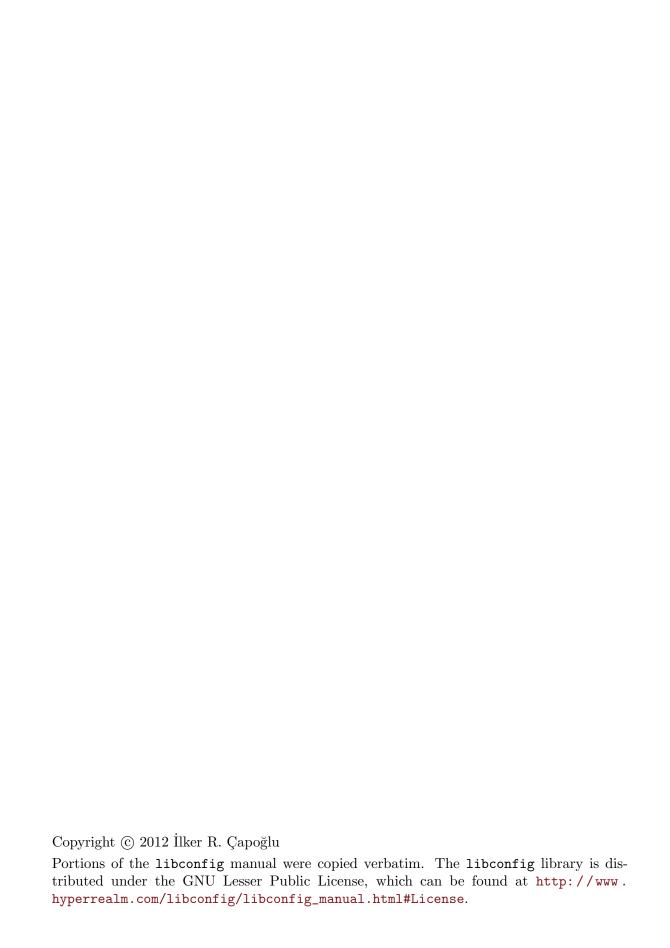
# Angora User's Guide

A finite-difference time-domain (FDTD) electromagnetic simulation software for version 0.18.8 and later, May 2012



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# Angora: A finite-difference time-domain simulation package

This is the user's guide for Angora, a software package that computes numerical solutions to electromagnetic radiation and scattering problems. It is based on the finite-difference time-domain (FDTD) method, which one of the most popular approaches for solving Maxwell's equations of electrodynamics.

# 1 Getting Started

Angora simulations are run by constructing a text file, called the *configuration file* that specifies all aspects of the simulation. This file is then given as a command-line option to the Angora executable angora; which reads the configuration file and produces the desired output (see Chapter 4 [Execution], page 9).

Let's start with a simple example. In the following, we will show how Angora can be used to solve the problem of electromagnetic scattering from a sphere illuminated by a plane wave. The geometry of the scattering problem is shown in Figure 1.1.

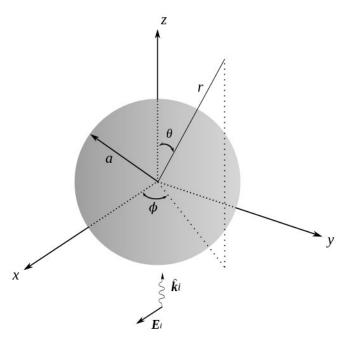


Figure 1.1: Scattering from a sphere illuminated by a plane wave incident from the -z direction.

We start by creating a configuration file; say 'sph\_sc.cfg'. This file will be populated by configuration options listed in the following. Some basic parameters of our simulation are determined by the following lines (see Section 6.2 [Grid Properties], page 14 for details):

```
dx = 20e-9;
courant = 0.98;
grid_dimension_x = 1e-6;
grid_dimension_y = 1e-6;
grid_dimension_z = 1e-6;
pml_thickness_in_cells = 5;
num_of_time_steps = 1500;
```

The first variable, dx, is the uniform spatial step size in the FDTD discretization. The second variable, courant, is the ratio of the time step to the maximum time step allowable by the Courant condition. The next three variables determine the physical size of the simulation grid in meters. The thickness of the absorbing layer (PML) is determined by the pml\_thickness\_in\_cells variable. The last line specifies the number of time steps in the simulation.

The sphere from which the electromagnetic plane wave will be scattered is created in two steps. First, we define a spherical "shape object" using the **Spheres** variable (see Section 6.3.2 [Spheres], page 20):

Next, the material filling the sphere is defined using the Materials variable (see Section 6.4 [Materials], page 21):

The shape and material definitions are then combined in the Objects variable, and the sphere is placed in the grid (see Section 6.5.1 [Objects], page 23):

With the above defitions, we have created a sphere of radius 320 nm and made of the material specified by "sph\_mat". Next, we define the waveform of the incident plane wave using the Waveforms variable:

```
Waveforms:
{
```

We then create the plane wave incident from the -z direction with the above waveform as its electric field using the PlaneWaves variable (see Section 6.10.1 [Plane Waves], page 64):

Finally, we create a near-field-to-far-field transformer to calculate the scattered field in the far zone using the PhasorDomainNFFFT variable (see Section 6.8 [Near-Field-to-Far-Field Transformer], page 40):

With the above definitions, the far field is calculated at the free-space wavelength 509.1 nm, and 360 equally-spaced angles on the xz plane. The output of the near-field-to-far-field transformer is in HDF5 format, which can be read and manipulated using freely-available tools. For more information, see Section 6.8 [Near-Field-to-Far-Field Transformer], page 40.

The absolute value of the phasor component of the far-zone electric field (normalized by 1/r) at 509.1 nm is shown in a polar plot in Figure 1.2.

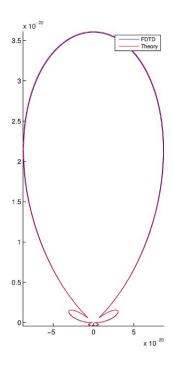


Figure 1.2: The absolute scattered electric field phasor amplitude on the xz plane at  $509.1~\mathrm{nm}$ .

The scattered electric field can also be obtained theoretically using Mie theory (see [Matzler02], page 90), which is shown alongside the Angora solution in the above figure.

# 2 Downloading

Angora is currently only available for the GNU/Linux operating system. If you would like to port Angora to another operating system, please contact us at capoglu@angorafdtd.org. Contributions are always welcome.

The latest version of Angora can be found at http://angorafdtd.org in source code format, as well as binary format for x86\_64 GNU/Linux systems.

# 3 Compilation and Installation

If you will be using Angora on a 64-bit x86 architecture with the GNU/Linux operating system, you can simply download the binary version (both non-parallel and OpenMPI-based parallel versions available) from the Angora website and start running simulations right away.

If there is no precompiled Angora binary available for your system, you will have to compile it from source. You will require the the following libraries on your system to compile Angora: blitz++, libconfig, hdf5, and boost. If possible, use the package manager for your specific GNU/Linux distribution (such as Synaptic in Ubuntu) to install the libraries directly from the package repository. Most major distributions provide these libraries in their package repositories. If you do not have root access to your system, you can install these libraries in your home directory. The installation instructions for the libraries usually provide detailed information on how to do this. For local installation, the usual trick is to set the installation path by specifying the prefix variable in the Makefiles. This is done either by using the '--prefix=local-path' option when calling the package's configure script, or customizing make at the final stage with the 'prefix=local-path' command option.

Once the dependency libraries are installed, the Angora package is ready for compilation. Extract the package 'angora-package-version.tar.gz' using tar, and enter the created directory:

```
johndoe@mysystem:~$ tar xvf angora-package-version.tar.gz
johndoe@mysystem:~$ cd angora-package-version
```

Run the configure script in this directory to create the Makefiles required to build the package:

```
johndoe@mysystem:~/angora-package-version$./configure
```

If any of the dependency libraries was installed in a local directory, then add the option '--with-library-name=local-path-to-library' to the above command line. For example, if the blitz++ library was installed in '/home/johndoe/blitz-0.9', then the option to add is '--with-blitz=/home/johndoe/blitz-0.9'. Type './configure --help' in the directory 'angora-package-version' for information on specifying the paths to the other dependency libraries.

After the configure script finishes execution, compile and install Angora using the make command:

```
johndoe@mysystem:~/angora-package-version$ make
```

If your system has multiple cores, you can speed up the compilation by executing make in parallel. For example, you can use all 4 cores of your system by typing, instead of the above line,

```
johndoe@mysystem:~/angora-package-version$ make -j 4
```

This might take a couple of minutes, depending on your system. After make finishes, the executable angora will be located in the directory 'angora-package-version'. If you wish to *install* the package globally so that it can be run from anywhere, type

```
johndoe@mysystem:~/angora-package-version$ sudo make install
```

Obviously, this requires super-user privileges on your system. By default, the package is installed in '/usr/local'; so the binary will reside in '/usr/local/bin'. If you don't have super-user privileges, you can install Angora in a local directory 'full-path-to-inst-dir' by typing

johndoe@mysystem:~/angora-package-version\$ make prefix=full-path-to-inst-dir install

The location 'full-path-to-inst-dir' should be an absolute path. After this, the binary angora will be located in the directory 'full-path-to-inst-dir/bin/'.

### 3.1 Enabling MPI Support

Parallel execution on multiple processors or cores is supported by Angora, provided that the MPI (Message Passing Interface) libraries are installed on your system (e.g., OpenMPI or MPICH2 or other). A precompiled binary version of Angora based on the OpenMPI implementation is available on the Angora website.

If you are compiling Angora from source, you'll have to enable the MPI feature at compile time. This feature is *disabled* by default. You can enable MPI functionality in Angora by adding the option '--with-mpi' to the configure command line:

```
johndoe@mysystem:~/angora-package-version$ ./configure --with-mpi
```

For more information on launching Angora simulations on multiple processors or cores using MPI, see Section 4.1 [Parallel Execution], page 9.

### 3.2 Building the Documentation

The GNU info documentation for Angora is automatically built and installed by make. If you have the texi2html and latex2html utilities installed, you can create an HTML version of the Angora documentation by typing

```
johndoe@mysystem:~/angora-package-version$ make html
```

If you have the texi2dvi command available (provided as part of the GNU Texinfo package), you can also build a PDF version of the Angora documentation by typing

```
johndoe@mysystem:~/angora-package-version$ make pdf
```

Once built, both the HTML and PDF versions of the documentation will be located in the subdirectory 'doc/'.

# 4 Execution

Angora operates by reading a text file, called the *configuration file*, that specifies the details of the simulation. Every aspect of the simulation is configured by a related *configuration variable* (or *variable* in short) in the configuration file; which comprises either a single line or a number of lines. In general, an Angora simulation is run by putting the name of the configuration file pertaining to the simulation as a command line option when calling the angora executable:

```
johndoe@mysystem:~/angora-package-version$ ./angora path-to-config-file
```

If the Angora executable is run without any command-line options, it looks for the configuration file named 'angora.cfg' in the same directory from which the executable is run. See Chapter 6 [Configuration Variables], page 14, for details on configuration files.

#### 4.1 Parallel Execution

If Angora is compiled with MPI support, then the standard MPI launcher (mpirun) can be used to execute the Angora binary angora in parallel:

```
\label{lem:config} johndoe@mysystem: $$^{angora-package-version$}$ mpirum -n num-of-processors ./angora path-to-config-file
```

For example, to run the simulation configured by 'mysimulation.cfg' using Angora version 0.9 on 8 processors, one should type

```
johndoe@mysystem:~/angora-package-version$ mpirun -n 8 ./angora mysimulation.cfg
```

MPI support should be enabled in compile time in order to run simulations in parallel. For details, see Section 3.1 [Enabling MPI Support], page 8. If you are using the OpenMPI-based precompiled binary version of Angora, then the OpenMPI shared libraries must be in your path before the binary 'angora' can be executed. This can either be done by installing OpenMPI globally (using a package manager etc.), or adding the path to the OpenMPI shared libraries to your LD\_LIBRARY\_PATH environment variable.

#### 4.2 Check Mode

Angora can check a configuration file for syntactic and semantic errors, without actually running the simulation. To do this, simply run Angora with the '--check' or '-c'option:

```
johndoe@mysystem:~/angora-package-version$ ./angora --check path-to-config-file
```

This reports any errors in the configuration-file syntax or invalid configuration options (see Section 6.1 [Template Configuration File], page 14). The actual size of the simulation does not have any effect on this operation; therefore it can be run on a single processor with little memory.

# 5 Configuration Format

Angora uses the libconfig library to read configuration variables regarding the simulation from a text file. The text file, called the *configuration file*, has to conform to the libconfig grammar; which is explained in greater detail at http://www.hyperrealm.com/libconfig/libconfig\_manual.html. Here, we will provide the minimum information necessary to write configuration files for Angora simulations.

# 5.1 Variable Assignment

A variable in a configuration file is set using the following assignment:

```
name=value;
or:
   name:value;
```

The trailing semicolon is required. Whitespace is not significant. Here, *name* is the name of the variable, and *value* is its value; which may be a scalar value, an array, a group, or a list. See Section 5.2 [Variable Types], page 10, for information on these value types.

The order in which variables are specified in the configuration file is insignificant, except within the SimulationSpace variable (see Section 6.5 [Simulation Space], page 23). The sub-variables of the SimulationSpace variable are processed in the order of appearance in the configuration file. This is necessary because the user needs to be able to control the order in which objects are placed in the grid, and predict the regions within an object that will be overwritten by another object.

# 5.2 Variable Types

Angora simulation variables can be assigned C++-type scalar values, as well as more complex values of type group, array, and list. The latter types are defined by the libconfig library. Some of the text in this section is copied verbatim from the libconfig manual. The libconfig library, along with its documentation, is distributed under the GNU Lesser Public License.

# 5.2.1 Integer Values

Integers can be represented in one of two ways: as a series of one or more decimal digits ('0' - '9'), with an optional leading sign character ('+' or '-'); or as a hexadecimal value consisting of the characters '0x' followed by a series of one or more hexadecimal digits ('0' - '9', 'A' - 'F', 'a' - 'f').

```
Examples:
    n_sx = 3;
    offset = -4;
    address = 0xFFFF;
```

# 5.2.2 Floating-Point Values

Floating point values consist of a series of one or more digits, one decimal point, an optional leading sign character ('+' or '-'), and an optional exponent. An exponent consists of the letter 'E' or 'e', an optional sign character, and a series of one or more digits.

Except in special circumstances, floating-point values in Angora are read and processed in 'double' precision, which corresponds to roughly 15 decimal digits.

Examples:

```
f = 1.0;
origin = -3e-6;
prefactor = 5E10;
```

#### 5.2.3 Boolean Values

Boolean values may have one of the following values: 'true', 'false', or any mixed-case variation thereof.

Examples:

```
include_first_value = true;
include_last_value = FaLsE;
```

#### 5.2.4 String Values

String values consist of arbitrary text delimited by double quotes. Literal double quotes can be escaped by preceding them with a backslash: '\"'. The escape sequences '\\', '\f', '\n', '\r', and '\t' are also recognized, and have the usual meaning.

In addition, the '\x' escape sequence is supported; this sequence must be followed by exactly two hexadecimal digits, which represent an 8-bit ASCII value. For example, '\xFF' represents the character with ASCII code 0xFF.

No other escape sequences are currently supported.

Adjacent strings are automatically concatenated, as in C/C++ source code. This is useful for formatting very long strings as sequences of shorter strings. For example, the following constructs are equivalent:

- "The quick brown fox jumped over the lazy dog."
- "The quick brown fox"
  " jumped over the lazy dog."
- "The quick" /\* comment \*/ " brown fox " // another comment "jumped over the lazy dog."

#### **5.2.5** Groups

A group has the form:

```
{
    name=value;
    other_name=other_value;
    ...
}
```

Notice the curly brackets '{}' around the variable assignments. Groups can contain any number of variable assignments (see Section 5.1 [Variable Assignment], page 10), but each variable must have a unique name within the group.

Example:

```
{
    shape_tag = "mysphere";
    center_coord_x = 5e-6;
    center_coord_y = 5e-6;
    center_coord_z = 5e-6;
    radius = 4e-6;
}
```

#### **5.2.6** Arrays

An array has the form:

```
[ value, value, ... ]
```

Notice the square brackets '[]' delimiting the comma-separated values. An array may have zero or more elements, but the elements must all be **scalar** values of the **same type**.

Examples:

```
disabled_runs = [0,1,3];
output_variables = ["Ex","Ey"];
```

#### 5.2.7 Lists

A list has the form:

```
( value, value, ... )
```

Notice the parantheses '()' delimiting the comma-separated values. A list may have zero or more elements, each of which can be a scalar value, an array, a group, or another list. The values in a list can be of different types; however, in Angora, the list type is exclusively used to contain a collection of group values. In Angora, the list type semantically represents a collection of objects, each with a collection of properties set within their respective group value. Here is an example:

Here, the list structure named Materials contains two groups (each delimited by curly brackets '{}') separated by a comma. This defines two materials with different sets of properties.

#### 5.2.8 Comments

Three types of comments are allowed within a configuration:

• Script-style comments. All text beginning with a '#' character to the end of the line is ignored.

- C-style comments. All text, including line breaks, between a starting '/\*' sequence and an ending '\*/' sequence is ignored.
- C++-style comments. All text beginning with a '//' sequence to the end of the line is ignored.

As expected, comment delimiters appearing within quoted strings are treated as literal text.

```
# Here's a comment
MyGroup:
(/* This is
    also a comment */
    {
        this_property = "myvalue";
        // Another comment
    }
);
```

#### 5.2.9 Include Directives

A configuration file may "include" the contents of another file using an *include directive*. This directive has the effect of inlining the contents of the named file at the point of inclusion.

An include directive must appear on its own line in the input. It has the form:

```
@include "filename"
```

Any backslashes or double quotes in the file name must be escaped as  $\$  and  $\$  respectively.

For example, consider the following two configuration files:

```
# file: limits.cfg
back_coord_x = -5e-6;
front_coord_x = 6e-6;
left_coord_y = -5e-6;
right_coord_y = 6e-6;
lower_coord_z = -3e-6;
upper_coord_z = 4e-6;
```

Include files may be nested to a maximum of 10 levels; exceeding this limit results in a runtime error.

# 6 Configuration Variables

The variable assignments (or settings in libconfig terminology) in a configuration file reside either at the uppermost level (called the Global level) or within a group structure (see Section 5.2.5 [Groups], page 11). In the following, configuration variables will be characterized as either being a Global variable, or a Sub-variable of ParentVariable; where Parent-Variable is the next parent variable upward in the hierarchy that has a name. The variable ParentVariable can either be a group or a list (see Section 5.2.5 [Groups], page 11 and Section 5.2.7 [Lists], page 12). Quite often, the immediate parent of a variable assignment is an unnamed group; therefore the ParentVariable of that assignment is the list that contains this unnamed group. For example, the ParentVariable of the variable material\_tag in the example in Section 5.2.7 [Lists], page 12 is Materials, since its immediate parent is an unnamed group, but the list structure containing the unnamed group has a name (which is Materials). On the other hand, the variable Materials is a Global variable; since it is assigned at the uppermost level in a configuration file, outside any enclosing structure.

The configuration variable names are case sensitive; meaning that Materials and materials are not the same.

Angora throws an error message for any missing variable or misspelled variable name. This is crucial for ensuring that no optional configuration variable is omitted because of a typo. The valid variable names are read into the Angora source code in compile time from a template file 'config\_all.cfg'. This file, although not required at the time of execution, is distributed with Angora for reference (see Section 6.1 [Template Configuration File], page 14).

# 6.1 Template Configuration File

A file named 'config\_all.cfg' is included in the Angora distribution, which includes all the valid configuration variables. All variables in a given configuration file are checked against 'config\_all.cfg' and labeled invalid if a corresponding variable does not exist in 'config\_all.cfg'. It should be stressed, however, that 'config\_all.cfg' is not necessary for the execution of Angora, but is necessary for its compilation. This is because 'config\_all.cfg' is read into the source code of Angora in the compilation stage. The file 'config\_all.cfg' is only distributed as a reference for the user's convenience.

The file 'config\_all.cfg' is installed in the directory '\$(prefix)/share/angora/' (see Chapter 3 [Compilation and Installation], page 7). If Angora was installed without any \$(prefix) configuration option, the default location is '/usr/local/share/angora/'.

# 6.2 Grid Properties

Angora currently only supports a rectangular, Cartesian FDTD grid with equal grid spacing in the x, y, and z directions. Mesh refinement is not yet supported; therefore the grid spacing is uniform across the grid.

#### 6.2.1 Courant Factor

#### floating-point courant

[Global variable]

Angora adopts a slightly modified form for the Courant factor, defined as

$$\sqrt{3} \frac{c\Delta t}{\Delta x}$$

where c=299792458 m/s is the speed of light in vacuum, and  $\Delta t$  and  $\Delta x$  are the temporal and spatial step sizes (see Section 6.2.2 [Spatial Step Size], page 15). The Courant factor should be less than 1.0 for stability. A common value for courant is 0.98.

#### 6.2.2 Spatial Step Size

#### floating-point dx (units: m)

[Global variable]

The spatial step size in the FDTD grid is specified by the dx variable. Currently only cubic FDTD cells are supported; therefore the spatial step sizes in the x, y, and z direction are all determined by dx.

#### 6.2.3 Grid Dimensions

floating-point grid\_dimension\_x (units: m) [Global variable]
floating-point grid\_dimension\_y (units: m) [Global variable]
floating-point grid\_dimension\_z (units: m) [Global variable]
integer grid\_dimension\_x\_in\_cells [Global variable]
integer grid\_dimension\_y\_in\_cells [Global variable]
integer grid\_dimension\_z\_in\_cells [Global variable]

These variables determine the size of the Cartesian FDTD grid. The dimensions of the grid can be specified either in meters, or in grid cells. For the latter, the <code>\_in\_cells</code> suffix should be appended to the variable name. If the dimensions are given in meters, the number of FDTD cells in the Cartesian FDTD grid in the x, y, and z directions are rounded to the closest integer. If no perfectly-matched layers are specified (see Section 6.2.4 [Perfectly-Matched Layer (PML)], page 15), the total number of FDTD cells in the three-dimensional FDTD grid is equal to (grid\_dimension\_x\_in\_cells) x (grid\_dimension\_y\_in\_cells) x (grid\_dimension\_z\_in\_cells).

### 6.2.4 Perfectly-Matched Layer (PML)

floating-point pml\_thickness (units: m)

[Global variable]

integer pml\_thickness\_in\_cells

[Global variable]

This variable sets the thickness of the perfectly-matched layers (PMLs) around the grid in all directions. Further customization of the PML thickness is not yet supported. The thickness can be specified either in meters, or in grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

Typical PML thicknesses are 5 to 10 grid cells. If you do not want to place a PML layer around the grid, just assign pml\_thickness=0. Without a PML layer, the boundary of

the FDTD grid acts as a perfect electric conductor (PEC). Other boundary conditions (perfect magnetic conductor, periodic, etc.) will also be supported in the future.

With a PML definition, the total number of FDTD cells in the three-dimensional FDTD grid becomes

(grid\_dimension\_x\_in\_cells+2\*pml\_thickness\_in\_cells)

x (grid\_dimension\_y\_in\_cells+2\*pml\_thickness\_in\_cells)

x (grid\_dimension\_z\_in\_cells+2\*pml\_thickness\_in\_cells)

The computational burden per FDTD cell associated with the PML layer is roughly three times that of the main grid.

Angora implements the convolution PML (CPML) formulation of the complex-frequency shifted (CFS) PML (see [Roden00], page 90; [Kuzuoglu96], page 90.)

This variable specifies the maximum size of the scattering or radiating structure in the FDTD grid. This size can be specified either in meters, or in grid cells. For the latter, the <code>\_in\_cells</code> suffix should be appended to the variable name.

This information is used to determine the frequency-shifting parameter  $\alpha$  in the CFS-PML formulation. Following Berenger's derivation (see [Berenger02], page 90), this parameter is defined as

$$\alpha = c\epsilon/w$$

where c is the velocity of propagation in the medium,  $\epsilon$  is the absolute permittivity (in F/m) in the medium, and w is the maximum size of the structure.

The above relationship follows essentially from the low-frequency behavior of the CFS-PML. At low frequencies where the evanescent field around the structure dominates, the CFS-PML reduces to a real stretch of coordinates without any absorption. This helps the termination of evanescent fields, which are poorly handled by ordinary PMLs.

#### 6.2.5 Number of Time Steps

integer num\_of\_time\_steps

[Global variable]

This variable determines the number of time steps in the FDTD simulation.

#### 6.2.6 Coordinate Origin

floating-point origin\_x (units:m, default: (grid\_dimension\_x+2\*pml\_thickness)/2+1)

[Global variable]

floating-point origin\_y (units:m, default: (grid\_dimension\_y+2\*pml\_thickness)/2+1)

[Global variable]

integer origin\_z\_in\_cells (default: [Global variable] (grid\_dimension\_z\_in\_cells+2\*pml\_thickness\_in\_cells)/2+1)

These variables set the origin of the coordinate system in the simulation. All other coordinates in a configuration file are taken as relative to this origin. The coordinates can be specified either in meters, or in grid cells. For the latter, the  $\_in\_cells$  suffix should be appended to the variable name. These three numbers represent the Cartesian coordinates of the origin from the back-left-lower corner of the grid. In Figure 6.1, the location of the coordinate origin in the FDTD grid is shown for (origin\_x\_in\_cells,origin\_y\_in\_cells,origin\_z\_in\_cells)=(2,3,2). The FDTD grid is composed of (3x5x3) grids, and only the back (y=z=0), left (x=z=0), and lower (x=y=0) surfaces are shown in the figure.

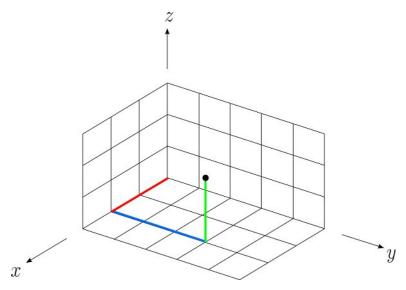


Figure 6.1: The location of the coordinate origin in the FDTD grid for (origin\_x\_in\_cells,origin\_y\_in\_cells,origin\_z\_in\_cells)=(2,3,2).

If the coordinates are given in meters, they are rounded to the closest integer multiple of the spatial step size (see Section 6.2.2 [Spatial Step Size], page 15).

#### 6.2.7 Dynamic Range

The following two variables are only relevant in movie recording (see Section 6.11.1 [Movie Recording], page 74), wherein the floating-point field values on the movie frames are sometimes discretized to fit into 1 byte.

#### floating-point max\_field\_value (default: 1.0)

[Global variable]

This value specifies the maximum field value used in the discretization for 1-byte movie recording (see Section 6.11.1 [Movie Recording], page 74).

#### floating-point dB\_accuracy (default: automatic)

[Global variable]

This value specifies the dynamic range (in dB) to be used in the discretization for 1-byte movie recording (see Section 6.11.1 [Movie Recording], page 74). For example,

```
dB_accuracy = -60;
```

tells Angora to discretize the field values in a dynamic range between the maximum field value (specified by max\_field\_value above) and 60dB below that value. If dB\_accuracy is not specified, Angora tries to set this value automatically, based on its best guess on the useful accuracy range in the simulation. This value can also be read from the output of the movie recorder (see Section 6.11.1 [Movie Recording], page 74).

### 6.3 Shapes

#### group Shapes

[Global variable]

In Angora, a geometrical shape and the material filling that shape are two distinct and independent elements of the definition of an object. The first of these elements is defined in the Shapes variable, which is a group (see Section 5.2.5 [Groups], page 11).

In this example, two sub-variables RectangularBoxes and Spheres of the Shapes group are shown. These are both list variables (see Section 5.2.7 [Lists], page 12).

Currently, rectangular boxes and spheres are the only basic shape classes defined in Angora. Unions, intersections, and geometrical transformations of shapes, as well as more basic shape classes will be added to Angora in the future. Please send any comments, suggestions, and requests to help@angorafdtd.org.

#### 6.3.1 Rectangular Boxes

#### group RectangularBoxes

[Sub-variable of Shapes]

Rectangular boxes are defined using the RectangularBoxes variable, which is a list structure under the Shapes group.

```
Shapes:
{
    RectangularBoxes:
    (
        {
            shape_tag = "mybox";
            back_coord_x = -5e-6;
            front_coord_x = 6e-6;
            left_coord_y = -5e-6;
            right_coord_y = 6e-6;
            lower\_coord\_z = -3e-6;
            upper_coord_z = 4e-6;
        },
        }
    );
};
```

In this example, two rectangular box shapes are defined in two respective unnamed groups; only the first being shown in complete detail.

#### string shape\_tag

[Sub-variable of RectangularBoxes]

This string variable assigns a *name* to the particular shape, so it can be referred to later in the configuration file.

```
floating-point back_coord_x (units:
                                           [Sub-variable of RectangularBoxes]
floating-point front_coord_x (units:
                                           [Sub-variable of RectangularBoxes]
floating-point left_coord_y (units:
                                            [Sub-variable of RectangularBoxes]
floating-point right_coord_y (units:
                                            [Sub-variable of RectangularBoxes]
floating-point lower_coord_z (units:
                                           [Sub-variable of RectangularBoxes]
floating-point upper_coord_z (units:
                                            [Sub-variable of RectangularBoxes]
         m)
floating-point
                                            [Sub-variable of RectangularBoxes]
         back_coord_x_in_cells
```

```
floating-point [Sub-variable of RectangularBoxes]
front_coord_x_in_cells

floating-point [Sub-variable of RectangularBoxes]
left_coord_y_in_cells

floating-point [Sub-variable of RectangularBoxes]
right_coord_y_in_cells

floating-point [Sub-variable of RectangularBoxes]
lower_coord_z_in_cells

floating-point [Sub-variable of RectangularBoxes]
lower_coord_z_in_cells

[Sub-variable of RectangularBoxes]
[Sub-variable of RectangularBoxes]
```

These variables determine the minimum and maximum Cartesian coordinates of the box in the x, y, and z directions relative to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

#### 6.3.2 Spheres

#### group Spheres

[Sub-variable of Shapes]

Spheres are defined using the Spheres variable, which is a list structure under the Shapes group.

In this example, two spherical shapes are defined in two respective unnamed groups; only the first being shown in complete detail.

#### string shape\_tag

[Sub-variable of Spheres]

This string variable assigns a *name* to the particular shape, so it can be referred to later in the configuration file.

```
floating-point center_coord_x (units: m) [Sub-variable of Spheres]
floating-point center_coord_y (units: m) [Sub-variable of Spheres]
floating-point center_coord_z (units: m) [Sub-variable of Spheres]
floating-point center_coord_x_in_cells [Sub-variable of Spheres]
floating-point center_coord_y_in_cells [Sub-variable of Spheres]
floating-point center_coord_z_in_cells [Sub-variable of Spheres]
```

These variables determine the Cartesian coordinate of the center of the sphere relative to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

```
floating-point radius (units: m) [Sub-variable of Spheres]

floating-point radius_in_cells [Sub-variable of Spheres]

This variable determines the radius of the sphere. The units are either in meters
```

This variable determines the radius of the sphere. The units are either in meters or grid cells. For the latter, the <u>\_in\_cells</u> suffix should be appended to the variable name.

#### 6.4 Materials

Currently, Angora only supports isotropic materials. Anisotropic materials may also be supported in the future. Please send any comments, suggestions, and requests to help@angorafdtd.org.

```
list Materials [Global variable]
```

The properties of a certain material type are specified in the Materials list (see Section 5.2.7 [Lists], page 12).

```
Materials:
(
    {
        material_tag = "this_material";
        rel_permittivity = 2.0;
        rel_permeability = 1.0;
        electric_conductivity = 0.0;
        magnetic_conductivity = 0.0;
        drude_pole_frequency = 0.0;
        drude_pole_relaxation_time = 0.0;
        transparent = false;
    },
        . . .
        . . .
    }
);
```

In this example, two materials are defined in two respective unnamed groups; only the first being shown in complete detail.

#### string material\_tag

[Sub-variable of Materials]

This string variable assigns a *name* to the particular material, so it can be referred to later in the configuration file.

floating-point rel\_permittivity (default: 1.0)

[Sub-variable of Materials]

This variable specifies the relative permittivity (or the dielectric constant) of the material. In SI units, the absolute permittivity of the material is this variable multiplied by the permittivity of free space (8.85418782E-12 F/m).

[Sub-variable of Materials]

This variable specifies the relative permeability (or the magnetic constant) of the material. In SI units, the absolute permeability of the material is this variable multiplied by the permeability of free space (4piE-7).

floating-point electric\_conductivity

[Sub-variable of Materials]

(units: S/m) (default: 0)

This variable specifies the electric conductivity (in Siemens/m or Mho/m) of the material.

floating-point magnetic\_conductivity

[Sub-variable of Materials]

(units: Ohm/m) (default: 0)

This variable specifies the magnetic conductivity (in Ohm/m) of the material.

[Sub-variable of Materials]

This variable specifies the Drude pole frequency (in radians) of the material (see Section 6.4.1 [Drude Dispersion], page 22).

floating-point drude\_pole\_relaxation\_time

[Sub-variable of Materials]

(units: sec) (default: 0)

This variable specifies the Drude pole relaxation time (in seconds) of the material (see Section 6.4.1 [Drude Dispersion], page 22).

boolean transparent (default: false)

[Sub-variable of Materials]

If set to false, any unspecified constitutive parameter is set to its default value. If set to true, unspecified constitutive parameters become *transparent*, meaning that when an object made up of this material is placed in the grid, the unspecified constitutive parameters are kept unchanged.

# 6.4.1 Drude Dispersion

Angora supports frequency-dependent permittivities described by a Drude dispersion model with a single pole. The relative permittivity of a material with a single Drude pole is given by the expression

$$\epsilon_r = \epsilon_{r_{\infty}} - \frac{\omega_p^2}{\omega^2 - j\omega/\tau_p}$$

where  $\omega$  is the radian frequency,  $\omega_p$  is the Drude pole frequency (also known as the plasma frequency) of the material, and  $\tau_p$  is the Drude pole relaxation time of the material.

Currently, Drude dispersion *cannot* be used for materials extending into the PML (see Section 6.2.4 [Perfectly-Matched Layer (PML)], page 15). Consequently, the plane-wave injector (see Section 6.10.1 [Plane Waves], page 64) and the near-field-to-far-field transformer (see Section 6.8 [Near-Field-to-Far-Field Transformer], page 40) *cannot* handle planar layers with Drude dispersion. This feature may be added in the future.

### 6.5 Simulation Space

#### group SimulationSpace

[Global variable]

The SimulationSpace group is where all the objects inside the simulation space are defined. If no SimulationSpace group is specified in the configuration file, the FDTD simulation space consists entirely of vacuum.

In the above example, only two of the sub-variables of the SimulationSpace group, Objects and RandomMaterials, are shown. The sub-variable Objects is a list (see Section 5.2.7 [Lists], page 12), whereas RandomMaterials is a group (see Section 5.2.5 [Groups], page 11).

The definitions in the SimulationSpace group are processed in the order of placement. Thus, the user has complete control over which object is placed in the simulation space first. As a consequence of this first-come-first-serve policy, objects can overwrite regions of the simulation space occupied by other objects.

# 6.5.1 Objects

#### list Objects

[Sub-variable of SimulationSpace]

The Objects list defines material objects to be placed in the simulation grid. An *object* in this context is defined as a combination of two abstract ingredients: A previously-defined shape (see Section 6.3 [Shapes], page 18), and a previously-defined material to fill that shape (see Section 6.4 [Materials], page 21). The shape and material are referred to using their shape and material tags, which are string variables assigned to them in their definitions.

#### string material\_tag

[Sub-variable of Objects]

This string variable specifies the material that makes up the object. It should match a previously-defined tag in a Materials definition (see Section 6.4 [Materials], page 21).

#### string shape\_tag

[Sub-variable of Objects]

This string variable specifies the geometrical shape of the object. It should match a previously-defined tag in a Shapes definition (see Section 6.3 [Shapes], page 18).

#### 6.5.2 Planar Layers

#### list MaterialSlabs

[Sub-variable of SimulationSpace]

The purpose of the MaterialSlab list is to introduce planar stratification into the simulation grid. Currently, Angora only supports planar stratification along the z direction. The handling of planar layers will be further improved in the future. Please send any comments, suggestions, and requests to help@angorafdtd.org.

Here is an example:

```
);
};
```

In the above example, a material slab composed of material1 is placed in the grid.

#### string material\_tag

[Sub-variable of MaterialSlabs]

This variable specifies the material that makes up the slab. It should match a previously-defined tag in a Materials definition (see Section 6.4 [Materials], page 21).

floating-point/string min\_coord [Sub-variable of MaterialSlabs]
floating-point/string max\_coord [Sub-variable of MaterialSlabs]
integer/string min\_coord\_in\_cells [Sub-variable of MaterialSlabs]
integer/string max\_coord\_in\_cells [Sub-variable of MaterialSlabs]

These two floating-point variables specify the lower and upper coordinates of the material slab with respect to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. These variables can also be assigned the string values "min" or "max"; which correspond to the lower and upper boundaries of the simulation grid, respectively. If the coordinates correspond to non-integer cell positions, they are rounded to the nearest multiple of the spatial step size. However, the tangential components of the electric tensor properties and the normal component of the magnetic tensor properties are suitably interpolated (see [Hwang01], page 90).

If the FDTD grid is terminated by absorbing PML boundaries (see Section 6.2.4 [Perfectly-Matched Layer (PML)], page 15), then the MaterialSlab definitions effectively create *infinite planar layers* that extend horizontally toward infinity. When the "min" or "max" strings are assigned as lower or upper coordinates of the slab, the MaterialSlab definition amounts to placing a *half space*. When the MaterialSlab variable is used, the incident beams (see Section 6.10 [Incident Beams], page 63) and the scattered far field (see Section 6.8 [Near-Field-to-Far-Field Transformer], page 40) are both calculated as if the material slab horizontally extends toward infinity.

#### 6.5.3 Random Materials

#### group RandomMaterials

[Sub-variable of SimulationSpace]

Independent samples from a random distribution of material properties with a specified correlation function can be generated and placed into the simulation grid using the RandomMaterials group. It contains sub-variables in the form of lists (see Section 5.2.7 [Lists], page 12) that correspond to specific correlation functions. Currently, only the *Whittle-Matern* family of correlation functions is supported. More correlation functions can be added in the future. Please send any comments, suggestions, and requests to help@angorafdtd.org.

Although the spatial correlation of the generated random material regions can vary, the joint probability density function of the material region is always a *multivariate* normal (Gaussian) function.

#### list WhittleMaternCorrelated

[Sub-variable of RandomMaterials]

The Whittle-Matern family of correlations (see [Rogers09], page 90) is a threeparameter isotropic stochastic model that can represent a wide range of spatial correlations. The Whittle-Matern correlation function B(r) for two points separated in space by a distance of r is given by the formula

$$B(r) = \sigma^2 \frac{2^{5/2 - m} (r/l_c)^{m - 3/2}}{\Gamma(m - 3/2)} K_{m - 3/2}(r/l_c)$$

where  $K_{m-3/2}(\cdot)$  is the modified Bessel function of the second kind and order (m-3/2).

- m: The shape parameter that determines the overall behavior of the correlation function. As m->infinity, the function approaches a Gaussian distribution. If m=2, the function reduces to a decaying exponential. For m<3/2, the distribution acquires an inverse power law dependence near the origin; approximating a fractal distribution. For more details, see [Rogers09], page 90.
- $l_c$ : (For m>3/2:) The correlation length. (For m<=3/2:) Loosely, the outer length scale where the fractal approximation no longer holds.
- $\sigma$ : (For m>3/2:) The standard deviation of the distribution at a given point (r=0). (For m<=3/2:) In this range, the correlation function enters the fractal regime with an inverse-power-law dependence at the origin (see [Rogers09], page 90). The meaning of  $\sigma$  becomes more subtle in this regime. It can loosely be associated with the amplitude of the correlation between two points separated by  $l_c$ .

The WhittleMaternCorrelated list creates regions with random material properties described by the Whittle-Matern correlation function above. Here is an example of its usage:

```
SimulationSpace:
    RandomMaterials:
    {
        WhittleMaternCorrelated:
        (
            {
                 constitutive_param_type = "rel_permittivity";
                 mean = 1.33;
                 std_dev = 0.05;
                 corr_len = 100e-9;
                 m = 2.0;
                 shape_tag = "rand_mat_shape";
                 random_seed = 0;
            },
            {
                 . . .
```

```
);
};
};
```

string

[Sub-variable of WhittleMaternCorrelated]

#### constitutive\_param\_type

The Whittle-Matern correlation function can describe the relative permittivity, relative permeability, electric conductivity (in Siemens/m), or magnetic conductivity (Ohm/m) of the material region. This is specified by assigning "rel\_permittivity", "rel\_permeability", "electric\_conductivity", or "magnetic\_conductivity" to the constitutive\_param\_type string variable.

The constitutive parameters other than the one specified are *not changed*. As a result, different random constitutive parameter distributions can be superimposed using multiple random material definitions:

```
SimulationSpace:
{
    RandomMaterials:
    {
        WhittleMaternCorrelated:
            {
                constitutive_param_type = "rel_permittivity";
                mean = 1.33;
                std_dev = 0.05;
                corr_len = 100e-9;
                m = 2.0;
                shape_tag = "rand_mat_shape";
            },
            {
                constitutive_param_type = "rel_permeability";
                mean = 1.1;
                std_dev = 0.05;
                corr_len = 100e-9;
                m = 2.0;
                shape_tag = "rand_mat_shape";
            }
        );
    };
};
```

Here, a random permittivity distribution and a random permeability distribution are overlaid within the same region in the grid.

#### floating-point mean

[Sub-variable of WhittleMaternCorrelated]

(units: none or S/m)

A baseline constant value equal to mean is added to the constitutive parameter described by the Whittle-Matern correlation function. If mean=0, then the generated random distribution will have zero mean. However, this will not necessarily be reflected to the actual constitutive parameter values in the grid; since Angora will automatically clip the constitutive parameters (permittivity, permeability, conductivity, etc.) from below to either unity or zero to avoid instabilities. For this reason, mean should be high enough to avoid this clipping as much as possible. As a rule of thumb, mean should be 5 to 6 times the standard deviation (std\_dev) above unity or zero.

#### floating-point std\_dev

[Sub-variable of WhittleMaternCorrelated]

(units: none or S/m)

This variable specifies the  $\sigma$  parameter in the definition of the Whittle-Matern correlation function.

# floating-point corr\_len (units: m)

[Sub-variable of WhittleMaternCorrelated]

#### floating-point

[Sub-variable of WhittleMaternCorrelated]

corr\_len\_in\_cells

This variable specifies the  $l_c$  parameter in the definition of the Whittle-Matern correlation function. The units are either in meters or grid cells. For the latter, the  $\tt in_cells$  suffix should be appended to the variable name.

#### floating-point m

[Sub-variable of WhittleMaternCorrelated]

This variable specifies the m parameter in the definition of the Whittle-Matern correlation function.

#### string shape\_tag

[Sub-variable of WhittleMaternCorrelated]

This string variable specifies the geometrical shape of the region occupied by the random material. It should match a previously-defined tag in a Shapes definition (see Section 6.3 [Shapes], page 18).

#### integer/string

[Sub-variable of WhittleMaternCorrelated]

random\_seed (default: determined by system time)

If you would like to create exactly the same random distribution each time the simulation is run, you can assign an integer value to the random\_seed variable. Otherwise, you should not define this variable. This value is used to initialize the random-number generator in Angora. If the same seed is used to initialize the random-number generator, the same sequence of random numbers will be generated each time, resulting in the same random distribution.

If multiple simulation runs are present (see Section 6.14 [Multiple Simulation Runs], page 87), you can create different random samples for each

simulation run by assigning the string value "run\_index" to random\_seed. This will initialize the intenal random-number generator with the run index (ranging from 0 to number\_of\_runs-1) of each run. This way, a different random distribution will be obtained in each simulation run; but a distribution for a given simulation run will be *fixed* in subsequent executions of Angora.

In Figure 6.2, a 2D slice of an example zero-mean sample distribution generated by WhittleMaternCorrelated is shown in grayscale.

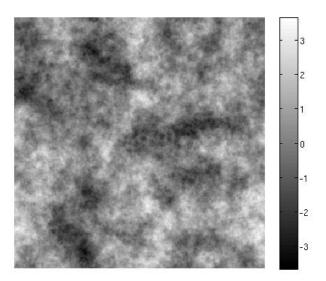


Figure 6.2: A 2D slice of an example zero-mean sample distribution. This distribution can be assigned to different constitutive parameters of a material.

## 6.5.4 File Input

#### list MaterialsFromFiles

[Sub-variable of SimulationSpace]

Material information within rectangular regions of the FDTD simulation grid can be read from files using a MaterialsFromFiles list. This feature of Angora is still under development. The user interface for this feature may change in the future, or be superseded by another, more general interface. Currently, only a single constitutive parameter can be read from a file; and dispersive or anisotropic materials are not supported. These issues will be handled more comprehensively in a future version. Please send any comments, suggestions, and requests to help@angorafdtd.org.

The material file should be in a simple custom binary format that Angora can recognize. The order and type of each variable in the file is explained below:

- 'x-extent': The extent of the array in the x direction in grid cells (integer, 4 bytes)
- 'y-extent': The extent of the array in the y direction in grid cells (integer, 4 bytes)

- 'z-extent': The extent of the array in the z direction in grid cells (integer, 4 bytes)
- A floating-point array of length (x-extent) x (y-extent) x (z-extent). Each value in this array is either of type double (8 bytes) or float (4 bytes), depending on the datatype variable (see [datatype], page 33). The floating-point array should be laid out in the file in *column-major* order, meaning that the x dimension is looped over first, then the y dimension, and finally the z dimension. This ordering is illustrated in Figure 6.3. The elements of the 2x2x2 array are numbered from 0 to 7. These elements should be laid out in the binary file in the same order:

..... 0 1 2 3 4 5 6 7 .....

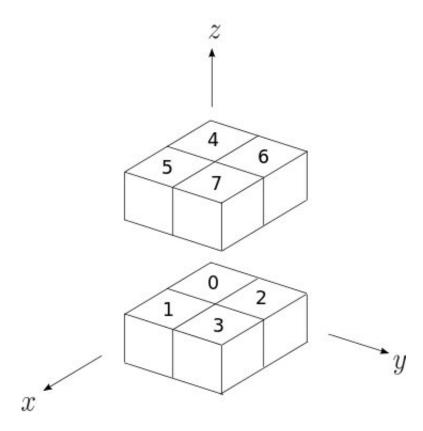


Figure 6.3: The illustration of the column-major ordering of a three-dimensional array. The values indicated by numbers should be laid out in the file in the same order.

Here is an example usage of MaterialsFromFiles:

```
SimulationSpace:
{
    MaterialsFromFiles:
    (
```

```
{
            file_name = "path_to_file/materialfile";
            append_run_index_to_name = true;
            file_extension = "mat";
            constitutive_param_type = "rel_permittivity";
            anchor = "center";
            coord_x = 0;
            coord_y = 0;
            coord_z = 0;
            datatype = "double";
            max_new_materials = 1000;
        },
        {
        }
    );
};
```

#### string file\_name

[Sub-variable of MaterialsFromFiles]

This string specifies the name of the binary file from which the material information will be read. Path information can be prepended to the file name, as shown in the example above. This path is interpreted as being relative to input\_dir (see Section 6.12 [Paths], page 86), unless it is preceded by a slash '/'.

string file\_extension (default: "") [Sub-variable of MaterialsFromFiles]

This is the extension of the material file to be read. In the above example, the file to be read is 'path\_to\_file/materialfile.mat'.

boolean append\_run\_index\_to\_name [Sub-variable of MaterialsFromFiles] This boolean flag becomes useful if there are multiple simulation runs (see Section 6.14 [Multiple Simulation Runs], page 87), and a different file needs to be read in each run. This can be accomplished by appending the run index (which ranges from 0 to number\_of\_runs-1) to the file name specified by file\_name. For example, if there are 3 simulation runs (number\_of\_runs is 3) the above assignment will tell Angora to read the file 'path\_to\_file/materialfile0.mat' in the first run, 'path\_to\_file/materialfile1.mat' in the second, and 'path\_to\_file/materialfile2.mat' in the third.

This variable is required for all simulations (hence no default value) to help the user prevent easy mistakes such as reading the same file for all simulation runs unintentionally, reading 'path\_to\_file/materialfile0.mat' instead of 'path\_to\_file/materialfile.mat', etc.

string constitutive\_param\_type [Sub-variable of MaterialsFromFiles]
The values read from the input file can be assigned to one of the following constitutive parameters: relative permittivity, relative permeability, electric conductivity, or magnetic conductivity. This is determined by assigning

"rel\_permittivity", "rel\_permeability", "electric\_conductivity", or "magnetic\_conductivity" to the constitutive\_param\_type string variable. Electric conductivity is assumed to be in Siemens/m, and magnetic conductivity is assumed to be in Ohm/m.

The constitutive parameters other than the one specified are *not changed*. As a result, different constitutive parameter distributions can be superimposed using multiple file-input definitions:

```
SimulationSpace:
{
    MaterialsFromFiles:
        {
            file_name = "permittivity_file";
            append_run_index_to_name = true;
            constitutive_param_type = "rel_permittivity";
            coord_x = 0;
            coord_y = 0;
            coord_z = 0;
            datatype = "double";
        },
            file_name = "conductivity_file";
            append_run_index_to_name = true;
            constitutive_param_type = "electric_conductivity";
            coord_x = 0;
            coord_y = 0;
            coord_z = 0;
            datatype = "double";
        }
    );
};
```

Here, the contents of the files 'permittivity\_file' and 'conductivity\_file' are interpreted as the relative permittivity and electric conductivity of the same region, respectively.

string anchor (default: "center") [Sub-variable of MaterialsFromFiles]
This string defines an anchor point inside the rectangular-box-shaped region
that is to be read from this file. This anchor is then assigned a coordinate in
the FDTD grid, determining the position of the rectangular box in the grid.
Valid values for anchor are:

- "center": center of the box
- "BLL": back-left-lower corner of the box
- "BLU": back-left-upper corner of the box
- "BRL": back-right-lower corner of the box
- "BRU": back-right-upper corner of the box

- "FLL": front-left-lower corner of the box
- "FLU": front-left-upper corner of the box
- "FRL": front-right-lower corner of the box
- "FRU": front-right-upper corner of the box

Here, as usual, "back"/"front" refers to the x coordinate, "left"/"right" refers to the y coordinate, and "lower"/"upper" refers to the z coordinate.

floating-point coord\_x (units: m) [Sub-variable of MaterialsFromFiles]
floating-point coord\_y (units: m) [Sub-variable of MaterialsFromFiles]
floating-point coord\_z (units: m) [Sub-variable of MaterialsFromFiles]
integer coord\_x\_in\_cells [Sub-variable of MaterialsFromFiles]
integer coord\_y\_in\_cells [Sub-variable of MaterialsFromFiles]
integer coord\_z\_in\_cells [Sub-variable of MaterialsFromFiles]

These values determine the Cartesian x,y, and z coordinates of the anchor point (see above) assigned to the rectangular region to be read from the file. The coordinates are measured with respect to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If the coordinates correspond to non-integer cell positions, the closest integer positions are chosen.

#### string datatype

[Sub-variable of MaterialsFromFiles]

The datatype for the values read from the file is determined by this variable. It should be either "double" (8 bytes) or "float" (4 bytes).

integer max\_new\_materials (default: [Sub-variable of MaterialsFromFiles] 1000)

Internally, Angora uses material indexing to reduce memory use for material arrays. Every constitutive parameter in the grid can only take a distinct set of values, represented by a variable of type unsigned short (2 bytes) that can range from 0 to 65,535. Instead of storing a floating-point value (which is usually 4 or 8 bytes) for a permittivity value at a point, Angora stores an index that represents the permittivity at that point. The same applies to other constitutive parameters (relative permeability, electric conductivity, etc.)

Each time a material region is read into the FDTD grid using MaterialsFromFiles, a fixed number of new constitutive parameter values are defined between the minimum and maximum values found in the file. Because of this discretization, some loss of information is inevitable. The number of new materials is determined by the variable max\_new\_materials; which is by equal to 1000 default. With the default value, the upper limit for the number of materials will be reached after about 65 material regions are inserted into the grid. If you wish to insert more material regions, and the dynamic ranges of constitutive parameters in your material files are not large, you can decrease max\_new\_materials. Alternatively, you may consider combining multiple material regions into a single region.

#### 6.5.5 Ground Planes

#### list GroundPlanes

[Sub-variable of SimulationSpace]

Infinitely thin perfect-electric-conductor (PEC) sheets can be placed in the grid using a GroundPlanes list. Currently, only z-oriented (parallel to the xy plane) sheets at integer (full-cell) positions are supported.

floating-point coord (units: m)

[Sub-variable of GroundPlanes]

integer coord\_in\_cells

[Sub-variable of GroundPlanes]

This variable specifies the z-coordinate of the ground plane with respect to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If the coordinate corresponds to a non-integer cell position, the closest integer position is chosen.

The GroundPlanes variable also updates the layering (stratification) information in the grid, much like MaterialSlabs (see Section 6.5.2 [Planar Layers], page 24).

#### 6.6 Waveforms

# group Waveforms

[Global variable]

In Angora, a *time waveform* is defined as a self-contained structure that can be used by other structures; such as a Hertzian dipole source or a plane-wave injector. The library of available time waveforms will be expanded in the future. Please send any comments, suggestions, and requests to help@angorafdtd.org.

An example usage of Waveforms:

```
Waveforms:
{
     GaussianWaveforms:
     (
          {
          ...
     }
    );
```

#### 6.6.1 Gaussian Waveforms

#### list GaussianWaveforms

[Sub-variable of Waveforms]

This variable is used to define Gaussian time waveforms given by the formula

$$f(t) = A \exp\left(\frac{-(t - n_{\tau}\tau)^2}{2\tau^2}\right)$$

The peak, 10%-amplitude (-20 dB power), and 1%-amplitude (-40 dB power) frequencies in the spectrum of the Gaussian are  $\omega=0,~\omega=2.15/\tau,~\omega=3.035/\tau$ , respectively.

Gaussian waveforms are defined as follows:

#### string waveform\_tag

[Sub-variable of GaussianWaveforms]

This is the string tag by which the waveform will later be referred to by another structure that requires a time waveform in its definition.

```
floating-point amplitude (default: [Sub-variable of Gaussian Waveforms] 1.0)
```

This specifies the variable A in the above equation defining the Gaussian waveform.

- floating-point tau (units: sec) [Sub-variable of Gaussian Waveforms] This specifies the variable  $\tau$  in the above equation defining the Gaussian waveform.
- floating-point delay (default: 0.0) [Sub-variable of Gaussian Waveforms] This specifies the variable  $n_{\tau}$  in the above equation defining the Gaussian waveform.

#### 6.6.2 Differentiated-Gaussian Waveforms

#### list DifferentiatedGaussianWaveforms

[Sub-variable of Waveforms]

This variable is used to define differentiated Gaussian time waveforms, given by the formula

$$f(t) = A \frac{d^n}{dt^n} \left[ \exp\left(\frac{-(t - n_\tau \tau)^2}{2\tau^2}\right) \right] = A \left(\frac{-1}{\tau \sqrt{2}}\right)^n H_n \left(\frac{t - n_\tau \tau}{\tau \sqrt{2}}\right) \exp\left(\frac{-(t - n_\tau \tau)^2}{2\tau^2}\right)$$

where  $H_n(x)$  are the (physicists') Hermite polynomials.

The peak frequency in the spectrum of the differentiated-Gaussian is  $\omega=1/\tau$ , the 10%-amplitude (-20 dB power) frequencies are  $\omega=0.06/\tau$  and  $\omega=2.76/\tau$ ; and the 1%-amplitude (-40 dB power) frequencies are  $\omega=0.006/\tau$  and  $\omega=3.57/\tau$ .

Differentiated Gaussian waveforms are defined as follows:

string waveform\_tag [Sub-variable of DifferentiatedGaussianWaveforms]

This is the string tag by which the waveform will later be referred to by another structure that requires a time waveform in its definition.

floating-point [Sub-variable of DifferentiatedGaussianWaveforms] amplitude (default: 1.0)

This specifies the variable A in the above equation defining the differentiated Gaussian waveform.

floating-point tau [Sub-variable of DifferentiatedGaussianWaveforms] (units: sec)

This specifies the variable  $\tau$  in the above equation defining the differentiated Gaussian waveform.

floating-point delay [Sub-variable of DifferentiatedGaussianWaveforms] (default: 0.0)

This specifies the variable  $n_{\tau}$  in the above equation defining the differentiated Gaussian waveform.

integer  $n_diff$  [Sub-variable of DifferentiatedGaussianWaveforms] This specifies the order of differentiation n in the above equation defining the differentiated Gaussian waveform.

## 6.6.3 Modulated-Gaussian Waveforms

#### list ModulatedGaussianWaveforms

[Sub-variable of Waveforms]

This variable is used to define sinusoidally-modulated Gaussian time waveforms, given by the formula

$$f(t) = A g(2\pi f_0(t - n_\tau \tau) + \phi) \exp\left(\frac{-(t - n_\tau \tau)^2}{2\tau^2}\right)$$

where the function g(t) is a sinusoidal function, being either  $\sin(t)$  or  $\cos(t)$ .

The peak frequency in the spectrum of the modulated-Gaussian is  $\omega = \omega_0 = 2\pi f_0$ , the 10%-amplitude (-20 dB power) frequencies are  $\omega = \omega_0 \pm 2.15/\tau$ ; and the 1%-amplitude (-40 dB power) frequencies are  $\omega = \omega_0 \pm 3.035/\tau$ . A MATLAB script named 'mod\_gaussian\_wf.m' is distributed as part of the Angora package, which calculates the center frequency  $f_0$  and the time constant  $\tau$  of a modulated-Gaussian waveform that has the desired lower and upper cutoff wavelengths, and the desired amount of attenuation at these wavelengths. It also outputs the -40 dB wavelength and the suggested maximum spatial time step in the simulation (which is the -40 dB wavelength divided by 15). This script is installed in the directory '\$(prefix)/share/angora/' (see Chapter 3 [Compilation and Installation], page 7). If Angora was installed without any \$(prefix) configuration option, the default location is '/usr/local/share/angora/'. This script can also be downloaded directly from the Angora website (link here).

Modulated Gaussian waveforms are defined as follows:

```
delay = 3;
    phase = 90;
    differentiated = false;
},
{
    ...
    ...
}
);
};
```

string waveform\_tag [Sub-variable of ModulatedGaussianWaveforms]

This is the string tag by which the waveform will later be referred to by another structure that requires a time waveform in its definition.

string modulation\_type [Sub-variable of ModulatedGaussianWaveforms] If assigned "sine", the modulation function g(t) in the above equation becomes a sine. If assigned "cosine", it becomes a cosine.

floating-point amplitude [Sub-variable of ModulatedGaussianWaveforms] (default: 1.0)

This specifies the variable A in the above equation defining the modulated Gaussian waveform.

floating-point tau (units: [Sub-variable of ModulatedGaussianWaveforms] sec)

This specifies the variable  $\tau$  in the above equation defining the modulated Gaussian waveform.

floating-point f\_0 (units: [Sub-variable of ModulatedGaussianWaveforms] Hz)

This specifies the modulation frequency  $f_0$  in the above equation defining the modulated Gaussian waveform.

floating-point delay [Sub-variable of ModulatedGaussianWaveforms] (default: 0.0)

This specifies the variable  $n_{\tau}$  in the above equation defining the modulated Gaussian waveform.

floating-point phase [Sub-variable of ModulatedGaussianWaveforms] (units: degrees, default: 0.0)

This specifies the extra phase  $\phi$  in the above equation defining the modulated Gaussian waveform. This phase should be specified in *degrees*, which is then converted internally to radians, which are the actual units of  $\phi$ .

boolean differentiated [Sub-variable of ModulatedGaussianWaveforms] (default: false)

If set to true, the waveform in the above equation is differentiated once with respect to time.

#### 6.7 Point Sources

#### list PointSources

[Global variable]

"Infinitesimal" electric dipole sources (also called *Hertzian* dipoles) can be simulated in Angora using the PointSources list.

A Hertzian dipole at position  $(x_0, y_0, z_0)$  is characterized by the following current distribution in space:

$$J(x, y, z; t) = \mathbf{a} j_0(t) \delta(x - x_0) \delta(y - y_0) \delta(z - z_0)$$

where  $\delta(x)$  is the Dirac delta function. The vector **a** determines the orientation of the dipole, which can be along the x, y, or z directions. The prefactor  $j_0(t)$  is called the current moment of the dipole, with the units (Ampere\*m).

Here is an example usage of PointSources:

```
floating-point coord_x (units: m) [Sub-variable of PointSources]
floating-point coord_y (units: m) [Sub-variable of PointSources]
floating-point coord_z (units: m) [Sub-variable of PointSources]
integer coord_x_in_cells [Sub-variable of PointSources]
integer coord_y_in_cells [Sub-variable of PointSources]
integer coord_z_in_cells [Sub-variable of PointSources]
```

These variables specify the Cartesian x, y, and z coordinates of the Hertzian dipole with respect to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If the coordinates correspond to non-integer cell positions, the closest integer positions are chosen.

```
string source_orientation
```

[Sub-variable of PointSources]

This string specifies the spatial orientation of the Hertzian dipole. It should be "x\_directed", "y\_directed", or "z\_directed".

#### string waveform\_tag

[Sub-variable of PointSources]

This string variable specifies the waveform of the current moment  $j_0(t)$ . The waveform is interpreted in (Ampere\*m) units. This should match a previously-defined tag in a Waveforms definition (see Section 6.6 [Waveforms], page 34).

floating-point j\_0 (units: Ampere/m, [Sub-variable of PointSources] default: 1.0)

This is an extra prefactor applied to the current moment waveform  $j_0(t)$ .

## 6.8 Near-Field-to-Far-Field Transformer

In many electromagnetic problems, it is of interest to calculate the radiated (or far-zone) field scattered from (or radiated by) the structures inside the grid. The radiated field is defined as the asymptotic form of the electric field at large distances, which decays as 1/r and propagates locally like a plane wave. Although the radial dependence is trivial in the far field, the angular dependence is highly variable. In finite numerical solution methods such as FDTD and FEM, it is only the near-field that is available in the computation grid. It is hugely impractical to extend the computation grid to large distances where the field assumes an asymptotic form. Luckily, certain theorems of electromagnetics (Huygens' principle, equivalence theorem, etc.) allow the calculation of the far field using this near field information. This procedure is called a **near-field-to-far-field transform** (NFFFT). There are two main types of NFFFTs. In the first type, the far-field waveforms are calculated directly in time domain. In the second, the frequency (or phasor) components in the Fourier decomposition of the far-field waveforms are calculated at a number of frequencies. Angora features both time-domain and phasor domain NFFFTs.

#### 6.8.1 Time-Domain Near-Field-to-Far-Field-Transformer

In the *time-domain* NFFFT, the far-field waveforms (normalized by the distance r, and advanced in time by r/c) are calculated directly using time-domain Green's functions for the particular space. Currently, the time-domain NFFFT supports up to *three* lossless infinite planar material layers with only permittivity variations.

The time-domain NFFFT should be used when the far-field waveforms are to be computed over only a few observation directions. The additional computational burden per observation direction is much larger than that of the phasor-domain NFFFT. The format used for the time-domain far-field output is **HDF5** (Hierarchical Data Format) (http://www.hdfgroup.org/HDF5/). The HDF5 format was chosen for its standard interface, and the availability of free software tools for inspecting and modifying HDF5 output. The HDF5 output created by the time-domain NFFFT is explained in more detail in Section 6.8.1.1 [HDF5 Content of Time-Domain NFFFT Output], page 44.

The radiated electric field can be expressed in the form

$$\bar{E}^r(r,\theta,\phi;t) = \bar{E}(\theta,\phi;t-r/c)/r$$
.

The time-domain NFFFT only calculates the angle and time-dependent part of the above expression, namely,  $\bar{E}(\theta, \phi; t)$ .

```
string td_nffft_output_dir (default: "nffft/td")
                                                                    [Global variable]
     This determines the subdirectory in which all the time-domain-NFFFT output will
     be placed. Unless it has a slash '/' up front; this path is interpreted as being relative
     to output_dir (see Section 6.12 [Paths], page 86).
           td_nffft_output_dir = "nffft/td";
           TimeDomainNFFFT:
           {
                    . . .
           };
list TimeDomainNFFFT
                                                                    [Global variable]
     Time-domain NFFFTs are defined inside a TimeDomainNFFFT list, each within its own
     group:
           TimeDomainNFFFT:
           (
               {
                   theta = 36;
                   phi = 57;
                   write_hertzian_dipole_far_field = false;
                   nffft_back_margin_x_in_cells = 3;
                   nffft_front_margin_x_in_cells = 3;
                   nffft_left_margin_y_in_cells = 3;
                   nffft_right_margin_y_in_cells = 3;
                   nffft_lower_margin_z_in_cells = 3;
                   nffft_upper_margin_z_in_cells = 3;
                   far_field_origin_x = 0;
                   far_field_origin_y = 0;
                   far_field_origin_z = 0;
                   far_field_dir = "my_dir";
                   far_field_file_name = "FarField_td";
                    far_field_file_extension = "hd5";
                    append_group_index_to_file_name = true;
               },
               {
               }
           );
     floating-point theta (units:
                                                [Sub-variable of TimeDomainNFFFT]
               degrees)
     floating-point phi (units: degrees)
                                                [Sub-variable of TimeDomainNFFFT]
           The direction at which the time-domain far field will be calculated is expressed
           in terms of the traditional spherical-coordinate variables (\theta, \phi). The first of
           these angles is the zenith angle, while the second is the azimuth angle. In
```

Figure 6.4, the definitions of these angles are shown schematically. The theta

variable specifies the zenith angle in degrees. Although this angle is traditionally defined between 0 and 180deg, theta can be assigned any negative or positive value. The phi variable specifies the azimuth angle in degrees. Although this angle is traditionally defined between 0 and 360deg, phi can be assigned any negative or positive value.

boolean [Sub-variable of TimeDomainNFFFT] write\_hertzian\_dipole\_far\_field (default: false)

If set to true, the theoretical far field waveforms due to the Hertzian point sources (see Section 6.7 [Point Sources], page 39) in the simulation grid are also written into the output file. Any planar stratification up to three lossless layers with permittivity variations is accounted for in the calculation of the theoretical far field, but the scattering from any other structure inside the grid is ignored. As such, this feature can be (and has been) used to test the timedomain NFFFT.

floating-point [Sub-variable of TimeDomainNFFFT] nffft\_right\_margin\_y (units:m)

The near field is collected over the surface of a rectangular prism in the grid, called the *NFFFT surface*. This surface should enclose all the scattering and/or radiating structures in the grid, as well as the total-field/scattered-field surface

(see Section 6.10 [Incident Beams], page 63). By default, this rectangular box is placed 3 grid cells away from the PML boundary (see Section 6.2.4 [Perfectly-Matched Layer (PML)], page 15). You can specify different margins to reduce the computational burden associated with the NFFFT. This burden is directly proportional to the surface area of the box. The margins can be specified in meters or in grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If given in meters, the margins are rounded to the nearest multiple of the spatial step size.

floating-point [Sub-variable of TimeDomainNFFFT] far\_field\_origin\_x (units: m, default: 0)

floating-point [Sub-variable of TimeDomainNFFFT] far\_field\_origin\_y\_in\_cells (default: 0)

These variables set the coordinates of the point relative to which the far field will be calculated. The distance r in [eq:far\_field\_angle\_dependence\_time\_domain], page 40 is with respect to this point. The coordinates of the far-field origin are with respect to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

string far\_field\_dir (default: "") [Sub-variable of TimeDomainNFFFT] This determines the subdirectory in which this individual far-field file will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to td\_nffft\_output\_dir (see [td\_nffft\_output\_dir], page 40). By default, no subdirectory is created inside td\_nffft\_output\_dir.

This determines the base string in the full name of the far-field file. Other information is appended to the name of the file to differentiate individual far-field files (see the example below).

This is the extension of the far-field file name. If assigned the value "", no extension is added to the file. The HDF5 extension "hd5" is applied by default.

Here is an example far-field file name:

#### FarField\_td\_0\_1.hd5

The base string in the name of the file ("FarField\_td") is specified by the far\_field\_file\_name variable. The two integers that follow are the run index (see Section 6.14 [Multiple Simulation Runs], page 87) and the index of the time-domain NFFFT inside the TimeDomainNFFFT list. For example, if there are two groups (two NFFFTs) in the TimeDomainNFFFT list, the first one will write into

FarField\_td\_0\_0.hd5

while the second will write into

FarField\_td\_0\_1.hd5

If there are two simulation runs (i.e., number\_of\_runs is equal to 2 – see Section 6.14 [Multiple Simulation Runs], page 87), then the files created in the second run will have 1 instead of 0 as the first integer in the above file names. Finally, the extension ("hd5") of the line files is determined by the variable far\_field\_file\_extension.

boolean

[Sub-variable of TimeDomainNFFFT]

append\_group\_index\_to\_file\_name (default: true)

If this is set to false, the second integer in the filename (see above) and the underscore preceding it are not included in the filename. It is set to true by default. If this variable is set to false and there are multiple groups (time-domain NFFFTs), there will be a name clash, and the output will be undefined.

# 6.8.1.1 HDF5 Content of Time-Domain NFFFT Output

The HDF5 file created as the output of the time-domain NFFFT can be viewed and modified using freely-available tools. One of these tools is HDFView, provided by the HDF Group. MATLAB also has built-in functions and tools that handle HDF5 files. For reference, a MATLAB script named 'hdf5\_read.m' is distributed as part of the Angora package, which reads an HDF5 dataset from an HDF5 file into a MATLAB array. This script is installed in the directory '\$(prefix)/share/angora/' (see Chapter 3 [Compilation and Installation], page 7). If Angora was installed without any \$(prefix) configuration option, the default location is '/usr/local/share/angora/'. This script can also be downloaded directly from the Angora website (link here). For example, if you want to read the dataset named theta from the file 'my\_file.hd5', use

```
>> theta = hdf5_read('my_file.hd5','theta');
```

In MATLAB R2011a and later, there is a high-level built-in function h5read that could be used for the same purpose.

The HDF5 datasets in the far-field file are the following:

- 'angora\_version': Integer array of length 3 with the major version, minor version, and revision numbers of the Angora package used to create the file.
- 'theta': A floating-point value for the spherical zenith angle at which the far field is calculated (in radians).
- 'phi': A floating-point value for the spherical azimuth angle at which the far field is calculated (in radians).
- 'time\_step': A floating-point value specifying the temporal step in the simulation (in sec).

- 'initial\_time\_value': A floating-point value specifying the time value corresponding to the beginning of the simulation (in sec). This is usually a negative value, since time waveforms frequently begin before t=0.
- Floating-point arrays with the waveforms of different components of the vector radiated electric field. See Figure 6.4 for a graphical illustration of the unit vectors in spherical coordinates. Note that only the angle and time-dependent part of the radiated electric field is calculated (see [eq:far\_field\_angle\_dependence\_time\_domain], page 40). Because the (1/r) dependence has been factored out, the units are in Volts.

'E\_theta': 1-D array with the theta component of the radiated electric field.

- 'E\_phi': 1-D array with the phi component of the radiated electric field.
- If the theoretical far field due to Hertzian point sources is also calculated (namely, write\_hertzian\_dipole\_far\_field is true):

'E\_theta\_th': 1-D array with the *theoretical* theta component of the radiated electric field created by the Hertzian dipoles in the simulation grid.

• 'E\_phi\_th': 1-D array with the *theoretical* phi component of the radiated electric field created by the Hertzian dipoles in the simulation grid.

## 6.8.2 Phasor-Domain Near-Field-to-Far-Field-Transformer

The *phasor-domain* NFFFT calculates the amplitude of the far field at individual frequencies using Fourier decomposition. This NFFFT supports free space as well as **infinite planar layered media** with arbitrary permittivity, permeability and conductivity profiles (see [Capoglu12], page 90). Infinite planar layers are created using the MaterialSlabs variable (see Section 6.5.2 [Planar Layers], page 24).

The phasor-domain NFFFT in Angora calculates far-field values over a two-dimensional array of observation directions and a range of wavelengths; resulting in a three-dimensional array. The spacing of the wavelengths and the arrangement of observation directions is highly configurable. The format used for the phasor-domain far-field output is **HDF5** (Hierarchical Data Format) (http://www.hdfgroup.org/HDF5/). The HDF5 format was chosen for its standard interface, and the availability of free software tools for inspecting and modifying HDF5 output. The HDF5 output created by the phasor-domain NFFFT is explained in more detail in Section 6.8.2.1 [HDF5 Content of Phasor-Domain NFFFT Output], page 52.

Angora uses the engineering convention  $\exp(j\omega t)$  for time-harmonic quantities. The time-domain data on the surface of a rectangular prism in the grid, called the NFFFT surface, is decomposed into its phasor components by a numerical approximation to the temporal Fourier transform  $F(\omega) = \frac{1}{2\pi} \int f(t) \exp(-j\omega t) dt$ . Because of the  $\frac{1}{2\pi}$  term, the phasor quantities  $F(\omega)$  correspond to the true Fourier components of the time-domain quantities on the NFFFT surface. These quantities are then inserted into phasor-domain electromagnetic theorems linking the near field to the far field. The complex phasor output data therefore also corresponds to the Fourier components of the far-field temporal waveforms.

In the phasor domain, the radiated electric field can be expressed in the form

$$\bar{E}^r(r,\theta,\phi) = \bar{E}(\theta,\phi) \exp(-jkr)/r$$
.

The phasor-domain NFFFT only calculates the *angle-dependent* part of the above expression, namely,  $\bar{E}(\theta,\phi)$ . In Figure 6.4, the angles and unit vectors are shown for spherical coordinates.

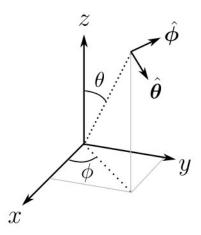


Figure 6.4: The angles and unit vectors for spherical coordinates.

# string pd\_nffft\_output\_dir (default: "nffft/pd") [Global variable]

This determines the subdirectory in which all the phasor-domain-NFFFT output will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to output\_dir (see Section 6.12 [Paths], page 86).

#### list PhasorDomainNFFFT

[Global variable]

Phasor-domain NFFFTs are defined inside a PhasorDomainNFFFT list, each within its own group:

```
dir2_min=0.0;
        dir2_max=360.0;
        limit_to_s = 1.0;
        write_hertzian_dipole_far_field = false;
        nffft_back_margin_x_in_cells = 3;
        nffft_front_margin_x_in_cells = 3;
        nffft_left_margin_y_in_cells = 3;
        nffft_right_margin_y_in_cells = 3;
        nffft_lower_margin_z_in_cells = 3;
        nffft_upper_margin_z_in_cells = 3;
        far_field_origin_x = 0.0;
        far_field_origin_y = 0.0;
        far_field_origin_z = 0.0;
        far_field_dir = "my_dir";
        far_field_file_name = "FarField_pd";
        far_field_file_extension = "hd5";
        append_group_index_to_file_name = true;
    },
    {
    }
);
```

integer num\_of\_lambdas

[Sub-variable of PhasorDomainNFFFT]

This specifies the number of wavelengths (in vacuum) at which the far field will be calculated.

```
floating-point lambda_min (units: [Sub-variable of PhasorDomainNFFFT] m)
```

floating-point

[Sub-variable of PhasorDomainNFFFT]

lambda\_min\_in\_cells

This value sets the lower limit of the wavelength range (in vacuum) over which the far field is calculated. The far field may or may not be calculated at the wavelength lambda\_min, depending on the variable do\_not\_include\_first\_lambda. The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

```
\begin{array}{ccc} \textbf{floating-point lambda\_max} & (units: & [Sub-variable of PhasorDomainNFFFT] \\ & & m) \end{array}
```

floating-point

[Sub-variable of PhasorDomainNFFFT]

lambda\_max\_in\_cells

This value sets the upper limit of the wavelength range (in vacuum) over which the far field is calculated. The far field may or may not be calculated at the wavelength lambda\_max, depending on the variable do\_not\_include\_last\_lambda. The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

### string lambda\_spacing\_type

[Sub-variable of PhasorDomainNFFFT] This string specifies how the wavelengths will be spaced between the two end points determined by lambda\_min, lambda\_max, do\_not\_include\_first\_

lambda, and do\_not\_include\_last\_lambda.

- "lambda-linear": The wavelengths are spaced lineary between the two end points.
- "k-linear": The wavenumbers  $k = 2\pi/\lambda$  are spaced linearly between the two end points. Since the wavenumber is also equal to  $k = \omega/c$ , where  $\omega$ is the radian frequency, this causes the frequencies to be spaced linearly as
- "log": The logarithms of the wavelengths (therefore the logarithms of the wavenumbers) are spaced linearly between the two end points.

boolean

[Sub-variable of PhasorDomainNFFFT]

do\_not\_include\_first\_lambda (default: false)

boolean

[Sub-variable of PhasorDomainNFFFT]

do\_not\_include\_last\_lambda (default: false)

Let's assume that lambda\_spacing\_type is lambda-linear. For k-linear and log, replace lambda\_min in the following by  $2\pi$  / lambda\_min and log(lambda\_ min), respectively. The same applies to lambda\_max.

- If do\_not\_include\_first\_lambda=false and do\_not\_include\_last\_ lambda=false: The interval between lambda\_min and lambda\_max is divided into (num\_of\_lambdas-1) equal intervals. A total of num\_of\_lambdas wavelengths are placed linearly at the boundaries between the intervals, including both endpoints lambda\_min and lambda\_max.
- If do\_not\_include\_first\_lambda=true and do\_not\_include\_last\_ lambda=false: The interval between lambda\_min and lambda\_max is divided into num\_of\_lambdas equal intervals. A total of num\_of\_lambdas wavelengths are placed linearly at the boundaries between the intervals, excluding the endpoint lambda\_min.
- If do\_not\_include\_first\_lambda=false and do\_not\_include\_last\_ lambda=true: The interval between lambda\_min and lambda\_max is divided into num\_of\_lambdas equal intervals. A total of num\_of\_lambdas wavelengths are placed linearly at the boundaries between the intervals, excluding the endpoint lambda\_max.
- If do\_not\_include\_first\_lambda=true and do\_not\_include\_last\_ lambda=true: The interval between lambda\_min and lambda\_max is divided into num\_of\_lambdas equal intervals. A total of num\_of\_lambdas wavelengths are placed at the midpoints of each interval.

## string direction\_spec

[Sub-variable of PhasorDomainNFFFT]

This string specifies how the observation directions are arranged in a twodimensional array.

• "theta-phi": The first dimension is the spherical polar angle  $\theta$ , defined as the angle between the observation direction and the z-axis. The second dimension is the spherical azimuth angle  $\phi$ , defined as the angle between the x-axis and the projection of the observation direction onto the xy-plane. See Figure 6.4 for a graphical illustration. These angles are spaced linearly between their respective endpoints.

• "dircosx-dircosy-upper" or "dircosx-dircosy-lower": The first dimension is the x-direction-cosine  $s_x = \sin\theta\cos\phi$  while the second dimension is the y-direction-cosine  $s_y = \sin\theta\sin\phi$ . These direction cosines are spaced linearly between their respective endpoints. The suffix "-upper" or "-lower" determines whether the observation direction is in the upper half space (+z direction) or the lower half space (-z direction).

#### integer num\_of\_dirs\_1

[Sub-variable of PhasorDomainNFFFT]

This is the number of observation directions over the first dimension of the two-dimensional observation-direction array. If direction\_spec is "theta-phi", this is the number of  $\theta$  values; otherwise, the number of x-direction-cosines  $s_x = \sin\theta\cos\phi$ .

floating-point dir1\_min

[Sub-variable of PhasorDomainNFFFT]

floating-point dir1\_max

[Sub-variable of PhasorDomainNFFFT]

These are the minimum/maximum values of either the  $\theta$  angle (in degrees), or the x-direction-cosine (between -1 and 1).

#### integer num\_of\_dirs\_2

[Sub-variable of PhasorDomainNFFFT]

This is the number of observation directions over the second dimension of the two-dimensional observation-direction array. If direction\_spec is "theta-phi", this is the number of  $\phi$  values; otherwise, the number of y-direction-cosines  $s_y = \sin\theta\sin\phi$ .

floating-point dir2\_min

[Sub-variable of PhasorDomainNFFFT]

floating-point dir2\_max

[Sub-variable of PhasorDomainNFFFT]

These are the minimum/maximum values of either the  $\phi$  angle (in degrees), or the y-direction-cosine (between -1 and 1).

# floating-point limit\_to\_s

[Sub-variable of PhasorDomainNFFFT]

(default: 1)

If direction\_spec is "dircosx-dircosy-upper" or "dircosx-dircosy-lower" (the direction cosines are used to specify the observation directions), it might happen that some combinations of  $s_x$  and  $s_y$  do not correspond to a real observation direction, since  $s_x^2 + s_y^2 > 1$ . Such direction cosines are automatically assigned a far-field value of zero. If you would like to limit the direction cosines further into a narrower observation cone, you can choose the value of limit\_to\_s to be smaller than 1.0. Then, the far field corresponding to the direction cosines satisfying  $s_x^2 + s_y^2 > (\text{limit_to_s})$  are assigned a zero value. Although this could also be done in post processing, eliminating some observation directions in this way removes the burden of computing them in the first place. Specifying a limit\_to\_s value corresponds to reducing the numerical aperture in a microscope objective.

```
boolean
                                         [Sub-variable of PhasorDomainNFFFT]
         write_hertzian_dipole_far_field (default: false)
     If set to true, the theoretical far field due to the Hertzian point sources (see
     Section 6.7 [Point Sources], page 39) in the simulation grid is also written into
     the output file. Any planar stratification is accounted for in the calculation of
     the theoretical far field, but the scattering from any other structure inside the
     grid is ignored. As such, this feature can be (and has been) used to test the
     phasor-domain NFFFT.
floating-point
                                         [Sub-variable of PhasorDomainNFFFT]
         nffft_back_margin_x (units:m)
floating-point
                                         [Sub-variable of PhasorDomainNFFFT]
         nffft_front_margin_x (units:m)
floating-point
                                          [Sub-variable of PhasorDomainNFFFT]
         nffft_left_margin_y (units:m)
floating-point
                                         [Sub-variable of PhasorDomainNFFFT]
         nffft_right_margin_y (units:m)
floating-point
                                         [Sub-variable of PhasorDomainNFFFT]
         nffft_lower_margin_z (units:m)
                                         [Sub-variable of PhasorDomainNFFFT]
floating-point
         nffft_upper_margin_z (units:m)
                                         [Sub-variable of PhasorDomainNFFFT]
integer
         nffft_back_margin_x_in_cells (default: 3)
                                         [Sub-variable of PhasorDomainNFFFT]
integer
         nffft_front_margin_x_in_cells (default: 3)
                                         [Sub-variable of PhasorDomainNFFFT]
integer
         nffft_left_margin_y_in_cells (default: 3)
                                          [Sub-variable of PhasorDomainNFFFT]
integer
         nffft_right_margin_y_in_cells (default: 3)
                                         [Sub-variable of PhasorDomainNFFFT]
integer
         nffft_lower_margin_z_in_cells (default: 3)
                                         [Sub-variable of PhasorDomainNFFFT]
integer
         nffft_upper_margin_z_in_cells (default: 3)
     The near field is collected over the surface of a rectangular prism in the grid,
     called the NFFFT surface. This surface should enclose all the scattering and/or
     radiating structures in the grid, as well as the total-field/scattered-field surface
     (see Section 6.10 [Incident Beams], page 63). By default, this rectangular box is
     placed 3 grid cells away from the PML boundary (see Section 6.2.4 Perfectly-
     Matched Layer (PML), page 15). You can specify different margins to reduce
     the computational burden associated with the NFFFT. This burden is directly
     proportional to the surface area of the box. The margins can be specified in
     meters or in grid cells. For the latter, the <u>_in_cells</u> suffix should be appended
```

to the variable name. If given in meters, the margins are rounded to the nearest

multiple of the spatial step size.

floating-point [Sub-variable of PhasorDomainNFFFT]

far\_field\_origin\_x (units: m, default: 0)

floating-point [Sub-variable of PhasorDomainNFFFT]

far\_field\_origin\_y (units: m, default: 0)

floating-point [Sub-variable of PhasorDomainNFFFT]

far\_field\_origin\_z (units: m, default: 0)

floating-point [Sub-variable of PhasorDomainNFFFT]

far\_field\_origin\_x\_in\_cells (default: 0)

floating-point [Sub-variable of PhasorDomainNFFFT]

far\_field\_origin\_y\_in\_cells (default: 0)

floating-point [Sub-variable of PhasorDomainNFFFT] far\_field\_origin\_z\_in\_cells (default: 0)

These variables set the coordinates of the point relative to which the far field will be calculated. The distance r in [eq:far\_field\_angle\_dependence], page 45 is with respect to this point. The coordinates of the far-field origin are with respect to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

string far\_field\_dir (default: "") [Sub-variable of PhasorDomainNFFFT] This determines the subdirectory in which this individual far-field file will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to pd\_nffft\_output\_dir (see [pd\_nffft\_output\_dir], page 46). By default, no subdirectory is created inside pd\_nffft\_output\_dir.

This determines the base string in the full name of the far-field file. Other information is appended to the name of the file to differentiate individual far-field files (see the example below).

This is the extension of the far-field file name. If assigned the value "", no extension is added to the file. The HDF5 extension "hd5" is applied by default.

Here is an example far-field file name:

FarField\_pd\_0\_1.hd5

The base string in the name of the file ("FarField\_pd") is specified by the far\_field\_file\_name variable. The two integers that follow are the run index (see Section 6.14 [Multiple Simulation Runs], page 87) and the index of the phasor-domain NFFFT inside the PhasorDomainNFFFT list. For example, if there are two groups (two NFFFTs) in the PhasorDomainNFFFT list, the first one will write into

FarField\_pd\_0\_0.hd5

while the second will write into

## FarField\_pd\_0\_1.hd5

If there are two simulation runs (i.e., number\_of\_runs is equal to 2 – see Section 6.14 [Multiple Simulation Runs], page 87), then the files created in the second run will have 1 instead of 0 as the first integer in the above file names. Finally, the extension ("hd5") of the line files is determined by the variable far\_field\_file\_extension.

boolean

[Sub-variable of PhasorDomainNFFFT]

append\_group\_index\_to\_file\_name (default: true)

If this is set to false, the second integer in the filename (see above) and the underscore preceding it are not included in the filename. It is set to true by default. If this variable is set to false and there are multiple groups (phasordomain NFFFTs), there will be a name clash, and the output will be undefined.

# 6.8.2.1 HDF5 Content of Phasor-Domain NFFFT Output

The HDF5 file created as the output of the phasor-domain NFFFT can be viewed and modified using freely-available tools. One of these tools is HDFView, provided by the HDF Group. MATLAB also has built-in functions and tools that handle HDF5 files. For reference, a MATLAB script named 'hdf5\_read.m' is distributed as part of the Angora package, which reads an HDF5 dataset from an HDF5 file into a MATLAB array. This script is installed in the directory '\$(prefix)/share/angora/' (see Chapter 3 [Compilation and Installation], page 7). If Angora was installed without any \$(prefix) configuration option, the default location is '/usr/local/share/angora/'. This script can also be downloaded directly from the Angora website (link here). For example, if you want to read the dataset named lambda from the file 'my\_file.hd5', use

```
>> lambda = hdf5_read('my_file.hd5','lambda');
```

In MATLAB R2011a and later, there is a high-level built-in function h5read that could be used for the same purpose.

The HDF5 datasets in the far-field file are the following:

- 'angora\_version': Integer array of length 3 with the major version, minor version, and revision numbers of the Angora package used to create the file.
- 'lambda': 1-D array with the recorded free-space wavelength values (in m).
- If direction\_spec is "theta-phi":
  - 'theta': 1-D array with the theta values.
  - 'phi': 1-D array with the phi values.
- If direction\_spec is "dircosx-dircosy-upper" or "dircosx-dircosy-lower":
  - 'dircos\_x': 1-D array with the x-direction-cosine values.
  - 'dircos\_y': 1-D array with the y-direction-cosine values.
- Floating-point arrays with the real and imaginary parts of different components of the vector radiated electric field. See Figure 6.4 for a graphical illustration of the unit vectors in spherical coordinates. Note that only the angle-dependent part of the radiated electric field is calculated (see [eq:far\_field\_angle\_dependence], page 45). Because the (1/r) dependence has been factored out, the units are in Volts. The first dimension is the wavelength, the second is either theta or the x-direction-cosine, and the third is either phi or the y-direction-cosine.

'E\_theta\_r', 'E\_theta\_i': 3-D arrays with the real and imaginary parts of the theta component of the radiated electric field.

- 'E\_phi\_r', 'E\_phi\_i': 3-D arrays with the real and imaginary parts of the phi component of the radiated electric field.
- If the theoretical far field due to Hertzian point sources is also calculated (namely, write\_hertzian\_dipole\_far\_field is true):

'E\_theta\_th\_r', 'E\_theta\_th\_i': 3-D arrays with the *theoretical* real and imaginary parts of the theta component of the radiated electric field created by the Hertzian dipoles in the simulation grid.

• 'E\_phi\_th\_r', 'E\_phi\_th\_i': 3-D arrays with the *theoretical* real and imaginary parts of the phi component of the radiated electric field created by the Hertzian dipoles in the simulation grid.

# 6.9 Optical Imaging

Angora can synthesize numerical **optical images** created by an ideal imaging system. The image is calculated in the form of a field distribution on a two-dimensional plane in the image space; which is assumed homogeneous. In photolithography, this image distribution is commonly called an *aerial image*.

The optical axis of the imaging system is currently limited to the z axis. The collection can be either through the +z or -z direction, allowing the simulation of reflection or transmission-mode imaging without changing the illumination scheme. Angora internally utilizes a near-field-to-far-field transformer (NFFFT) (see Section 6.8 [Near-Field-to-Far-Field Transformer], page 40) to calculate the optical image.

In Figure 6.5, a simplified representation is shown for the optical imaging geometry. The illumination scheme is not shown in the figure, and the collection is assumed to be through the upper half space. The entire optical system is represented by a single lens, although the system may comprise multiple lenses, apertures, stops, etc. The only assumptions regarding the optical system is that it satisfies Abbe's sine condition, and it is telecentric (see [Capoglu12b], page 90). Telecentricity implies that the entrance pupil is actually at infinity, although it is shown at a finite distance for ease of presentation in the figure.

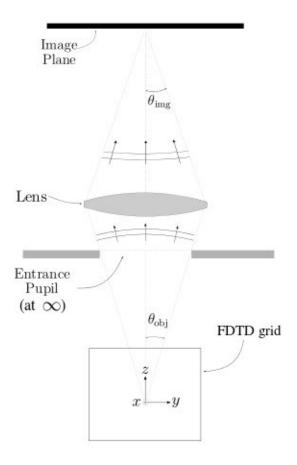


Figure 6.5: A simplified depiction of the optical imaging geometry.

The format used for the optical imaging output is **HDF5** (Hierarchical Data Format) (http://www.hdfgroup.org/HDF5/). The HDF5 format was chosen for its standard interface, and the availability of free software tools for inspecting and modifying HDF5 output. The HDF5 content of the optical image file is explained in more detail in Section 6.9.1 [Optical Image File HDF5 Content], page 61.

```
string imaging_output_dir (default: "imaging/") [Global variable]
This determines the subdirectory in which all the optical-imaging output will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to output_dir (see Section 6.12 [Paths], page 86).
```

#### list OpticalImages

[Global variable]

Optical images are defined in an OpticalImages list:

```
OpticalImages:
    {
        output_data = ["E_x_tot", "E_y_tot", "E_z_tot",
                        "E_x_sca", "E_y_sca", "E_z_sca",
                        "E_x_unsca", "E_y_unsca", "E_z_unsca",
                        "intensity_tot",
                        "intensity_sca",
                        "intensity_unsca"];
        num_of_lambdas = 5;
        lambda_min = 400e-9;
        lambda_max = 700e-9;
        lambda_spacing_type = "k-linear";
        do_not_include_first_lambda = false;
        do_not_include_last_lambda = false;
        ap_half_angle = 36.87;
        magnification = 40.0;
        image_space_refr_index = 1.0;
        image_expansion_factor_x = 1.0;
        image_expansion_factor_y = 1.0;
        image_oversampling_rate_x = 1.0;
        image_oversampling_rate_y = 1.0;
        coll_half_space = "upper";
        nffft_back_margin_x_in_cells = 3;
        nffft_front_margin_x_in_cells = 3;
        nffft_left_margin_y_in_cells = 3;
        nffft_right_margin_y_in_cells = 3;
        nffft_lower_margin_z_in_cells = 3;
        nffft_upper_margin_z_in_cells = 3;
        image_origin_x = 0.0;
        image_origin_y = 0.0;
        image_origin_z = 0.0;
        image_dir = "";
        image_file_name = "Image";
        image_file_extension = "hd5";
        append_group_index_to_file_name = true;
    },
        . . .
        . . .
    }
);
```

# string-array output\_data

[Sub-variable of OpticalImages]

This array of strings determines what will be included in the final output file. Any combination of the following strings can be listed in the array.

• "E\_x\_sca", "E\_y\_sca", "E\_z\_sca": The x, y, and z components of the

scattered electric field of the image. This is the electric field that is scattered or generated by the structures inside the simulation grid. The incident beams (see Section 6.10 [Incident Beams], page 63) and the reflections and transmissions from the infinite planar layer interfaces are *not* included in the scattered field.

- "E\_x\_unsca", "E\_y\_unsca", "E\_z\_unsca": The x, y, and z components of the *unscattered* electric field of the image. This is the electric field that would be created at the image plane in the absence of any scatterer inside the simulation grid except the infinite planar layers. The portion of the incident beams (see Section 6.10 [Incident Beams], page 63) and the reflections and transmissions from the infinite planar layer interfaces that fall into the collection aperture contribute to the unscattered field.
- "E\_x\_tot", "E\_y\_tot", "E\_z\_tot": The x, y, and z components of the total electric field of the image, defined as the sum of the scattered and unscattered fields above.
- "intensity\_sca": The scattered light intensity at the image plane (in W/m^2), defined as  $I_{sca} = n_{img}|E_{sca}|^2/\eta_0$  where  $n_{img}$  is the image-side refractive index, and  $\eta_0$  is the free-space wave impedance (=376.7303...Ohms).  $E_{sca}$  is the scattered electric field vector.
- "intensity\_unsca": The unscattered light intensity at the image plane (in W/m^2), defined as  $I_{unsca} = n_{img}|E_{unsca}|^2/\eta_0$  where  $n_{img}$  is the image-side refractive index, and  $\eta_0$  is the free-space wave impedance (=376.7303...Ohms).  $E_{unsca}$  is the unscattered electric field vector.
- "intensity\_tot": The total light intensity at the image plane (in W/m^2), defined as  $I_{tot} = n_{img}|E_{tot}|^2/\eta_0$  where  $n_{img}$  is the image-side refractive index, and  $\eta_0$  is the free-space wave impedance (=376.7303...Ohms).  $E_{tot}$  is the total electric field vector.

For example, if the output\_data array is

```
output_data = ["E_x_sca","intensity_tot"];
```

then only the x-component of the scattered electric field of the image and the total light intensity of the image are recorded in the output.

#### integer num\_of\_lambdas

[Sub-variable of OpticalImages]

This specifies the number of wavelengths (in vacuum) at which the optical image will be calculated.

floating-point lambda\_min (units: m) [Sub-variable of OpticalImages]

floating-point lambda\_min\_in\_cells [Sub-variable of OpticalImages]

This value sets the lower limit of the wavelength range (in vacuum) over which the optical image is calculated. The optical image may or may not be calculated at the wavelength lambda\_min, depending on the variable do\_not\_include\_first\_lambda. The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

floating-point lambda\_max (units: m) [Sub-variable of OpticalImages]

floating-point lambda\_max\_in\_cells [Sub-variable of OpticalImages]

This value sets the upper limit of the wavelength range (in vacuum) over which the optical image is calculated. The optical image may or may not be calculated at the wavelength lambda\_max, depending on the variable do\_not\_include\_last\_lambda. The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

#### string lambda\_spacing\_type

[Sub-variable of OpticalImages]

This string specifies how the wavelengths will be spaced between the two end points determined by lambda\_min, lambda\_max, do\_not\_include\_first\_lambda, and do\_not\_include\_last\_lambda.

- "lambda-linear": The wavelengths are spaced lineary between the two end points.
- "k-linear": The wavenumbers  $k=2\pi/\lambda$  are spaced linearly between the two end points. Since the wavenumber is also equal to  $k=\omega/c$ , where  $\omega$  is the radian frequency, this causes the frequencies to be spaced linearly as well.
- "log": The logarithms of the wavelengths (therefore the logarithms of the wavenumbers) are spaced linearly between the two end points.

boolean do\_not\_include\_first\_lambda [Sub-variable of OpticalImages] (default: false)

boolean do\_not\_include\_last\_lambda [Sub-variable of OpticalImages] (default: false)

Let's assume that lambda\_spacing\_type is lambda-linear. For k-linear and log, replace lambda\_min in the following by  $2\pi/$  lambda\_min and log(lambda\_min), respectively. The same applies to lambda\_max.

- If do\_not\_include\_first\_lambda=false and do\_not\_include\_last\_ lambda=false: The interval between lambda\_min and lambda\_max is divided into (num\_of\_lambdas-1) equal intervals. A total of num\_of\_lambdas wavelengths are placed linearly at the boundaries between the intervals, including both endpoints lambda\_min and lambda\_max.
- If do\_not\_include\_first\_lambda=true and do\_not\_include\_last\_ lambda=false: The interval between lambda\_min and lambda\_max is divided into num\_of\_lambdas equal intervals. A total of num\_of\_lambdas wavelengths are placed linearly at the boundaries between the intervals, excluding the endpoint lambda\_min.
- If do\_not\_include\_first\_lambda=false and do\_not\_include\_last\_ lambda=true: The interval between lambda\_min and lambda\_max is divided into num\_of\_lambdas equal intervals. A total of num\_of\_lambdas wavelengths are placed linearly at the boundaries between the intervals, excluding the endpoint lambda\_max.

• If do\_not\_include\_first\_lambda=true and do\_not\_include\_last\_ lambda=true: The interval between lambda\_min and lambda\_max is divided into num\_of\_lambdas equal intervals. A total of num\_of\_lambdas wavelengths are placed at the midpoints of each interval.

# floating-point ap\_half\_angle (units: [Sub-variable of OpticalImages] degrees)

This is the half-angle of the collection cone over which the far field is collected. This angle is represented by  $\theta_{\rm obj}$  in Figure 6.5

```
floating-point magnification (default: [Sub-variable of OpticalImages]

1)
```

This is the absolute value of the *lateral magnification* of the optical imaging system. If greater than 1, the imaging system shows a magnified image of the object. This is the case in *microscopy*, where the magnification ranges from 10 to 100. If less than 1, the image is a de-magnified version of the object, This is the case in *photolithography*, where a de-magnified image of a mask is projected on a photoresist. Typical magnifications in photolithography are 0.1 to 0.25.

# floating-point image\_space\_refr\_index [Sub-variable of OpticalImages] (default: 1)

This variable specifies the refractive index of the image space, assumed to be homogeneous.

# floating-point [Sub-variable of OpticalImages] image\_expansion\_factor\_y (default: 1)

By default, the optical image will only span the lateral (x-y) dimensions of the FDTD grid. The x and y dimensions of the image can be increased or decreased using these two factors. Setting these factors greater than 1 will reduce the aliasing effects in the numerical computation of the image, but linearly increase the computational burden associated with the far-field computation. This is because the far-field has to be collected at a denser set of observation directions for a larger image. The technical details of this are the subject of *sampling theory*, and are explained in [Capoglu12b], page 90.

```
floating-point [Sub-variable of OpticalImages]
    image_oversampling_rate_x (default: 1)
```

```
floating-point [Sub-variable of OpticalImages]
    image_oversampling_rate_y (default: 1)
```

Angora tries to automatically determine the minimum number of far-field collection directions to accurately synthesize the optical image. By default, the number of pixels in the final image is the same as the number of far-field collection directions. As a result, the image is sampled very economically; causing a pixelated appearance. A finer image can be synthesized by scaling the sampling rate in the x and y directions by modifying image\_oversampling\_rate\_x and image\_oversampling\_rate\_y, respectively. For example, setting

image\_oversampling\_rate\_x=10 results in 10 times the default number of pixels in the x direction. Choosing high values for these two factors do not really cause much degradation in performance, since only the post-processing (post-simulation) computational burden is affected. The post-processing burden is usually a small fraction of the burden associated with the whole simulation.

In sampling theory, the minimum number of pixels needed to represent the image is determined by the *Nyquist sampling rate* for the image (see [Capoglu12b], page 90). There is a well-defined Nyquist sampling rate associated with every optical image, since they are constrained in spatial frequency content by the wavelength of illumination. If desired, the default image (the one obtained with image\_oversampling\_rate\_x=image\_oversampling\_rate\_y=1) can be made arbitrarily fine through *bandlimited interpolation* in post-processing.

#### string coll\_half\_space

[Sub-variable of OpticalImages]

Although the collection apparatus seems to be situated in the upper (+z) half space in Figure 6.5, it can also be situated in the lower (-z) half space. This is specified by assigning the string "upper" or "lower" to the coll\_half\_space variable, respectively. In Figure 6.6, these two imaging geometries are shown separately. Note that the image is inverted, but the image-space coordinates (x' and y') are also inverted with respect to the object space.

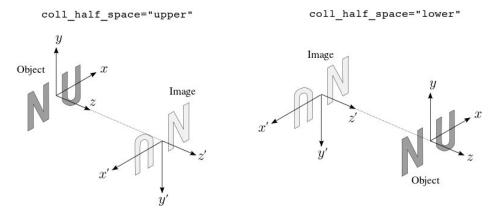


Figure 6.6: Collection of the scattered light in the upper half space (left figure), or the lower half space (right figure) for the calculation of the optical image.

floating-point nffft_back_margin_x (units:m)	[Sub-variable of OpticalImages]
<pre>floating-point nffft_front_margin_x</pre>	[Sub-variable of OpticalImages]
<pre>floating-point nffft_left_margin_y</pre>	[Sub-variable of OpticalImages]
<pre>floating-point nffft_right_margin_y</pre>	[Sub-variable of OpticalImages]

```
floating-point nffft_lower_margin_z
                                                  [Sub-variable of OpticalImages]
         (units:m)
floating-point nffft_upper_margin_z
                                                  [Sub-variable of OpticalImages]
         (units:m)
integer nffft_back_margin_x_in_cells
                                                  [Sub-variable of OpticalImages]
         (default: 3)
integer nffft_front_margin_x_in_cells
                                                  [Sub-variable of OpticalImages]
         (default: 3)
integer nffft_left_margin_y_in_cells
                                                  [Sub-variable of OpticalImages]
         (default: 3)
integer nffft_right_margin_y_in_cells
                                                  [Sub-variable of OpticalImages]
         (default: 3)
integer nffft_lower_margin_z_in_cells
                                                  [Sub-variable of OpticalImages]
         (default: 3)
integer nffft_upper_margin_z_in_cells
                                                  [Sub-variable of OpticalImages]
         (default: 3)
     In the collection stage of optical imaging (see Figure 6.5), the far field scat-
     tered from the sample is calculated using a near-field-to-far-field transformer
     (NFFFT). These variables determine the surface over which the near field is col-
     lected for the calculation of the far field. For more information, see Section 6.8
     [Near-Field-to-Far-Field Transformer], page 40.
floating-point image_origin_x (units: m,
                                                  [Sub-variable of OpticalImages]
         default: 0)
floating-point image_origin_y (units: m,
                                                  [Sub-variable of OpticalImages]
         default: 0)
floating-point image_origin_z (units: m,
                                                  [Sub-variable of OpticalImages]
         default: 0)
                                                  [Sub-variable of OpticalImages]
floating-point
         image_origin_x_in_cells (default: 0)
floating-point
                                                  [Sub-variable of OpticalImages]
         image_origin_y_in_cells (default: 0)
floating-point
                                                  [Sub-variable of OpticalImages]
          {	t image\_origin\_z\_in\_cells} (default: 0)
     These variables set the coordinates of the optical conjugate of the center of
     the image plane. Changing these values amounts to focusing at different posi-
     tions and depths in the sample using the focusing knob on a microscope. The
     coordinates are with respect to the grid origin (see Section 6.2.6 [Coordinate
     Origin, page 16). The units are either in meters or grid cells. For the latter,
     the _in_cells suffix should be appended to the variable name.
```

### string image\_dir (default: "")

[Sub-variable of OpticalImages]

This determines the subdirectory in which this individual image file will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to imaging\_output\_dir (see [imaging\_output\_dir], page 54). By default, no subdirectory is created inside imaging\_output\_dir.

# 

[Sub-variable of OpticalImages]

This determines the base string in the full name of the image file. Other information is appended to the name of the file to differentiate individual image files (see the example below).

[Sub-variable of OpticalImages]

This is the extension of the image file name. If assigned the value "", no extension is added to the file.

Here is an example image file name:

The base string in the name of the file ("Image") is specified by the image\_file\_name variable. The two integers that follow are the run index (see Section 6.14 [Multiple Simulation Runs], page 87) and the index of the image inside the OpticalImages list. For example, if there are two groups (two images) in the OpticalImages list, the first one will write into

Image\_0\_0.hd5

while the second will write into

Image\_0\_1.hd5

If there are two simulation runs (i.e., number\_of\_runs is equal to 2 – see Section 6.14 [Multiple Simulation Runs], page 87), then the files created in the second run will have 1 instead of 0 as the first integer in the above file names. Finally, the extension ("hd5") of the movie files is determined by the variable image\_file\_extension.

boolean

[Sub-variable of OpticalImages]

append\_group\_index\_to\_file\_name (default: true)

If this is set to false, the second integer in the filename (see above) and the underscore preceding it are not included in the filename. It is set to true by default. If this variable is set to false and there are multiple groups (optical images), there will be a name clash, and the output will be undefined.

# 6.9.1 Optical Image File HDF5 Content

The HDF5 file created as the output of optical imaging can be viewed and modified using freely-available tools. One of these tools is HDFView, provided by the HDF Group. MATLAB also has built-in functions and tools that handle HDF5 files. For reference, a MATLAB script named 'hdf5\_read.m' is distributed as part of the Angora package, which reads an HDF5 dataset from an HDF5 file into a MATLAB array. This script is installed in the directory '\$(prefix)/share/angora/' (see Chapter 3 [Compilation and Installation], page 7). If Angora was installed without any \$(prefix) configuration option, the default

location is '/usr/local/share/angora/'. This script can also be downloaded directly from the Angora website (link here). For example, if you want to read the dataset named lambda from the file 'my\_file.hd5', use

```
>> lambda = hdf5_read('my_file.hd5','lambda');
```

In MATLAB R2011a and later, there is a high-level built-in function h5read that could be used for the same purpose.

The HDF5 datasets in the optical image file are the following:

- 'angora\_version': Integer array of length 3 with the major version, minor version, and revision numbers of the Angora package used to create the file.
- 'wv\_range': 1-D array with the recorded free-space wavelength values (in m).
- 'k\_range': 1-D array with the recorded free-space wavenumber values (in 1/m).
- 'x\_range', 'y\_range': 1-D arrays with the x and y coordinates of the image (in m).
- 'n\_obj', 'n\_img': Refractive indices of the object and image spaces, respectively.
- 'magnification': Absolute value of the lateral magnification of the imaging system.
- 'ap\_half\_angle': The half-angle of the collection cone over which the scattered light is collected (in degrees).
- 'E\_x\_sca\_r', 'E\_x\_sca\_i': 3-D arrays with the real and imaginary parts of the x component of the scattered electric field in the image. (if "E\_x\_sca" is included in the array output\_data)
- 'E\_x\_unsca\_r', 'E\_x\_unsca\_i': 3-D arrays with the real and imaginary parts of the x component of the unscattered electric field in the image. (if "E\_x\_unsca" is included in the array output\_data)
- 'E\_x\_tot\_r', 'E\_x\_tot\_i': 3-D arrays with the real and imaginary parts of the x component of the total electric field in the image. (if "E\_x\_tot" is included in the array output\_data)
- 'E\_y\_sca\_r', 'E\_y\_sca\_i': 3-D arrays with the real and imaginary parts of the y component of the scattered electric field in the image. (if "E\_y\_sca" is included in the array output\_data)
- 'E\_y\_unsca\_r', 'E\_y\_unsca\_i': 3-D arrays with the real and imaginary parts of the y component of the unscattered electric field in the image. (if "E\_y\_unsca" is included in the array output\_data)
- 'E\_y\_tot\_r', 'E\_y\_tot\_i': 3-D arrays with the real and imaginary parts of the y component of the total electric field in the image. (if "E\_y\_tot" is included in the array output\_data)
- 'E\_z\_sca\_r', 'E\_z\_sca\_i': 3-D arrays with the real and imaginary parts of the z component of the scattered electric field in the image. (if "E\_z\_sca" is included in the array output\_data)
- 'E\_z\_unsca\_r', 'E\_z\_unsca\_i': 3-D arrays with the real and imaginary parts of the z component of the unscattered electric field in the image. (if "E\_z\_unsca" is included in the array output\_data)
- 'E\_z\_tot\_r', 'E\_z\_tot\_i': 3-D arrays with the real and imaginary parts of the z component of the total electric field in the image. (if "E\_z\_tot" is included in the array output\_data)

- 'intensity\_sca': 3-D array with the intensity of the scattered light at the image plane (if "intensity\_sca" is included in the array output\_data). See above for the definition of 'intensity\_sca'.
- 'intensity\_unsca': 3-D array with the intensity of the unscattered light at the image plane (if "intensity\_unsca" is included in the array output\_data). See above for the definition of 'intensity\_unsca'.
- 'intensity\_tot': 3-D array with the intensity of the total light at the image plane (if "intensity\_tot" is included in the array output\_data) See above for the definition of 'intensity\_tot'.

•

#### 6.10 Incident Beams

Different types of incident beams can be sourced into the simulation grid using the TFSF group.

group TFSF [Global variable]

The TFSF group contains definitions for various types of incident electromagnetic beams required for scattering problems. Angora uses the total-field/scattered-field (TF/SF) technique to source incident beams into the simulation grid (see [TafloveHagness], page 90). In this technique, a rectangular surface surrounding the scatterer is designated the total-field/scattered-field boundary (or the TF/SF box in short); and the electromagnetic field on this surface is supplemented by certain terms proportional to the incident electromagnetic field. These additional terms create the incident field inside the surface (suggesting the term injection), while maintaining a very small electromagnetic field outside the surface. The region outside the TF/SF box only harbors the scattered field created by the scatterers inside the TF/SF box. The field inside the box is the total field, which is a sum of the incident field and the scattered field. Since the boundary divides the grid into total-field and scattered-field regions, the term "TF/SF boundary" is justified.

TF/SF incident beam injection is supported for **infinite planar layered media**. Infinite planar layers are created using the MaterialSlabs variable (see Section 6.5.2 [Planar Layers], page 24). Currently, only layers with different permittivities and electrical conductivities are supported. Permeability variations across layers will also be supported in the future. Angora also supports **evanescent plane waves** resulting from plane waves passing from a high-permittivity layer to a low-permittivity one at a low grazing angle. Angora supports evanescent waves only for *narrowband* plane waves, which have appreciable frequency components only in a small band around a center frequency. A modulated Gaussian waveform with a large  $f_0\tau$  can be used as a narrowband waveform in cases where evanescent waves might be present (see Section 6.6.3 [Modulated-Gaussian Waveforms], page 37).

Different types of incident beams are defined in their respective lists inside the TFSF group. These are explained in the following subsections.

```
TFSF:
{
    PlaneWaves:
```

# 6.10.1 Plane Waves

A plane wave is one of the simplest solutions of Maxwell's equations; with the electric field

$$\bar{\mathbf{E}}(\bar{\mathbf{r}},t) = \hat{\mathbf{e}}E_0 f(t - \bar{\mathbf{r}} \cdot \hat{\mathbf{k}}^i/v_p)$$

where  $\hat{\mathbf{k}}^i$  is the unit vector in the direction of propagation,  $\hat{\mathbf{e}}$  is the electric-field unit vector,  $E_0$  is the electric field amplitude, and  $\bar{\mathbf{r}}$  is the distance vector. The velocity of propagation  $v_p$  is determined by the material properties in the direction from which the plane wave is incident. The time waveform f(t) is arbitrary. Inserting the above expression into Maxwell's equations, it is found that the electric-field unit vector  $\hat{\mathbf{e}}$  is perpendicular to the direction of propagation, as well as the magnetic-field unit vector.

In a discrete FDTD grid, a plane wave propagates at a slightly lower velocity than in continuum. Furthermore, there is an intrinsic grid velocity anisotropy that results from the inherent rotational asymmetry of the rectangular FDTD grid. These are partially alleviated in Angora by the use of the *matched numerical dispersion* (MND) technique (see [TafloveHagness], page 90).

#### list PlaneWaves

[Sub-variable of TFSF]

Plane waves are defined inside a PlaneWaves list inside the TFSF group:

```
tfsf_right_margin_y_in_cells = 6;
tfsf_lower_margin_z_in_cells = 6;
tfsf_upper_margin_z_in_cells = 6;
pw_origin_x = 0.0;
pw_origin_y = 0.0;
pw_origin_z = 0.0;
display_warnings = true;
min_cells_per_lambda = 15.0;
},
{
...
},
{
...
}
);
};
```

floating-point theta (units: degrees)

[Sub-variable of PlaneWaves]

floating-point phi (units: degrees)

[Sub-variable of PlaneWaves]

The incidence angles of the plane waves are defined in terms of the traditional spherical-coordinate variables  $(\theta, \phi)$ . The first of these angles is the *zenith angle*, while the second is the *azimuth angle*. In Figure 6.7, the definitions of these angles are shown schematically. The theta variable specifies the zenith angle in degrees. Although this angle is traditionally defined between 0 and 180deg, theta can be assigned any negative or positive value. The phi variable specifies the azimuth angle in degrees. Although this angle is traditionally defined between 0 and 360deg, phi can be assigned any negative or positive value.

Note that the incidence angles  $(\theta, \phi)$  specify the direction from which the plane wave is incident; **not** the direction in which it propagates.

floating-point psi (units: degrees)

[Sub-variable of PlaneWaves]

This variable is used to specify the polarization of the electric field of the incident plane wave. Maxwell's equations dictate that the electric field is **perpendicular** to the incidence vector  $\hat{\mathbf{k}}^i$ . In order to define the orientation of the electric vector unambiguously, a local coordinate system  $(\xi, \eta)$  is defined, such that  $\hat{\xi} = \hat{\mathbf{k}}^i \times \hat{z}$  and  $\hat{\eta} = \hat{\xi} \times \hat{\mathbf{k}}^i$  The unit vectors  $(\hat{\xi}, \hat{\eta})$  are perpendicular to each other, and lie in the plane perpendicular to the incidence vector  $\hat{\mathbf{k}}^i$ . The polarization angle  $\psi$  of the electric-field unit vector  $\hat{\mathbf{e}}$  is defined as the left-handed (clockwise) rotation angle around the axis defined by the incidence vector  $\hat{\mathbf{k}}^i$ . The variable psi sets this angle in degrees.

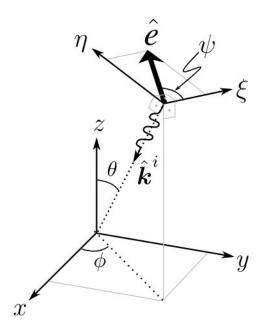


Figure 6.7: Graphical description of the incidence and polarization angles associated with a plane wave.

# string waveform\_tag

[Sub-variable of PlaneWaves]

This string variable specifies the electric-field waveform f(t) in [eq:pw\_E\_field], page 64. The waveform is interpreted in (Volts/m) units. This should match a previously-defined tag in a Waveforms definition (see Section 6.6 [Waveforms], page 34).

floating-point pw\_extra\_amplitude (units: [Sub-variable of PlaneWaves] V/m, default: 1.0)

This variable sets the electric field amplitude  $E_0$  in [eq:pw\_E\_field], page 64.

floating-point tfsf\_back\_margin\_x (units: [Sub-variable of PlaneWaves] m)

floating-point tfsf\_front\_margin\_x [Sub-variable of PlaneWaves] (units: m)

floating-point tfsf\_left\_margin\_y (units: [Sub-variable of PlaneWaves]
m)

floating-point tfsf\_right\_margin\_y [Sub-variable of PlaneWaves] (units: m)

floating-point tfsf\_lower\_margin\_z [Sub-variable of PlaneWaves] (units: m)

integer	<pre>tfsf_back_margin_x_in_cells (default: 6)</pre>	[Sub-variable of PlaneWaves]
integer	<pre>tfsf_front_margin_x_in_cells (default: 6)</pre>	[Sub-variable of PlaneWaves]
integer	<pre>tfsf_left_margin_y_in_cells (default: 6)</pre>	[Sub-variable of PlaneWaves]
integer	<pre>tfsf_right_margin_y_in_cells (default: 6)</pre>	[Sub-variable of PlaneWaves]
integer	<pre>tfsf_lower_margin_z_in_cells (default: 6)</pre>	[Sub-variable of PlaneWaves]
integer	<pre>tfsf_upper_margin_z_in_cells (default: 6)</pre>	[Sub-variable of PlaneWaves]

By default, the total-field/scattered-field (TF/SF) surface is placed 6 grid cells away from the PML boundary (see Section 6.2.4 [Perfectly-Matched Layer (PML)], page 15). You can specify different margins to reduce the computational burden associated with the TF/SF operation. This burden is directly proportional to the area of the TF/SF surface. The margins can be specified in meters or in grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If given in meters, the margins are rounded to the nearest multiple of the spatial step size.

These variables set the coordinates of the point relative to which the distance  $\bar{\mathbf{r}}$  is defined in [eq:pw\_E\_field], page 64. The coordinates are with respect to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name.

```
boolean display_warnings (default: true) [Sub-variable of PlaneWaves]

floating-point min_cells_per_lambda [Sub-variable of PlaneWaves]

(default: 15)
```

The boolean variable display\_warnings enables or disables the printing of warning messages. Currently, a warning is displayed only when there are not enough grid cells per "minimum" wavelength in the excitation waveform. This minimum wavelength is defined to be the one at which the spectrum of the

waveform falls to -40dB below its maximum. The number of required grid cells per the minimum wavelength is determined by the min\_cells\_per\_lambda variable.

## 6.10.2 Focused Laser Beams

Angora can synthesize focused laser beams created by an aplanatic optical system (i.e., free of spherical aberration and coma) illuminated by a normally-incident paraxial Hermite-Gaussian laser mode. The electromagnetic formulation of the focused beam is based on the classic work of Richards and Wolf (see [Richards59], page 90). This formulation is interpreted as a sum of plane waves, and approximated by a finite sum in the FDTD implementation (see [Capoglu08], page 90). It is assumed that the Hermite-Gaussian laser mode filling the entrance pupil of the optical system has a beam width much larger than the wavelength, and is therefore in the paraxial regime. In this regime, the wavefronts are almost planar, perpendicular to the optical axis, and the electric field of the beam has a negligible longitudinal component.

The incidence geometry for the laser mode illuminating the entrance pupil of the system is shown on the upper right in Figure 6.8. A local coordinate system  $(\xi, \eta)$  is defined on the plane of the entrance pupil, such that  $\hat{\xi} = \mathbf{k}^i \times \hat{z}$  and  $\hat{\eta} = \hat{\xi} \times \mathbf{k}^i$  The unit vectors  $(\hat{\xi}, \hat{\eta})$  are perpendicular to each other, and lie in the plane perpendicular to the incidence vector  $\mathbf{k}^i$ . The symmetry axes (x', y') of the Hermite-Gaussian beam are rotated at an angle of  $\alpha$  with respect to the  $\xi$  axis, in a clock-wise (left-handed) sense with respect to  $\mathbf{k}^i$ .

On the plane of the entrance pupil, which is assumed to coincide with the waist of the Hermite-Gaussian beam, the electric field is given by

$$\bar{\mathbf{E}}(\bar{\mathbf{r}},t) = \hat{\mathbf{e}}E_0 f(t) H_m(\sqrt{2}\frac{x'}{w_0}) H_n(\sqrt{2}\frac{y'}{w_0}) \exp(-\frac{(x')^2 + (y')^2}{w_0^2})$$

where  $w_0$  is the beam half width (or beam waist radius),  $\hat{e}$  is the electric-field unit vector,  $E_0$  is the electric field amplitude, and  $H_m(\cdot)$  are the (physicists') Hermite polynomials of order m. The first few Hermite polynomials are

$$H_0(x) = 1$$
,  $H_1(x) = 2x$ ,  $H_2(x) = 4x^2 - 2$ 

The time waveform f(t) is arbitrary. Since we assume that the width of the beam at the entrance pupil is much larger than the wavelengths contained in the waveform f(t), it is reasonable to employ the *paraxial* approximation, in which the rays propagate parallel to the optical axis and the electric-field unit vector  $\hat{\mathbf{e}}$  is perpendicular to the direction of propagation  $\hat{\mathbf{k}}^i$ .

The focusing optical system between the entrance pupil and the exit pupil is assumed aplanatic. This means that, in addition to focusing on-axis points stigmatically (without spherical aberration), the system also correctly focuses off-axis points up to the first order in off-axis distance. The latter condition corresponds to the absence of circular coma. The sine condition, first derived by Ernst Abbe in 1881, is an expression of this in mathematical terms. The sine condition reads

$$h = f \sin(\theta_{\rm ill})$$

where h is the radius of the entrance pupil, and f is the back focal length of the focusing system. The sine condition is also shown geometrically in Figure 6.8.

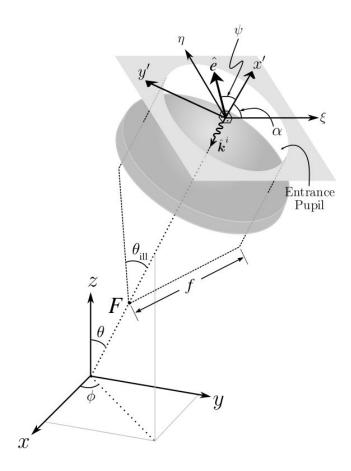


Figure 6.8: Geometry of the focused laser beam.

#### list FocusedLaserBeams

[Sub-variable of TFSF]

Focused laser beams are defined inside a FocusedLaserBeams list inside the TFSF group:

```
filling_factor = 1;
            object_space_refr_index = 1.0;
            tfsf_back_margin_x_in_cells = 6;
            tfsf_front_margin_x_in_cells = 6;
            tfsf_left_margin_y_in_cells = 6;
            tfsf_right_margin_y_in_cells = 6;
            tfsf_lower_margin_z_in_cells = 6;
            tfsf_upper_margin_z_in_cells = 6;
            flb_origin_x = 0.0;
            flb_origin_y = 0.0;
            flb_origin_z = 0.0;
            display_warnings = true;
            min_cells_per_lambda = 15.0;
        },
        {
        }
    );
};
```

floating-point theta (units: degrees) [Sub-variable of FocusedLaserBeams]

The incidence angles for the focused laser beam are defined in reference to the paraxial beam that hits the entrance pupil (see Figure 6.8). The incidence angles are defined in terms of the traditional spherical-coordinate variables  $(\theta, \phi)$ . The first of these angles is the zenith angle, while the second is the azimuth angle. The theta variable specifies the zenith angle in degrees. Although this angle is traditionally defined between 0 and 180deg, theta can be assigned any negative or positive value. The phi variable specifies the azimuth angle in degrees. Although this angle is traditionally defined between 0 and 360deg, phi can be assigned any negative or positive value.

Note that the incidence angles  $(\theta, \phi)$  specify the direction from which the paraxial beam is incident; **not** the direction in which it propagates.

floating-point psi (units: degrees) [Sub-variable of FocusedLaserBeams] This variable is used to specify the polarization of the transverse electric field of the paraxial beam on the entrance pupil. The electric field is perpendicular to the incidence vector  $\mathbf{\hat{k}}^i$ . The polarization angle  $\psi$  is defined as the left-handed (clockwise) rotation angle with respect to the incidence vector  $\mathbf{\hat{k}}^i$  between the symmetry axis x' and the electric-field unit vector  $\mathbf{\hat{e}}$  (see Figure 6.8). The variable psi sets this angle in degrees.

floating-point alpha (units: degrees) [Sub-variable of FocusedLaserBeams] (default: 0)

This angle specifies the rotation of the symmetry axes (x', y') of the Hermite-Gaussian beam with respect to the local coordinate axes  $(\xi, \eta)$ . The rotation is clock-wise (left-handed) with respect to the incidence vector  $\hat{k}^i$  (see Figure 6.8).

integer x\_order

[Sub-variable of FocusedLaserBeams]

integer y\_order

[Sub-variable of FocusedLaserBeams]

These positive integers specify the orders of the Hermite polynomials  $H_m(x), H_n(y)$  in the definition of the Hermite-Gaussian beam in [eq:fb\_incident\_E\_field], page 68. x\_order and y\_order correspond to m and n, respectively.

#### string waveform\_tag

[Sub-variable of FocusedLaserBeams]

This string variable specifies the electric-field waveform f(t) in [eq:fb\_incident\_E\_field], page 68, except a time advance  $t_0$  equal to the time of propagation from the entrance pupil to the focal point F. In other words, the actual waveform f(t) on the entrance pupil is advanced in time by  $t_0$  with respect to the waveform represented by waveform\_tag. This is needed because we simulate the fields around the focus F; not the entrance pupil. The waveform is interpreted in (Volts/m) units. The string waveform\_tag should match a previously-defined string tag in a Waveforms definition (see Section 6.6 [Waveforms], page 34).

#### floating-point

[Sub-variable of FocusedLaserBeams]

 $flb_{extra_amplitude}$  (units: V/m, default: 1.0)

This variable sets the electric field amplitude  $E_0$  in [eq:fb\_incident\_E\_field], page 68.

# floating-point ap\_half\_angle

[Sub-variable of FocusedLaserBeams]

(units: degrees)

This variable sets the half-angle  $\theta_{ill}$  of the illumination cone in degrees (see Figure 6.8).

If a planar layered medium is present in the grid (see Section 6.5.2 [Planar Layers], page 24), the incidence cone bounded by the angle  $\theta_{\rm ill}$  should lie entirely within the upper or lower half space. In other words, the incidence cone cannot cut across the grazing direction ( $\theta = \pi/2$ ). Angora will throw an error if this is found to be the case.

# floating-point back\_focal\_length (units: m)

[Sub-variable of FocusedLaserBeams]

floating-point

[Sub-variable of FocusedLaserBeams]

back\_focal\_length\_in\_cells

This variable specifies the back focal length f of the optical system. The units are either in meters or grid cells. For the latter, the  ${\tt in\_cells}$  suffix should be appended to the variable name.

#### floating-point filling\_factor

[Sub-variable of FocusedLaserBeams]

This dimensionless parameter represents the ratio between the half-width of the incident paraxial beam and the radius of the entrance pupil. The larger this ratio, the more overfilled the pupil, and vice versa. This parameter is defined as

$$f_0 = \frac{w_0}{f \sin(\theta_{\rm ill})}$$

```
floating-point
                                           [Sub-variable of FocusedLaserBeams]
         object_space_refr_index (default: 1.0)
     This variable specifies the refractive index of the object space of the optical
     system; i.e., the space from which the paraxial beam is incident. Note that the
     FDTD simulation grid is in the image space of the optical system; therefore
     the refractive index of the image space is determined by the material filling the
     FDTD grid. If you want to simulate an oil immersion scenario, for example,
     you should fill the FDTD simulation space with the material representing the
     immersion oil. The object-side refractive index object_space_refr_index is
     seldom different than 1.0, which is the default value.
floating-point tfsf_back_margin_x
                                           [Sub-variable of FocusedLaserBeams]
         (units: m)
floating-point
                                            [Sub-variable of FocusedLaserBeams]
         tfsf_front_margin_x (units: m)
floating-point tfsf_left_margin_y
                                           [Sub-variable of FocusedLaserBeams]
         (units: m)
floating-point
                                            [Sub-variable of FocusedLaserBeams]
         tfsf_right_margin_y (units: m)
floating-point
                                           [Sub-variable of FocusedLaserBeams]
         tfsf_lower_margin_z (units: m)
floating-point
                                           [Sub-variable of FocusedLaserBeams]
         tfsf_upper_margin_z (units: m)
                                           [Sub-variable of FocusedLaserBeams]
integer
         tfsf_back_margin_x_in_cells (default: 6)
                                           [Sub-variable of FocusedLaserBeams]
integer
         tfsf_front_margin_x_in_cells (default: 6)
                                            [Sub-variable of FocusedLaserBeams]
integer
         tfsf_left_margin_y_in_cells (default: 6)
                                           [Sub-variable of FocusedLaserBeams]
integer
         tfsf_right_margin_y_in_cells (default: 6)
                                            [Sub-variable of FocusedLaserBeams]
integer
         tfsf_lower_margin_z_in_cells (default: 6)
                                           [Sub-variable of FocusedLaserBeams]
integer
         tfsf_upper_margin_z_in_cells (default: 6)
```

By default, the total-field/scattered-field (TF/SF) surface is placed 6 grid cells away from the PML boundary (see Section 6.2.4 [Perfectly-Matched Layer (PML)], page 15). You can specify different margins to reduce the computational burden associated with the TF/SF operation. This burden is directly proportional to the area of the TF/SF surface. Because the focused beam is actually a collection of many (often hundreds) of plane waves, the reduction of the surface area of the TF/SF box greatly helps the simulation performance.

The margins can be specified in meters or in grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If given in meters, the margins are rounded to the nearest multiple of the spatial step size.

floating-point flb\_origin\_x (units: [Sub-variable of FocusedLaserBeams]
m)

floating-point flb\_origin\_y (units: [Sub-variable of FocusedLaserBeams] m)

floating-point flb\_origin\_z (units: [Sub-variable of FocusedLaserBeams]
m)

These variables set the coordinates of the back focal point F of the focusing lens. (see Figure 6.8). The coordinates are with respect to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the  $\tt in\_cells$  suffix should be appended to the variable name.

boolean display\_warnings (default: [Sub-variable of FocusedLaserBeams] true)

The boolean variable display\_warnings enables or disables the printing of warning messages. Currently, a warning is displayed only when there are not enough grid cells per "minimum" wavelength in the excitation waveform. This minimum wavelength is defined to be the one at which the spectrum of the waveform falls to -40dB below its maximum. The number of required grid cells per the minimum wavelength is determined by the min\_cells\_per\_lambda variable.

# 6.11 Recording

Angora can record field values computed during a simulation into a file in a variety of ways. Field values can be recorded on a cross-section of the grid, along a line through the grid, or at a given point in the grid. Currently, Angora only supports the recording of the electric or the magnetic field. Recording of other field-related quantities such as energy, flux, Poynting's vector, etc. will be implemented in the future. Please send any comments, suggestions, and requests to help@angorafdtd.org.

```
string recorder_output_dir (default: "recorder") [Global variable]
This determines the subdirectory in which all the recording-related stuff will be placed.
Unless it has a slash '/' up front; this path is interpreted as being relative to output_
dir (see Section 6.12 [Paths], page 86).
```

group Recorder

[Global variable]

The Recorder group contains the sub-variables related to different types of field recording. These are explained in the following subsections.

```
Recorder:
{
     MovieRecorders:
          {
               . . .
          }
     );
     LineRecorders:
          {
               . . .
               . . .
          }
     );
     FieldValueRecorders:
          {
               . . .
          }
     );
};
```

# 6.11.1 Movie Recording

Angora can record field components on a two-dimensional cross section of the grid into a custom movie file. The binary format used for movie recording is described in more detail in Section 6.11.1.1 [Movie File Format], page 77.

#### list MovieRecorders

[Sub-variable of Recorder]

Field values on a two-dimensional cross section of the FDTD grid can be recorded using the MovieRecorders list.

```
Recorder:
{
    MovieRecorders:
    (
        {
            recorded_section = "xz";
            recorded_position = 0;
            recorded_component = "Ex";
            recording_scale = "dB";
            recording_type = "uchar1";
            movie_dir = "this_movie_dir";
            movie_file_name = "MovieFile"
            movie_file_extension = "amv";
            append_group_index_to_file_name = true;
            only_records_material_info = false;
        },
        }
    );
};
```

#### string recorded\_section

[Sub-variable of MovieRecorders]

This determines the cross section of the grid over which the field is recorded. Currently, only xz, yz, and xy cross sections are supported. These are represented by the string values "xz", "yz", and "xy", respectively.

```
floating-point recorded_position [Sub-variable of MovieRecorders] (units: m)
```

integer recorded\_position\_in\_cells [Sub-variable of MovieRecorders]

This value specifies the coordinate of the recorded cross section along the perpendicular direction (e.g., the z direction if recorded\_section is "xy"). The coordinate is relative to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_ in\_cells suffix should be appended to the variable name. If the coordinate corresponds to a non-integer cell position, the closest integer position is chosen.

#### string recorded\_component

[Sub-variable of MovieRecorders]

An individual movie recorder (in a group delineated by the curly brackets '{}') only records a single scalar value extracted from the vector-valued electromagnetic field. This could be one of the Cartesian components or the absolute value of the electric or the magnetic field. These are represented by the string values "Ex", "Ey", "Ez", "E", "Hx", "Hy", "Hz", and "H". If you would like to record multiple Cartesian components of a vector field, simply add other movie recorders (i.e., other groups, see Section 5.2.5 [Groups], page 11) to the MovieRecorders list with the desired recorded\_component values.

## string recording\_scale

[Sub-variable of MovieRecorders]

If "linear", the raw values are recorded. If "absolute", the absolute value is taken before recording. If "dB", the decibel value  $(20 \log_{10}(|\cdot|))$  is recorded.

#### string recording\_type

[Sub-variable of MovieRecorders]

Movies can either be recorded either in raw floating-point format, or in a single-byte compressed format. This is specified by assigning the string values "db18" or "uchar1" to the recording\_type variable, respectively. Using the single-byte format reduces the file size considerably, but results in some data loss.

If recording\_type is "db18", then the field values are recorded in 8-byte double datatype, after processed in accordance with the recording\_scale specification above. This provides practically lossless recording, albeit with increased computational burden and file size.

With the "uchar1" option, the field values are reduced to 256 discrete bins within a fixed *dynamic range*. This requires only a single byte per field value; reducing the storage requirement by a factor of 8.

• If recording\_type is "dB", the maximum and minimum values in this dynamic range are determined by the global variables max\_field\_value and dB\_accuracy (see Section 6.2.7 [Dynamic Range], page 17):

 $\max : 20 \log_{10}(|\max_{\text{field-value}}|) \quad \min : 20 \log_{10}(|\max_{\text{field-value}}|) + (dB_{\text{accuracy}})$ 

The dB\_accuracy variable should always be negative; therefore the minimum value in the dynamic range is lower than the maximum.

• If recording\_type is "linear" or "absolute", the maximum and minimum values are determined only by the global variable max\_field\_value (see Section 6.2.7 [Dynamic Range], page 17):

max: max\_field\_value min: (-max\_field\_value) or 0

### string movie\_dir (default: "")

[Sub-variable of MovieRecorders]

This determines the subdirectory in which this individual movie file will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to movie\_recorder\_output\_dir (see [movie\_recorder\_output\_dir], page 74). By default, no subdirectory is created inside movie\_recorder\_output\_dir.

This determines the base string in the full name of the movie file. Other information is appended to the name of the file to differentiate individual movie files (see the example below).

This is the extension of the movie file name. If assigned the value "", no extension is added to the file.

Here is an example movie file name:

MovieFile\_Ex\_0\_1.amv

The base string in the name of the file ("MovieFile") is specified by the movie\_file\_name variable. The second part of the file name, "Ex", is determined by the recorded field component. The two integers that follow are the run index (see Section 6.14 [Multiple Simulation Runs], page 87) and the index of the movie inside the MovieRecorders list. For example, if there are two groups (two movies) in the MovieRecorders list, the first one will write into

MovieFile\_Ex\_0\_0.amv

while the second will write into

MovieFile\_Ex\_0\_1.amv

If there are two simulation runs (i.e., number\_of\_runs is equal to 2 – see Section 6.14 [Multiple Simulation Runs], page 87), then the files created in the second run will have 1 instead of 0 as the first integer in the above file names. Finally, the extension ("amv") of the movie files is determined by the variable movie\_file\_extension.

boolean [Sub-variable of MovieRecorders] append\_group\_index\_to\_file\_name (default: true)

If this is set to false, the second integer in the filename (see above) and the underscore preceding it are not included in the filename. It is set to true by default. If this variable is set to false and there are multiple groups (movie recorders), there will be a name clash, and the output will be undefined.

boolean only\_records\_material\_info [Sub-variable of MovieRecorders] (default: false)

If set to true, only the material information is recorded into the file, and no field recording is performed during the simulation.

### 6.11.1.1 Movie File Format

Angora records movies in a custom binary format for better speed and performance. Please be aware that this format is subject to modification. The changes in the format will be documented in this manual as necessary. You may refer to the 'ChangeLog' file in the Angora distribution for recent changes in the movie recording format.

The MATLAB script 'angora\_movie.m', distributed as part of the Angora package, reads an Angora movie file and displays it as a MATLAB movie. It can also save the movie in AVI

format. This script is installed in the directory '\$(prefix)/share/angora/' (see Chapter 3 [Compilation and Installation], page 7). If Angora was installed without any \$(prefix) configuration option, the default location is '/usr/local/share/angora/'. This script can also be downloaded directly from the Angora website (link here).

The movie file is composed of chunks of data, ordered as follows. For each chunk, a short explanation (and maybe an alias) is given, followed by a description of the datatype in parantheses.

- major package version (integer, 4 bytes)
- minor package version (integer, 4 bytes)
- package revision number (integer, 4 bytes)
- number of bytes used to record each field component (integer, 4 bytes): This is either equal to 1 or 8, depending on the recording\_type variable.
- spatial step size (double, 8 bytes)
- temporal step size (double, 8 bytes)
- time value that corresponds to the beginning of the simulation (double, 8 bytes): This is usually a negative value, since time waveforms frequently begin before t=0.
- maximum value in the field discretization range (double, 8 bytes): This is the maximum value in the discretization dynamic range for single-byte recording (i.e., recording\_type is "uchar1"). If recording\_type is "dbl8", this value is irrelevant. Same applies to the next value in the file.
- minimum value in the field discretization range (double, 8 bytes)
- 'length\_1': length along the first dimension of the recorded array (integer, 4 bytes): If the xy section were recorded, this would be the length of the array in the x dimension. This includes the thickness of the PML sections in both directions.
- 'length\_2': length along the second dimension of the recorded array (integer, 4 bytes): If the xy section were recorded, this would be the length of the array in the y dimension. This includes the thickness of the PML sections in both directions.
- 'length\_time': number of time steps in the simulation (integer, 4 bytes)
- thickness of the PML region, in grid cells (integer, 4 bytes): See Section 6.2.4 [Perfectly-Matched Layer (PML)], page 15 for more information on the PML. The PML sections are included in the recorded cross sectional area. They can easily be removed in post-processing.
- an array of length length\_1 with the actual physical coordinates (in m) along the first dimension of the recorded cross section (double, 8 bytes)
- an array of length length\_2 with the actual physical coordinates (in m) along the second dimension of the recorded cross section (double, 8 bytes)
- an array of length (length\_2 x length\_1) holding the relative permittivity (if the electric field is recorded) or the relative permeability (if the magnetic field is recorded) values on the recorded cross section (double, 8 bytes): In Figure 6.9, it is assumed that the xy section is recorded, and the field positions are numbered from 0 to 11. It is seen that the second dimension (here, the y-dimension) is looped through first. These positions are laid out in the movie file in the same order:

0 1 2 3 4 5 6 7 8 9 10 11

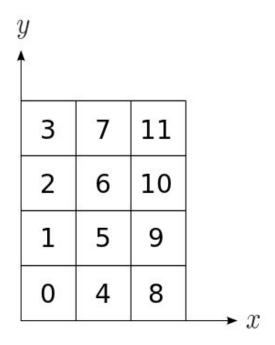


Figure 6.9: The layout of the field positions on the recorded cross section in the movie file

- an array of length (length\_2 x length\_1) holding the electric conductivity values (in Siemens/m, if the electric field is recorded) or the magnetic conductivity values (in Ohm/m, if the magnetic field is recorded) on the recorded cross section (double, 8 bytes): The 2D cross section is laid out in the movie file in the same way as the previous array.
- arrays (movie frames) of length (length\_2 x length\_1) holding the field values on the recorded cross section (double, 8 bytes OR unsigned char, 1 byte depending on recording\_type): The total number of these movie frames is equal to length\_time, read earlier from the binary file. Each of these frames is laid out in the movie file in the same way as the previous arrays.

## 6.11.2 Line Recording

Angora can record field components along a line into a file. The binary format used for line recording is described in more detail in Section 6.11.2.1 [Line File Format], page 82.

```
string line_recorder_output_dir (default: "") [Sub-variable of Recorder]
This determines the subdirectory in which all the recorded line files will be placed.
Unless it has a slash '/' up front; this path is interpreted as being relative to recorder_output_dir (see [recorder_output_dir], page 73).

Recorder:
{
```

line\_recorder\_output\_dir = "lines";

```
LineRecorders:
              );
          };
list LineRecorders
                                                        [Sub-variable of Recorder]
          Recorder:
          {
              LineRecorders:
               (
                   {
                       line_orientation = "y_directed";
                       line_position_x1 = 0;
                       line_position_x2 = 0;
                       recorded_component = "Ex";
                       recording_scale = "linear";
                       line_dir = "this_line_dir";
                       line_file_name = "LineFile";
                       line_file_extension = "aln";
                       append_group_index_to_file_name = true;
                  },
                   }
              );
          };
```

### string line\_orientation

[Sub-variable of LineRecorders]

There are three possible orientations for the line over which the field values are recorded .These orientations are along the three principal axes of the grid; namely, the x,y, and z directions. These are specified by the strings "x\_directed", "y\_directed", and "z\_directed", respectively.

floating-point line\_position\_x1 (units: [Sub-variable of LineRecorders] m)

integer line\_position\_x1\_in\_cells [Sub-variable of LineRecorders]

This is the first of the remaining two coordinates that specify the position of the recorded line. The coordinate is relative to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). For example, if the line is oriented in the y direction (line\_orientation is "y\_directed"), then line\_position\_x1\_in\_cells specifies the x coordinate of the line. The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If the coordinate corresponds to a non-integer cell position, the closest integer position is chosen.

floating-point line\_position\_x2 (units: [Sub-variable of LineRecorders]

## integer line\_position\_x2\_in\_cells

closest integer position is chosen.

[Sub-variable of LineRecorders] This is the second of the remaining two coordinates that specify the position of the recorded line. The coordinate is relative to the grid origin (see Section 6.2.6) [Coordinate Origin], page 16). For example, if the line is oriented in the y direction (line\_orientation is "y\_directed"), then line\_position\_x2\_in\_ cells specifies the z coordinate of the line. The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If the coordinate corresponds to a non-integer cell position, the

### string recorded\_component

[Sub-variable of LineRecorders]

An individual line recorder (in a group delineated by the curly brackets '{}') only records a single scalar value extracted from the vector-valued electromagnetic field. This could be one of the Cartesian components or the absolute value of the electric or the magnetic field. These are represented by the string values "Ex", "Ey", "Ez", "E", "Hx", "Hy", "Hz", and "H". If you would like to record multiple Cartesian components of a vector field, simply add other line recorders (i.e., other groups, see Section 5.2.5 [Groups], page 11) to the LineRecorders list with the desired recorded\_component values.

#### string recording\_scale

[Sub-variable of LineRecorders]

If "linear", the raw values are recorded. If "absolute", the absolute value is taken before recording. If "dB", the decibel value  $(20 \log_{10}(|\cdot|))$  is recorded.

#### string line\_dir (default: "")

[Sub-variable of LineRecorders]

This determines the subdirectory in which this individual line file will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to line\_recorder\_output\_dir (see [line\_recorder\_output\_dir], page 79). By default, no subdirectory is created inside line\_recorder\_output\_dir.

### string line\_file\_name (default: "LineFile")

[Sub-variable of LineRecorders]

This determines the base string in the full name of the line file. Other information is appended to the name of the file to differentiate individual line files (see the example below).

# string line\_file\_extension (default:

[Sub-variable of LineRecorders]

This is the extension of the line file name. If assigned the value "", no extension is added to the file.

Here is an example line file name:

The base string in the name of the file ("LineFile") is specified by the line\_file\_ name variable. The second part of the file name, "Ey", is determined by the recorded field component. The following string "Y" indicates the orientation of the line, which is y-directed for this example. The two integers that follow are the run index (see Section 6.14 [Multiple Simulation Runs], page 87) and the index of the line recorder inside the LineRecorders list. For example, if there are two groups (two line recorders) in the LineRecorders list, the first one will write into

LineFile\_Ey\_Y\_0\_0.aln

while the second will write into

LineFile\_Ey\_Y\_0\_1.aln

If there are two simulation runs (i.e., number\_of\_runs is equal to 2 – see Section 6.14 [Multiple Simulation Runs], page 87), then the files created in the second run will have 1 instead of 0 as the first integer in the above file names. Finally, the extension ("aln") of the line files is determined by the variable line\_file\_extension.

boolean

[Sub-variable of LineRecorders]

append\_group\_index\_to\_file\_name (default: true)

If this is set to false, the second integer in the filename (see above) and the underscore preceding it are not included in the filename. It is set to true by default. If this variable is set to false and there are multiple groups (line recorders), there will be a name clash, and the output will be undefined.

#### 6.11.2.1 Line File Format

As with movies, Angora records the line files in a custom binary format for better speed and performance. Please be aware that this format is subject to modification. The changes in the format will be documented in this manual as necessary. You may refer to the 'ChangeLog' file in the Angora distribution for recent changes in the line recording format.

The MATLAB script 'angora\_line.m', distributed as part of the Angora package, reads an Angora line file and displays it as a MATLAB movie. This script is installed in the directory '\$(prefix)/share/angora/' (see Chapter 3 [Compilation and Installation], page 7). If Angora was installed without any \$(prefix) configuration option, the default location is '/usr/local/share/angora/'. This script can also be downloaded directly from the Angora website (link here).

The line file is composed of chunks of data, ordered as follows. For each chunk, a short explanation (and maybe an alias) is given, followed by a description of the datatype in parantheses.

- major package version (integer, 4 bytes)
- minor package version (integer, 4 bytes)
- package revision number (integer, 4 bytes)
- temporal step size (double, 8 bytes)
- time value that corresponds to the beginning of the simulation (double, 8 bytes): This is usually a negative value, since time waveforms frequently begin before t=0.
- 'total\_length': the number of recorded elements on each line snapshot (integer, 4 bytes)
- 'length\_time': number of time steps in the simulation (integer, 4 bytes)
- thickness of the PML region, in grid cells (integer, 4 bytes): See Section 6.2.4 [Perfectly-Matched Layer (PML)], page 15 for more information on the PML. The recorded line

includes two PML sections on opposite ends, each with this length. These sections can easily be removed in post-processing.

• arrays (line snapshots) of length total\_length holding the field values on the recorded line (double, 8 bytes): The total number of these line snapshots is equal to length\_time, read earlier from the binary file.

## 6.11.3 Field-Value Recording

Angora can record the time history of the field at a given position in the simulation grid. The format used for this sort of recording is **HDF5** (Hierarchical Data Format) (http://www.hdfgroup.org/HDF5/). The HDF5 format was chosen for its standard interface, and the availability of free software tools for inspecting and modifying HDF5 output. The HDF5 output created by the field-value recorder is explained in more detail in Section 6.11.3.1 [Field-Value File HDF5 Content], page 85.

This determines the subdirectory in which all the recorded field-value files will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to recorder\_output\_dir (see [recorder\_output\_dir], page 73).

. . .

); };

floating-point coord\_x (units: m) [Sub-variable of FieldValueRecorders]

integer coord\_x\_in\_cells [Sub-variable of FieldValueRecorders] This is the x coordinate of the recorded position in the simulation grid. It is relative to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If the coordinate corresponds to a non-integer cell position, the closest integer position is chosen.

floating-point coord\_y (units: m) [Sub-variable of FieldValueRecorders]
integer coord\_y\_in\_cells [Sub-variable of FieldValueRecorders]

This is the y coordinate of the recorded position in the simulation grid. It is relative to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the \_in\_cells suffix should be appended to the variable name. If the coordinate corresponds to a non-integer cell position, the closest integer position is chosen.

floating-point coord\_z (units: m) [Sub-variable of FieldValueRecorders]
integer coord\_z\_in\_cells [Sub-variable of FieldValueRecorders]

This is the z coordinate of the recorded position in the simulation grid. It is relative to the grid origin (see Section 6.2.6 [Coordinate Origin], page 16). The units are either in meters or grid cells. For the latter, the <code>\_in\_cells</code> suffix should be appended to the variable name. If the coordinate corresponds to a non-integer cell position, the closest integer position is chosen.

string recorded\_component [Sub-variable of FieldValueRecorders]

An individual field-value recorder (in a group delineated by the curly brackets '{}') only records a single scalar value extracted from the vector-valued electromagnetic field. This could be one of the Cartesian components or the absolute value of the electric or the magnetic field. These are represented by the string values "Ex", "Ey", "Ez", "E", "Hx", "Hy", "Hz", and "H". If you would like to record multiple Cartesian components of a vector field, simply add other field-value recorders (i.e., other groups, see Section 5.2.5 [Groups], page 11) to the FieldValueRecorders list with the desired recorded\_component values.

string recording\_scale [Sub-variable of FieldValueRecorders] If "linear", the raw values are recorded. If "absolute", the absolute value is taken before recording. If "dB", the decibel value  $(20 \log_{10}(|\cdot|))$  is recorded.

string field\_value\_dir (default: "") [Sub-variable of FieldValueRecorders] This determines the subdirectory in which this individual field-value file will be placed. Unless it has a slash '/' up front; this path is interpreted as being relative to field\_value\_recorder\_output\_dir (see [field\_value\_recorder\_output\_dir], page 83). By default, no subdirectory is created inside field\_value\_recorder\_output\_dir.

This determines the base string in the full name of the field-value file. Other information is appended to the name of the file to differentiate individual field-value files (see the example below).

```
string [Sub-variable of FieldValueRecorders] field_value_file_extension (default: "hd5")
```

This is the extension of the field-value file name. If assigned the value "", no extension is added to the file. The HDF5 extension "hd5" is applied by default.

Here is an example field-value file name:

```
FieldValueFile_Ex_0_1.hd5
```

The base string in the name of the file ("FieldValueFile") is specified by the field\_value\_file\_name variable. The second part of the file name, "Ex", is determined by the recorded field component. The two integers that follow are the run index (see Section 6.14 [Multiple Simulation Runs], page 87) and the index of the field-value recorder inside the FieldValueRecorders list. For example, if there are two groups (two field-value recorders) in the FieldValueRecorders list, the first one will write into

```
FieldValueFile_Ex_0_0.hd5
```

while the second will write into

```
FieldValueFile_Ex_0_1.hd5
```

If there are two simulation runs (i.e., number\_of\_runs is equal to 2 – see Section 6.14 [Multiple Simulation Runs], page 87), then the files created in the second run will have 1 instead of 0 as the first integer in the above file names. Finally, the extension ("hd5") of the line files is determined by the variable field\_value\_file\_extension.

```
boolean [Sub-variable of FieldValueRecorders] append_group_index_to_file_name (default: true)
```

If this is set to false, the second integer in the filename (see above) and the underscore preceding it are not included in the filename. It is set to true by default. If this variable is set to false and there are multiple groups (field-value recorders), there will be a name clash, and the output will be undefined.

#### 6.11.3.1 Field-Value File HDF5 Content

The HDF5 file created as the output of the field-value recorder can be viewed and modified using freely-available tools. One of these tools is HDFView, provided by the HDF Group. MATLAB also has built-in functions and tools that handle HDF5 files. For reference, a MATLAB script named 'angora\_fieldvalue.m' is distributed as part of the Angora package, which reads an Angora field-value file and plots the recorded waveform. This script is installed in the directory '\$(prefix)/share/angora/' (see Chapter 3 [Compilation and Installation], page 7). If Angora was installed without any \$(prefix) configuration option, the default location is '/usr/local/share/angora/'. This script can also be downloaded directly from the Angora website (link here).

The HDF5 datasets in the field-value file are the following:

- 'angora\_version': An integer array of length 3 with the major version, minor version, and revision numbers of the Angora package used to create the file.
- 'time\_step': A floating-point value specifying the temporal step in the simulation (in sec).
- 'initial\_time\_value': A floating-point value specifying the time value corresponding to the beginning of the simulation (in sec). This is usually a negative value, since time waveforms frequently begin before t=0.
- 'field\_values': A 1-D floating-point array with the recorded field values.

#### 6.12 Paths

```
string angora_basepath (default: ".")
```

[Global variable]

This variable specifies the base directory for all the input-output operations in Angora. If there is no slash '/' in front of the path, it is interpreted as a relative path starting from the working directory (i.e, the one from which Angora is launched.)

Any other input or output directory will be assumed *relative* to angora\_basepath. An overarching exception is when a directory is specified with a slash '/' up front; in which case that directory will be taken as an *absolute path*, and not relative to angora\_basepath.

```
string output_dir (default: "output")
```

[Global variable]

This is the base directory for all the output that will result from Angora. It is interpreted as being relative to angora\_basepath, unless it is preceded by a slash '/'. All other output directories are created as subdirectories of this directory.

Example:

```
angora_basepath = "angora_stuff";
output_dir = "data";
```

With these variable assignments, all the output will be written into subdirectories within './angora\_stuff/data/'.

#### string input\_dir

[Global variable]

This is the base directory for all the input that will be read by Angora. It is interpreted as being relative to angora\_basepath, unless it is preceded by a slash '/'. Unless the path to an input file is absolute (i.e., preceded by a slash '/'), it is interpreted as being relative to input\_dir.

Example:

```
angora_basepath = "angora_stuff";
input_dir = "input_data";
```

With these variable assignments, the input base directory becomes './angora\_stuff/input\_data/'.

# 6.13 Logging

You can keep a log of the simulations run by Angora in a log file, which contains several lines of information for each simulation. First, an estimate of the finishing time and duration of

the simulation is written into the log entry. The actual finishing time and duration is added to the log entry upon completion of the simulation.

Here is an example entry for a simulation in the log file:

```
johndoe started Angora on 02/22/12 11:54:36AM
Estimated to finish on 02/22/12 11:54:42AM
Estimated duration : 6 seconds.
Simulation finished on 02/22/12 11:54:42AM
Elapsed time : 6 seconds.
```

## boolean enable\_logging (default: "true")

[Global variable]

If set to 'true', Angora will keep a record of the simulations that it runs in a log file. The name of this log file is specified by the log\_file\_name variable, and the directory in which this file resides is specified by the log\_output\_dir variable.

```
string log_file_name (default: "angora.log")
```

[Global variable]

This is the name of the Angora log file. It resides in the directory specified by the log\_output\_dir variable.

```
string log_output_dir (default: "log")
```

[Global variable]

This is the directory in which the Angora log file is kept. Unless it is preceded by a slash '/', it is taken as relative to the base output directory output\_dir (see Section 6.12 [Paths], page 86).

# 6.14 Multiple Simulation Runs

A number of consecutive Angora simulations can be set up in a single configuration file.

```
integer number_of_runs (default: 1)
```

[Global variable]

The number of simulation runs is specified by the number\_of\_runs variable. The simulation runs (or *runs* for short) are indexed from 0 to number\_of\_runs-1. You can refer to these indices later in the configuration file for enabling or disabling certain configuration variables for certain runs (see [enabled\_for\_runs], page 88).

```
integer-array disabled_runs (default: none)
```

[Global variable]

This array of integers (see Section 5.2.6 [Arrays], page 12) lists the run indices for simulations that will be skipped.

Example:

```
disabled_runs = [1,2,3,4,5];
```

If number\_of\_runs was 7, the above variable will cause only the simulations with indices 0 and 6 to be run.

```
integer-array disabled_run_range (default: none)
```

[Global variable]

If you would like to disable simulations that correspond to a *range* of run indices, you can use this variable. This has to be an array of integers with only two elements (see Section 5.2.6 [Arrays], page 12). Simulations with run indices between (and including) these two integers will be skipped.

The following variable assignment has the same effect as the one in the previous example:

```
disabled_run_range = [1,5];
```

Certain variables can be *enabled* or *disabled* for any of the simulation runs using the <code>enabled\_for\_runs</code> or <code>enabled\_for\_run\_range</code> arrays. These arrays can be used inside any group structure (see Section 5.2.5 [Groups], page 11) to specify the run indices for which that group is enabled.

The enabled\_for\_runs array simply lists the run indices for which the specific group is enabled. For example,

```
number_of_runs = 4;
PointSources:
(
    {
        //point source #1
        enabled_for_runs = [0,1,2];
        coord_x_in_cells = 0;
        coord_y_in_cells = 0;
        coord_z_in_cells = 0;
        source_orientation = "x_directed";
        waveform_tag = "waveform1";
    },
        //point source #2
        enabled_for_runs = [3];
        coord_x_in_cells = 0;
        coord_y_in_cells = 0;
        coord_z_in_cells = 0;
        source_orientation = "x_directed";
        waveform_tag = "waveform2";
    }
);
```

In this example, each group represents a collection of variable assignments that characterize an individual point source. With the enabled\_for\_runs variables set as shown, simulations 0, 1, and 2 will be run with the first point source; whereas simulation 3 will be run with the second point source.

Alternatively, the enabled\_for\_run\_range array can be used to specify a range of run indices for which the group is enabled. This should be an integer array of length two. It specifies the lower and upper limits of the range of run indices for the specific group. For example,

```
coord_y_in_cells = 0;
coord_z_in_cells = 0;
source_orientation = "x_directed";
waveform_tag = "waveform1";
}
);
```

This point source will only be enabled for run indices 0, 1, 2, 3, 4, and 5.

#### 6.15 Miscellaneous

## 6.15.1 Auto-Saving the Configuration

Angora can automatically save a record of every simulation configuration that it processes.

```
boolean auto_save_cfg (default: "false")
```

[Global variable]

If set to 'true', Angora will automatically write every simulation configuration it runs into another configuration file, and save it in the directory specified by cfg\_output\_dir. A time/date string is appended to the name of the saved file to differentiate between subsequent executions of the same configuration file.

```
string cfg_output_dir (default: "cfg")
```

[Global variable]

This is the directory in which the auto-saved configuration files are placed. Unless it is preceded by a slash '/', it is taken as relative to the base output directory output\_dir (see Section 6.12 [Paths], page 86).

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