or even better, ask Steven...

## 5.3 Baby's First Bandstructure

In this example we calculate the lowest four TE modes of a simple hollow metallic waveguide of radius one.

```
int main(int argc, char *argv[]) {
  initialize mpi(argc, argv);
  FILE *ban = master_fopen("bands", "w");
  structure s(volcyl(1.0, 0.0, rad), eps);
  for (int m=0;m<3;m++) {
    for (double k=0.0; k<= 1.01; k += 0.25) {
      master_printf("Working on k of %g and m = %d with a=%d...\n",
                    k, m, rad);
      fields f(&s, m);
      f.use_bloch(k);
```

There are a few tricks you should know before you decide to go about calculating a band structure. One of the biggest problems in calculating a band structure in a time domain code is that of exciting all the modes you are interested in. Meep makes this easy with a couple of "fields" methods, `initialize_with_n_te`, and `initialize_with_n_tm`. These initialize the field with the n lowest TE and TM modes respectively.

```
      f.initialize_with_n_te(4);
```

The band structure code itself begins with a call to `prepare_for_bands`, which allocates space to store the field data, which is later used for the band structure calculation. Its third argument is the maximum frequency you are interested in.

```
      double fmax = 1.0, qmin = 200;
      f.prepare_for_bands(0, ttot, fmax, qmin);
      for (int t=0;t<ttot;t++) {
```

The second band structure function is `record_bands`, which just copies the fields into the already allocated arrays for future use.

```
        f.record_bands();
        f.step();
      }
```

Finally, the band structure is actually computed and output by the method `output_bands`. The key thing to know about `output_bands` is that its last argument should be something like twice the number of modes which have a frequency below your maximum. Rounding this number up slows the code down considerably, but can sometimes fix problems where harminv (which is used internally) doesn't find the modes correctly. Usually, however, when harminv fails it means you are misunderstanding something (for example, fmax may be less than the lowest frequency mode).

```
      f.output_bands(ban, "band", 35);
    }
  }
  master_fclose(ban);
}
```

## 5.4 Computing the band structure of an omniguide

In this section we give as an example of a more complicated band structure, a computation of the band structure of an omniguide. The output of this program is shown in Figure 5.4.

```
const int num_layers = 3;
const double rcore = 3.0;

double guided_eps(const vec &v) {
  double rr = v.r() - rcore;
  if (rr > num_layers + 0.3) return 1.0; // outside the entire waveguide
  if (rr < 0.0) return 1.0;   // vacuum in the core
  while (rr > 1.0) rr -= 1.0; // calculate (r - rcore) % 1
  if (rr < 0.3) return 21.16; // in the high dielectric
  return 1.6*1.6;             // in the low dielectric
}
double vacuum_eps(const vec &v) { return 1.0; }
```

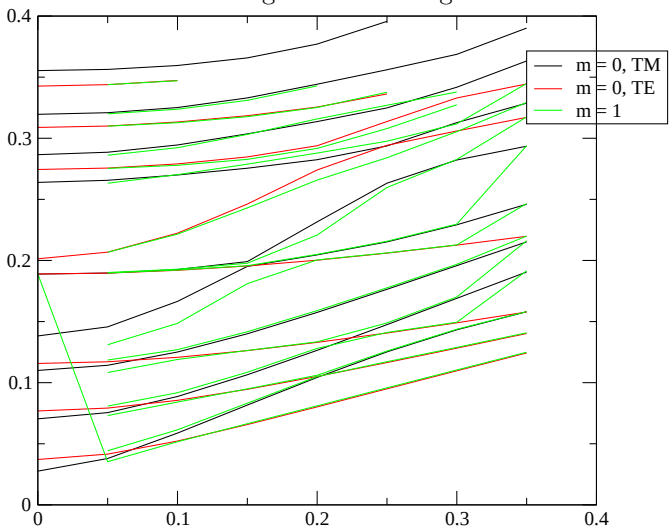
For this band structure example, we use the grace object to create our plot.

```
  grace g("bands", dirname);
  g.set_range(0.0, 0.35, 0.0, 0.35);
```

Since the m = 0 modes are pure TE or TM, it makes sense to calculate the two polarizations separately. Not only does this give us more interesting output, but it doesn't cost us any time, to speak of, and actually makes the band structure much easier to converge. However, for brevity, I won't include here in the manual computation of the TM modes, but will skip straight to the TE modes.

```
  for (int m=0;m<2 && !interrupt;m++) {
    g.new_set();
    char m_string[30];
    if (m) snprintf(m_string, 30, "m = %d", m);
    else snprintf(m_string, 30, "m = 0, TE");
    g.set_legend(m_string);
    for (double k=0.0;k<0.351 && !interrupt;k+=0.05) {
```

Figure 5.3: Omniguide band structure.




In order to populate the modes that we are interested in, we first populate the modes of an empty waveguide (whose modes are known), and then adiabatically transform from that waveguide into our omniguide structure.

```
printf("Working on k of %g and %s with a=%d...\n", k, m_string, a);
fields f(&vac, m);
f.use_bloch(k);
f.verbose(1);
f.phase_in_material(&s, 1000);
```

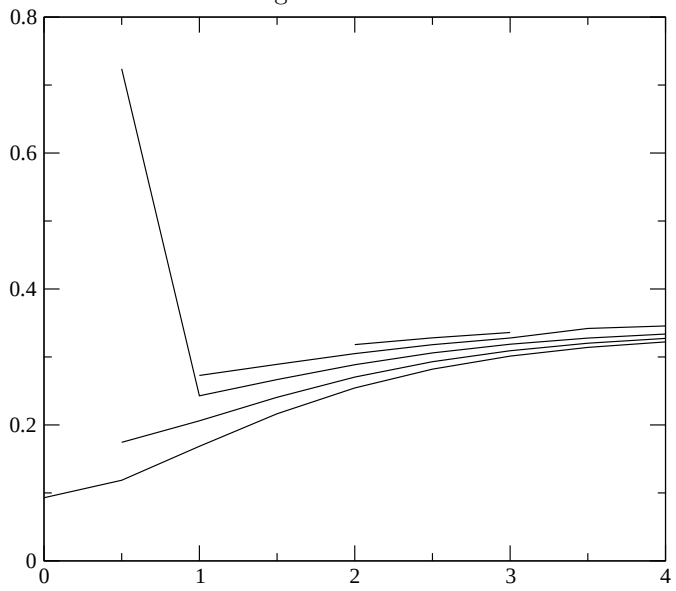
We initialize the fields with both TE and TM modes, and then phase in the epsilon as usual, and then do the actual phasing in of the structure.

```
f.initialize_with_n_te(9);
if (m) f.initialize_with_n_tm(9);
while (f.is_phasing() && !interrupt) f.step();
```

Again, the band structure code is pretty normal, with the only real difference being that in this case we *really* want to have specify a large $Q_{min}$, to help meep to distinguish between real modes and spurious noise. Note that we are using metallic boundary conditions, so all physical modes should have infinite lifetime.

```
f.prepare_for_bands(veccyl(4.801,0.0), ttot, .35, 300, 0.0);
f.prepare_for_bands(veccyl(1.801,0.0), ttot, .35, 300, 0.0);
f.prepare_for_bands(veccyl(2.801,0.0), ttot, .35, 300, 0.0);
const double stoptime = f.time() + ttot;
while (f.time() < stoptime && !interrupt) {
```

Figure 5.4: Polariton band structure.




```
    f.record_bands();
    f.step();
  }
```

Finally, we just need to compute and output the bands. We are careful here to keep in mind that when $m > 0$, there are twice as many bands, since there are both TM and TE modes.

```
  f.grace_bands(&g, m?80:40);
}
```

The band is actually printed to disk only when the grace object is destroyed, which in this case happens just before the program exits.

## 5.5 Band structure of a polariton

Here we compute and plot the band structure of a polariton material. We look at a simple metallic waveguide filled with a polaritonic material. The material we look at has an epsilon of 13.4 and a longitudinal phonon frequency of 0.7 and a transverse phonon frequency of 0.4.

```
double eps(const vec &) { return 13.4; }
double one(const vec &) { return 1; }
```

To create the polaritonic material, we add the polarizability to the material after we have created it.

```
double freq = 0.4, gamma = 0.01, delta_eps = 27.63;
s.add_polarizability(one, freq, gamma, delta_eps);

for (k=0.0;k<4.01 && !interrupt;k+=.5) {
  master_printf("Working on k of %g and m = %d...\n", k, m);
  fields f(&s, m);
  f.use_bloch(k);
```

Now we excite the first TE mode (we are only looking at m = 0 here), and remember to excite along with it the phonon with which it couples.

```
  f.initialize_with_nth_te(1);
  f.initialize_polarizations();
```

Finally, we compute the band structure as usual.

```
  f.prepare_for_bands(veccyl(0.501,0.0), ttot, .7+.15*k/3.0, 50, 1e-4);
  f.prepare_for_bands(veccyl(0.301,0.0), ttot, .7+.15*k/3.0, 50, 1e-4);

  while (f.time() < ttot && !interrupt) {
    f.record_bands();
    f.step();
  }
  f.grace_bands(&g, 16);
```

The final output of this routine (as calculated using the "plot" program) is shown in Figure 5.5.

## 5.6 Energy conservation in cylindrical coordinates

In this example, we compute the total energy over time for a polaritonic material in cylindrical coordinates. Eventually I figure I may extend this example to demonstrate energy/flux conservation using PML. That would definitely be more impressive.

For our example polaritonic material, we'll use an $\epsilon(0)$ of 13.4. We will put the polaritons in just one quarter of our system to add a little extra excitement.

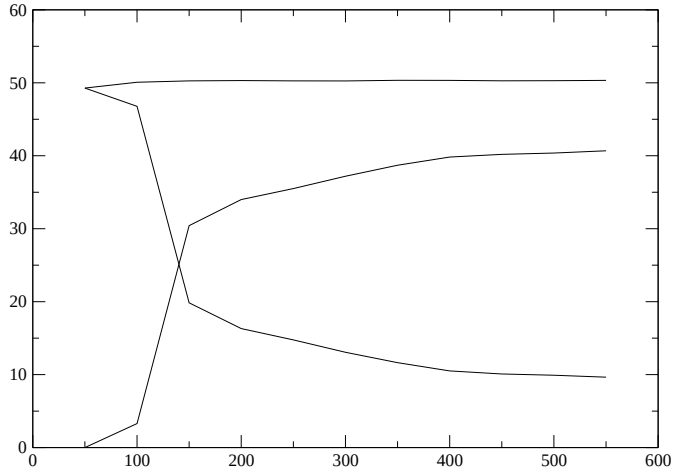
```
double eps(const vec &) { return 13.4; }
double one(const vec &p) { return (p.z() > 15.0)?1:0; }
```

We use a long and skinny system so as to exaggerate any errors that may crop up at small $r$.

```
structure s(volcyl(1.0,20.0, a), eps);
```

We use several point sources, to cover a broad frequency range, just for the heck of it.

Figure 5.5: Energy vs. Time.




```
f.add_point_source(Ep, 0.6 , 1.8, 0.0, 8.0, veccyl(0.5,2.0));
f.add_point_source(Ep, 0.4 , 1.8, 0.0, 8.0, veccyl(0.5,2.0));
f.add_point_source(Ep, 0.33, 1.8, 0.0, 8.0, veccyl(0.5,2.0));
```

We plot the total energy, the electromagnetic energy and the "thermodynamic energy" which is the energy that is either stored in the polarization, or has been converted into heat, or (if we had a saturating gain system) perhaps is stored in a population inversion.

```
g.output_out_of_order(0, f.time(), f.total_energy());
g.output_out_of_order(1, f.time(), f.field_energy_in_box(f.v.surroundings()));
g.output_out_of_order(2, f.time(), f.thermo_energy_in_box(f.v.surroundings()));
```

## 5.7 Energy conservation in one dimension

In this example, we compute the total energy over time for a polaritonic material in one dimension to verify that it is indeed conserved. This also demonstrates how to use a 1D system.

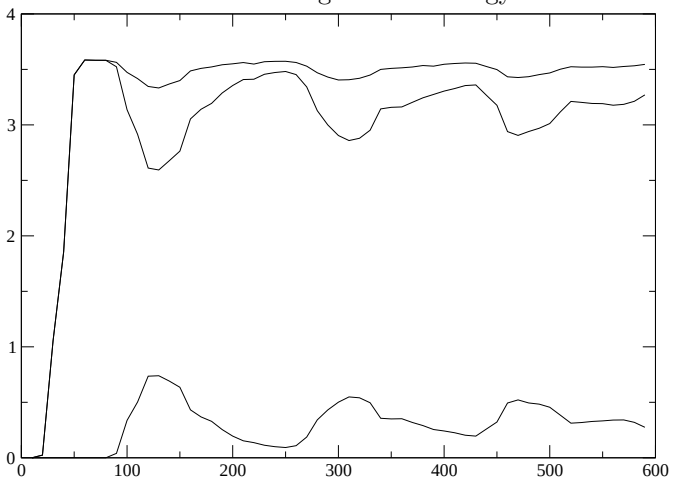
For our example polaritonic material, we'll use an $\epsilon(0)$ of 13.4. We will put the polaritons in just one quarter of our system to add a little extra excitement.

```
double eps(const vec &) { return 13.4; }
double one(const vec &p) { return (p.z() > 15.0)?1:0; }
```

We create a 1D system by making the volume with the "`volone`" function, and making sure any vecs we use are one dimensional.

```
structure s(volone(20.0, a), eps);
```

Figure 5.6: Energy vs. Time.




The polarizability is added as usual... in this case we use a very sharp resonance, which means that our energy will only be very slowly absorbed.

```
s.add_polarizability(one, 0.25, 0.0001, 3.0);
fields f(&s);
grace g("energy", dirname);
```

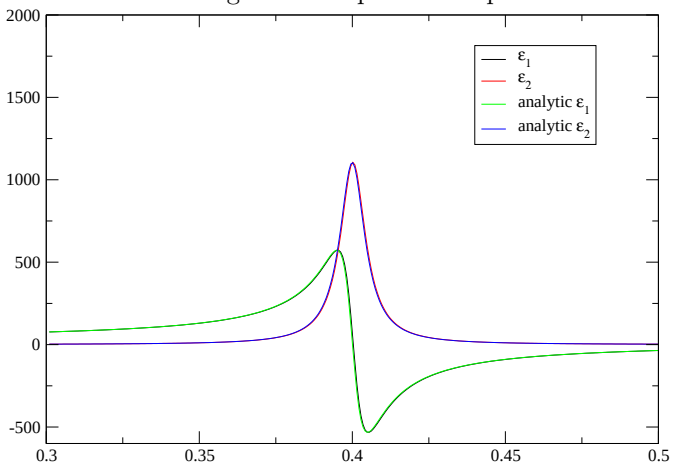
We use several point sources, to cover a broad frequency range, just for the heck of it.

```
f.add_point_source(Ex, 0.6 , 1.8, 0.0, 8.0, vec(2.0));
f.add_point_source(Ex, 0.4 , 1.8, 0.0, 8.0, vec(2.0));
f.add_point_source(Ex, 0.33, 1.8, 0.0, 8.0, vec(2.0));
```

We plot the total energy, the electromagnetic energy and the "thermodynamic energy" which is the energy that is either stored in the polarization, or has been converted into heat, or (if we had a saturating gain system) perhaps is stored in a population inversion.

```
    g.output_out_of_order(0, f.time(), f.total_energy() - ezero);
    g.output_out_of_order(1, f.time(),
                          f.electric_energy_in_box(f.v.surroundings())
                        + f.magnetic_energy_in_box(f.v.surroundings()));
    g.output_out_of_order(2, f.time(),
                          f.thermo_energy_in_box(f.v.surroundings()) - ezero);
```

Figure 5.7: Epsilon of a polaritonic material.




## 5.8 Epsilon of a polaritonic material in one dimension

In this example, we compute epsilon as a function of frequency for a simple polaritonic material. This example is done in one dimension for speed purposes.

One thing to be aware of when using polaritonic materials, is that generally you will be needing a rather higher grid resolution than you may be used to in order to properly model the material. Here I am using an $a$ of 40.

Altough in this calculation the polaritonic material will not be within the PML, it is all right to have polaritonic material within PML regions.

```
s.add_polarizability(one, 0.4, 0.01, 27.63);
```

We use a single rather high frequency (and very broad) point source, to cover a broad frequency range.

```
f.add_point_source(Ex, 0.9, 0.8, 0.0, 8.0, vec(sourceloc));
```

We use a couple of monitor points to determine epsilon.

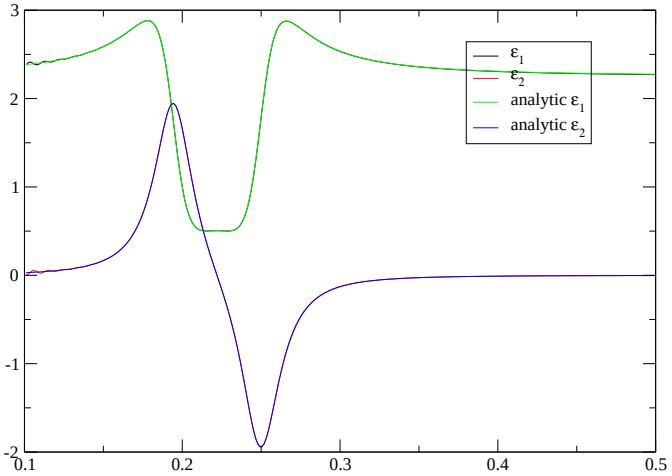
```
monitor_point *left = NULL, *right = NULL, *middle = NULL;
```

The monitor points are located one grid spacing from one another. The `get_new_point` method appends the fields at a given time to a monitor point linked list.

```
left  = f.get_new_point(vec(sourceloc+1.0/a), left );
middle = f.get_new_point(vec(sourceloc+2.0/a), middle);
right = f.get_new_point(vec(sourceloc+3.0/a), right);
```

When the time stepping is over, we take a fourier transform of the fields at the two monitor points.

Figure 5.8: Dielectric function of a material with loss and gain.




```
left->fourier_transform(Ex, &al, &freqs, &numl, 0.301, 0.5, 300);
```

Finally we calculate epsilon from the second derivative of the field using

$$-k^2 H_z(\omega) = \nabla^2 H_z(\omega) = \nabla^2$$

```
complex<double> *epsilon = new complex<double>[numl];
for (int i=0;i<numl;i++) {
  complex<double> ksqr = -(ar[i]+al[i]-2.0*am[i])*a*a/am[i];
  epsilon[i] = ksqr/freqs[i]/freqs[i]/(2*pi*2*pi);
}
for (int i=0;i<numl;i++)
  g.output_point(real(freqs[i]), real(epsilon[i]));
g.new_set();
g.set_legend("\\x\\e\\s2\\N");
for (int i=0;i<numl;i++)
  g.output_point(real(freqs[i]), imag(epsilon[i]));
```

## 5.9 Dielectric function of a material with loss and gain

In this section, we demonstrate a better way to calculate the dielectric function, and illustrate it by computing the dielectric function of a material with a normal lossy resonance as well as a gain line. Gain in the PML is a bad idea, so we restrict the polarizabilities to exist only in the middle of the system (which is surrounded by PML).

```
s.add_polarizability(one_in_middle, 0.195, 0.03, 0.25*.25/.195);
s.add_polarizability(one_in_middle, 0.25, 0.03,-0.25);
```

For sources, we use a series of broad point sources covering the frequency range of interest.

```
f.add_point_source(Ep, 0.3,  0.8, 0.0, 8.0, veccyl(rmax*0.5,sourceloc));
```

The calculation proceeds as usual, except that we now keep track of a set of monitor points that will allow us to take a laplacian of the $H_z$ field component. We choose $m = 0$, so we won't have to deal with the $\phi$ derivative.

```
  left   = f.get_new_point(veccyl(r_look    , z_look - d), left);
  middle = f.get_new_point(veccyl(r_look    , z_look    ), middle);
  top    = f.get_new_point(veccyl(r_look + d, z_look    ), top);
  bottom = f.get_new_point(veccyl(r_look - d, z_look    ), bottom);
  right  = f.get_new_point(veccyl(r_look    , z_look + d), right);
```

We fourier transform $H_z$ at each point:

```
left->fourier_transform(Hz, &al, &freqs, &numl, minfreq, maxfreq, numfreqs);
```

Finally, we calculate the laplacian of $H_z(\omega)$, which is equal to $-k^2 H_z(\omega)$, from which we extract epsilon.

```
for (int i=0;i<numl;i++) {
  complex<double> ksqr = -(ar[i]+al[i]-2.0*am[i]
                           + at[i]*0.5*(1+(r_look+d)/r_look) +
                             ab[i]*0.5*(1+(r_look-d)/r_look) - 2.0*am[i]
                           - m*m*1.0*am[i]/r_look/r_look*a*a
                           )*a*a/am[i];
  epsilon[i] = ksqr/freqs[i]/freqs[i]/(2*pi*2*pi);
}
```

I've left out the bulk of this example from the manual itself, since it is pretty much the same as the previous examples. Among other features, we use the grace functions to plot the result, which can be seen in Figure 5.9.

## 5.10 Nonlinear materials

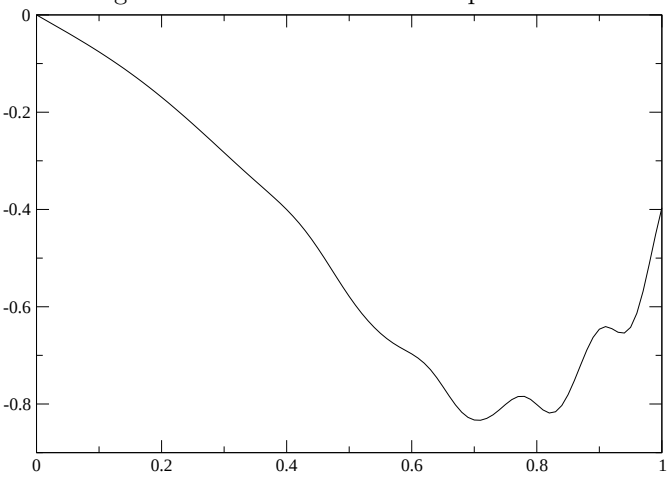
FIXME: Add a nice discussion of nonlinear materials here...

In this example, we will use a CW source and compute the amplitude of the field at a given position and time as a function of the source amplitude. The result will be linear as long as the material remains in the linear regime. Once we have departed from the linear regime, we get more complicated behavior. Yes, this is a stupid example...

The system is shown in Figure 5.10. It is a 2D metallic waveguide with vacuum $\epsilon$ of 2.25. In the center of the cell is a small region that is linear which contains the source, and the rest of the waveguide contains a nonlinear material. Both ends of the waveguide have PML absorbing boundary conditions.

Figure 5.9: Field vs. source amplitude with nonlinear material

Figure 5.10: Field vs. source amplitude with nonlinear material




```
const double alpha_value = 0.07;
double alpha(const vec &v) {
  if (fabs(v.x() - xmax/2.0) < .51) return 0.0;
  return alpha_value;
}
```

The set_chi3 method is used to set the chi3 coefficient.

```
  s.set_chi3(alpha);
```

We use a CW source at a frequency of 0.4, which gives single-mode behavior when the amplitude is small. Also note that we use real fields, since complex fields are incorrect for nonlinear materials.

```
  continuous_src_time my_source(0.4,  0.8);
  for (double amp = 0.05; amp <= 1.01 && !interrupt; amp += 0.01) {
    fields f(&s, m);
    f.use_real_fields();
    f.add_point_source(Ez, my_source, vec(xmax*0.5,ymax*0.5), amp);
```

Time stepping, etc, is done as usual. We monitor the field at one end of the cell, which gives Figure 5.10, which show the field versus source amplitude.

# Appendix A

# GNU General Public License

## Version 2, June 1991



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