User's Manual

GSolver

Diffraction Grating Analysis for Windows

Version 5.2

Grating Solver Development Company

www.gsolver.com

GSolver Version 5.2 User's Guide

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This Manual

7th Edition, July 2012, updated to reflect version 5.2.1.4 of code.

Grating Solver Development Company

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1 Introduction

1.1 Overview

Introduced in 1994, GSolver is a full vector implementation of a class of algorithms known as Rigorous Coupled Wave (RCW) Analysis. These algorithms give a numerical solution of Maxwell's equations for a periodic grating structure that lies at the boundary between two homogeneous linear isotropic infinite half spaces: the substrate, and the superstrate. The solution is rigorous in the sense that the full set of vector Maxwell's equations are solved with only the following two simplifying assumptions: 1) a piecewise-linear approximation to the grating construction, and 2) a truncation parameter for the Fourier series representation of the permittivity (and impermitivity) within each grating layer. GSolver is set up to work with linear isotropic homogeneous materials.

Within GSolver, a grating is specified by a series of thin layers. Each layer consists of (box shaped) regions of constant indices of refraction. By allowing the scale of this approximation to decrease, a spatially-continuous grating structure can be approximated to any desired accuracy.

Version 5.1 uses the same hardware key system as previous versions of GSolver, and is forward compatible with the older keys (32-bit parallel port, and USB type keys).

In general, the GSolver executable is static linked. This means that it is a stand-alone application and does not rely on a host of Microsoft© DLLs. However the basic graphics (charting) engine requires the ChartFX© clientserver.core.dll as well as the GDI library (which is a native component for most Microsoft OS). These additional libraries are installed in the local GSolver directory (%install directory%/support) to minimize possible conflicts with the host system and other applications.

GSolver uses the system registry to store the user tool bar and menu selections, basic form layouts, and working file names. The materials catalog is called GSolver.ini. (The 'ini' file type is a hold over from earlier versions of GSolver.)

1.1.1 New V5.1 Features

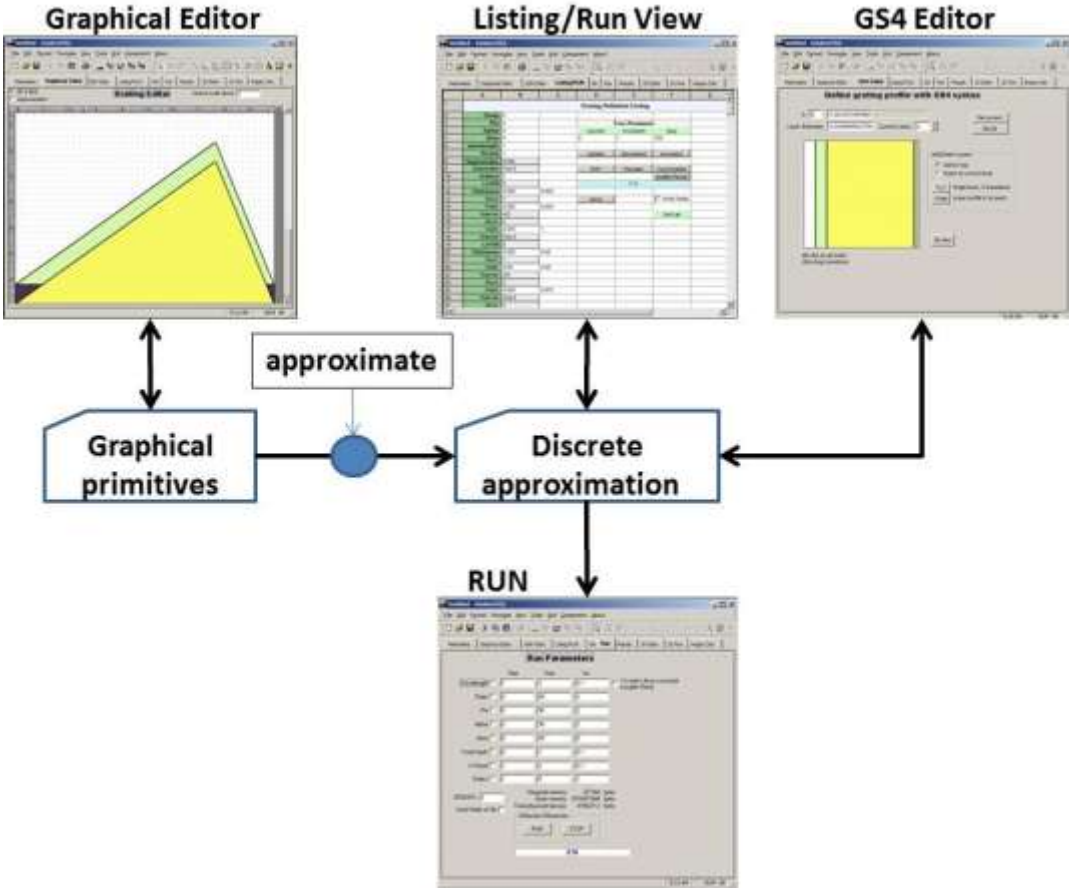
Version 5.1 represents a major rework of previous versions of GSolver. (V4.20c is the prior version.) Many features have been added, many others expanded. Following is a list of the principal differences between V5.1 and previous versions:

- Graphical Grating Editor
- Automatic piecewise approximation construction
- Greatly expanded genetic algorithm for automatic design
- General algebraic constraints and equation editor
- Improved graphing
- Object linking and embedding (for interfacing to other programs with drag and drop capability)
- Modified interface with independent floating GSolver windows
- The materials file (Gsolver.ini) is now written to the root directory (location of the GsolverV51.exe file)
- More consistent use of units. All forms now expect input in the user Units selection (made on the Parameters tab).
- The genetic algorithm merit function has been expanded to allow for summing a result over a set of angles or wavelengths. This allows for optimization over certain parameter ranges.
- The results of a Grating Listing run or a GA run can now be copied to the internal piecewise grating structure allowing for the results of (say) a GA run to then be used directly in a Grating Listing run or from Run.

1.1.2 New V5.2 Features

Version 5.1 release included some 30 interim upgrades with various bug fixes and addition of new features. Version 5.2 release includes a new editor, patterned on the legacy V4.20 editor. A clear understanding of the interrelation between the various grating definition editors and the internal grating array is essential. The various user interactions are described in the following section

1.2 GSolver Grating Definition



All calculations are performed on the ‘Discrete approximation’ of the grating structure. This is best viewed/examined from the Listing/RUN view tab. Note that changes made on the List/RUN view grid are copied to the ‘Discrete approximation’ data structure with the Copy/Update button on the Listing/RUN grid. The ‘Populate’ button copies the ‘Discrete/approximation’ data structure to the Listing/RUN grid.

All horizontal dimensions of the 'Discrete approximation' **are relative to the Period** which set on the Parameters tab. Thus all Widths for each layer must total to 1.0.

All vertical dimensions are absolute (based on the Units set on the Parameters tab).

Remembering the above two principles will alleviate many sources of confusion when designing gratings. In general it is good practice to 'populate' the Listing/RUN grid and do a quick chech the the physical dimentions are as expected.

The RUN command (on the Listing/RUN, GA, and Run tabs) operate on the 'Discrete approximation' data structure.

1.3 Example Run (Quick Start)

The GSolver V5.1 install directory should include GsolverV50.exe, Gsolver.ini (the materials catalog), this users guide, and a subdirectory that contains ChartFX.ClientServer.core.dll (for graphics, and other graphics related dll files). If an INI file is not found, GSolver will create one with a default for each material class. Prior version INI files can be used if a [CONSTANT] section, such as shown below, is added.

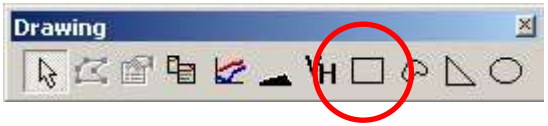
```
[CONSTANTS]
total = 3
Ones: 1, 0
One.25: 1.25, 0
One.5: 1.5, 0
```

This identifies three materials of the following constant refractive indices: 1.0, 1.25, and 1.5. Besides the [CONSTANTS] section, V5.1 INI files **must** also contain the following sections: [DRUDE], [SELLMEIER], [HERZBERGER], [SCHOTT], [POLYNOMIAL], [TABLE] with at least one entry in for each type.

1.3.1 Binary Grating Example

This section gives a step-by-step example for creating a single binary layer grating (one layer with one index transition).

1. Open GsolverV5.1
2. The Parameters form is the global settings home. The substrate and superstrate materials may be selected here. (More details are found in the Dialogs chapter.) Select a substrate and superstrate material by clicking on the appropriate select buttons.
3. Enter the grating period (or lines/mm), wavelength, and other parameters. (A discussion of the angles is given in the Parameters Tab chapter.)
4. Click on the Editor tab. Shown on this tab is the graphical working area called the canvas (see chapter 4). The substrate is located at 0 and below, referenced to the ruler on the left, and is not shown on the canvas.
5. This example employs the square (rectangle) shape button to draw a rectangular structure. If not already present, use the menu item Tools→Customize to add the drawing tools to the toolbar. (See the section on toolbars if needed.)



Drawing Tools

6. Click on the square tool button. Place the mouse cursor anywhere on the active area of the canvas, and, while holding down the left mouse button, drag the mouse to create a rectangle on the canvas.
7. Move the mouse cursor into the interior of the rectangle and right click. This brings up an item property menu. Select Properties.
8. Select a material for the rectangular region just created. In principle, any shape may be made, and assigned a property. For overlapping shapes, the region on top is used when making the grating definition.
9. Drag the rectangle to the bottom of the canvas so it rests on the substrate region.
10. The units of the canvas are normalized to 1 grating period. The view region can be sized to any reasonable size, however the width

of the canvas is 1 period no matter how the canvas is sized for display purposes. This is explained in detail in the Editor chapter.

11. Recalling that periodic boundary conditions are assumed, the single rectangle drawn in the canvas represents a binary grating looking edge on. Once the grating is defined with the graphical editor, an internal piecewise-constant approximation can be created. This gives the representation used in the RCW analysis.
12. Click on the Approximation radio button in the upper left corner of the canvas area to create the piecewise constant approximation. Each time this button is clicked, and only then, the internal representation of the piecewise constant construct is recalculated.
13. The spatial resolution of the piecewise constant construct is determined by the canvas grid (see Editor Tab for greater detail). It can be made finer in two ways: 1) by changing the grid spacing by selecting Grid Properties from the Grid menu, which can also be activated by right clicking in the canvas area; or 2) by changing the canvas resolution (a number of view units equals one grating period), which can be accessed under the menu entry Edit→Canvas Properties. Also, the actual layer and inter-layer geometric dimensions of any piecewise constant feature are accessible, and modifiable on the Listing/RUN tab.
14. Click the Run tab. This brings up the standard global parameter list similar to that of prior versions of GSolver. Using the check boxes, select one or several parameters, enter limits and then click the RUN button. The calculated results are shown on the Results Tab.
15. Alternatively, click on the Listing/RUN tab to bring up the single parameter editable list option.
16. On the Listing/RUN tab click the Populate button to load the list from the current internal piecewise constant construct. If the ‘Approximation’ button on the Editor form has not been clicked, this construct is empty, and so nothing will change. The piecewise constant listing is discussed in the Listing/RUN chapter.
17. For this example the Listing/RUN will be used for a couple of simple calculations. To create a run with the angle of incidence changing. Enter the following formula into grid B2

    =D5/2

All cell formulas begin with an equals sign (=) and are calculated immediately. [To toggle between formula view, and value view use the menu Formulas→Formula View.] The formula engine included in GSolver is very extensive and powerful. It includes all common functions, and logicals, with logical conditional constructs. The formula engine is discussed in the Grid Formula chapter. Any cell can be used in any formula as long as nested iterations and a few restricted cells are avoided.

18. This Listing/RUN grid comes equipped with a single free parameter in cell D5. Enter the parameter increment and stop values as indicated in E5 and F5; set them to 0 and 80 respectively. This will cause the value of theta (formula entered in B2) to change from 0 to 40 degrees in steps of 0.5 degrees.
19. Now click on the RUN button in cell D9. The first thing that happens is that GSolver cycles through the parameter range. For complicated formulas the increment and decrement buttons may be used to single step the grid computation to verify correct behavior.
20. After the first run through, the parameter loop is reset, and then on each parameter increment the current grating list, as defined on the grid, is sent to the solver routines. The solution is written to the Results grid (Results tab).
21. At the completion of the loop, the Results tab is displayed. Select any column(s) to graph by clicking on their headings. Multiple columns are selected using the shift and ctrl keys along with the mouse in the usual manner. The many options available for graphical display are discussed in the Graphing Options chapter.
22. Return to the Listing/RUN tab. Reset the parameter D5 to 0 and change cell B2 to 10 for a fixed 10 degree incidence angle.
23. Enter the following formula in cell B6 (wavelength):

    =if(D5/100>.5,D5/100,.5)

    This is a from of a conditional entry. The wavelength remains constant (0.5 microns) if D5/100<=0.5. Otherwise it changes linearly with D5 as given in the formula.
24. In cell B7 enter the following formula

    =1.+D5/100.

This formula changes the grating period from 1 to 2 linearly as D5 changes from 0 to 100.

25. Change the orders field to 5.
26. Click the Run button and examine the results.

Note that the thickness of any layer can be entered as a constant or through a formula on the grid listing. With this capability all film thicknesses (layers) can be accurately set; the finite grid resolution of the canvas does not limit layer thicknesses.

1.3.2 Blaze Grating Example

For the Blaze grating use the tool button that shows a Blaze profile in black. This is a general tool that includes common grating design tasks. [Note that the dimensions need to be considered carefully as pointed out in section 1.2.]

Blaze Tool Button

1. From within the Editor tab, click on the Blaze tool button. This brings up the Custom Profile Construction dialog which includes Blaze, Triangle, Sinusoidal, Piecewise linear, and Piecewise spline.
2. In the Blaze grid profile, select the desired blaze angle (change the default 35 in cell C3, or leave it as 35). Click OK.
3. A blazed profile is created. A blaze grating profile is a right triangle. Select a material property for the triangle by right clicking it.
4. At this point it is easy to create a conformal layer for this profile. Select the triangle shape just created with a mouse click, then hold down the control key, and click and drag the triangle. A copy of the triangle is created. Change the properties of the new triangle. Then send it behind the original triangle by right clicking the new triangle and using Order→Send to Back. Move the second triangle so that a thin conformal layer is created around the original triangle. The small gaps left in the lower right and left sides can be filled in with rectangles of the appropriate material settings.

5. Click the Approximation button to create the piecewise constant approximation used by GSolver.
6. Perform a grating calculation using the RUN or Listing/RUN tab.

1.3.3 Alternative Blaze Procedure[1]

Here, we describe how to set up a blazed surface-relief transmission grating with the facets towards incident light. This example is for a 125 line/mm grating with a blaze angle of 30°, with light incident at 30°.

1. Begin by filling in the appropriate information on the parameters tab:

Vacuum wavelength	1.5 microns	Can be changed at will
Grating lines/mm	125	Or enter grating period of 8 microns
Theta	30	Angle of incidence
Alpha	45	Unpolarized light
Superstrate index	1	Light incident in vacuum
Substrate index	1.5	Grating material index

2. Select the editor tab. At the upper left you will see the 2D editor button selected.

3. Press the custom profile selection button (the sawtooth icon). The default is a blazed grating. Change the angle (C3) to 30 degrees and press OK.

4. You will now see a grating facet in 2D editor mode. The next step is approximate the ideal grating shape by a number of layers. You can control the number of layers by selecting the grid button, then grid properties, and then changing the grid spacing parameters. A smaller grid spacing number gives more layers.

[1] Provided by Daniel Fabricant, e-mail 23 Nov 2010.

5. You now need to set the scale of the grating facet. For an 8 micron period, you need to enter an 8 in the vertical scale factor box in the editor window so that the layers will have the correct physical scale.

6. You can now select the approximation button in the editor window and a layered approximation of the grating is drawn. This approximation will be used for the grating calculations.

7. Now select the Listing/Run tab, and press the populate button. You can now see the grating layers described numerically on the spreadsheet.

8. Now you can select the run tab. If you check the wavelength box and enter appropriate parameters you can calculate the grating performance in various orders as a function of wavelength. Now press the run button. When the calculation is complete, the results screen pops up. Highlight a column and press the chart button to get a plot of efficiency versus wavelength in the chosen order.

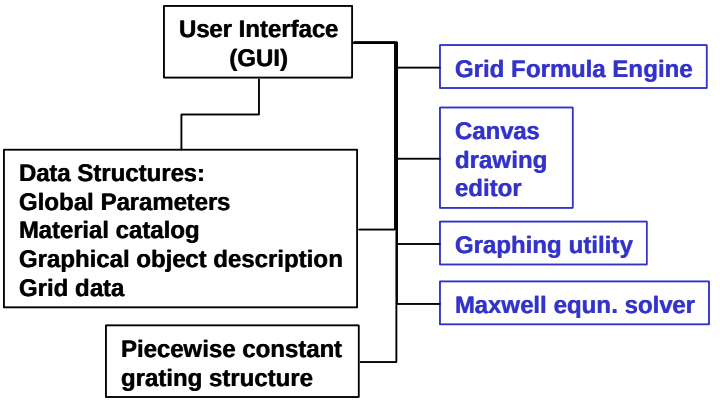
1.3.4 Yet Another Blaze Procedure

1. Set the superstrate, substrate, Period, wavelength and so forth on the Parameters tab.
2. Click over to the GS4 Editor and click on the N-ties option. This brings up a GS4 dialog (more on this in the GS4 section below).
3. Enter the desired blaze angle in the Balze angle calculator, press the ‘enter’ key to display the result. Not the ‘pct’ value. This is the position of the apex of the ‘triangle’ profile relative to the current Period.
4. Click on the handle in the graphic and drag it to so the x: position is either the pct value of 1-pct value (depending on left/right orientation).
5. Enter the h: value in the Total thickness box (which translates to the maximum y-dimension for the profile).

6. Decide on the number of level you want for the discrete approximation.
7. Set the base and top index values and click OK.

2 General Principles

2.1 Overview



Each top-level GSolver window, as depicted in the figure above, is designed to operate on a single grating structure.

The objects in blue are shared components. The objects on the left are unique to each top level GSolver window. Therefore if multiple GSolver windows are open, each with some grating structure entered, then all parameter settings are unique to that window's particular grating.

When GSolver is started, the first order of operation is to look for the INI file in the local directory where GSolver was launched. If GSolver does not find one, it creates a new one with default materials of each type.

When GSolver shuts down, its final operation is to rewrite the INI file with the current material structure. Thus, if there are multiple GSolver windows open from the same directory, the last one closed will overwrite the INI file. This should be kept in mind when using the GSolver material editor to add or otherwise change the material catalog.

2.2 Drag and Drop

GSolver V5.1 is built as an OLE (Object Linking and Embedding) object. This permits the various graphical fields to be dragged between different

GSolver windows, as well as any other OLE enabled application (such as the Microsoft© Office applications).

2.3 Importing grating defitinion by text file

A grating may be defined in text format external to GSolver and imported using the

File → Import Text

menu item when the Editor tab is active.

2.3.1 Grating Text File Format

Following is an example grating definition file format for a two layer grating structure. The first layer has two regions, and the second layer has four regions.

```
[LAYER]
 0.213
 0.2 DRUDE Lead true
 0.8 CONSTANT Ones false
[LAYER]
 0.132
 0.12 SCHOTT BSC4h true
 0.22 HERZBERGER KCL true
 0.26 TABLE SIPOLY10 true
 0.4  CONSTANT Ones false
[END]
```

Layers are numberd starting with the substrate and moving up. The LAYER description starts with the first layer on top of the substrate (which is defined within GSolver on the Parameters tab) and is identified with the

[LAYER]

keyword. The first line following the [LAYER] keyword is the THICKNESS of the layer in MICRONS (be sure to leave the default GSolver units on the parameters tab as Microns).

Following the thickness line is a line for each block of material within a single period. There must be at least one block definition (a uniform layer will have width 1.0).

A block definition consists of four entries on the same line: a relative width (based on grating period), a material catalog type which must be one of

CONSTANT, TABLE, SCHOTT, SELLMEIER, DRUDE, HERZBERGER, and POLYNOMIAL

which are the seven index models used in GSolver; the catalog entry NAME of the material, which must be listed in your GSolver.ini (and loaded into GSolver). The final entry is a flag (true/false) which tells GSolver to update the index value if the wavelength changes or not.

If a block definition line does not have four entries errors will occur.

The sum of the block widths must total 1.0 otherwise an error condition is set and the file read aborts.

A typical file import would proceed as follows: Open a new GSolver instance, set the Parameters to some nominal values (using microns) then click on the Editor tab and then click (from the menu)

File → Import Text

This action will initiate a file read dialog box. Navigate to the text file which contains your grating definition as explained above and open it. GSolver will read the file and update the Editor window.

NOTE: DO NOT CLICK the APPROXIMATION button if you do not want GSolver to approximate the layer widths and thicknesses to the Editor grid spacing. Rather go directly to either Run or Listing/Run and populate the grid.

When the text file is read in, the grating is already defined as a piecewise constant structure. Therefore the internal grating structure is updated automatically and there is no reason to 'approximate' it using the Editor tool.

2.4 Importing V4.20c

GSolver V5.1 incorporates an entirely new user interface with new features and expanded capabilities. In particular, all materials are now tied to material properties that assign indices of refraction for each region, including the superstrate and the substrate. This requires new data structures that do not exist in previous versions of GSolver.

An import function is provided to attempt conversion of V4.20c binary grating files (*.gs4) into the V5.1 format. In many cases the material index of refraction properties are assigned constant values in V4.20c. On import, the constant index of refraction properties are translated into material type CONSTANT (see Gsolver.ini file format), and this property is added to the current material list automatically if it is not found.

Holographic gratings are approximated as a set of constant index of refraction regions. Depending on the granularity of the index modulation, this may lead to a very large number of materials of type CONSTANT.

To import a V4.20 GSolver object, open a new GSolver window and click on the Editor tab. Then click on the menu item File→Import GS4.20c. A file open dialog is created in which you should select the existing *.gs4 file. After selection and clicking the OK button, GSolver creates a dummy 4.0 data structure and loads the *.gs4 binary object into it. It then reads through the data structure and creates a V5.1 data structure from it, using default values for any information that are not assigned. In particular, V5.1 must assign a material type (INI model and model entry property) to each material region. V4.20 objects are generally of constant value, so new

material entries are created as needed for these types. If a V4.20c binary file contains saved catalog materials these may not be converted correctly. This situation can also occasionally cause a program crash (see the known bugs section) which is being addressed.

2.5 Forms

GSolver is a form-driven application. The various data fields that define a grating, and the intended calculations, are arranged by class on different forms. The forms are labeled **Parameters, Editor, Listing/RUN, GA (Genetic Algorithm), Run, Results, 3D Editor, 3D Run, and Angles Calculation**. Separate chapters are devoted to the descriptions of each.

Forms are activated by clicking on tabs, and the data fields in each form provide interfaces to the internal data structure (of which there is one for each top-level GSolver window). Each data document represents one grating structure with its related global and calculation run parameters.

2.6 Toolbars and Menus

Several toolbars are provided for access to various GSolver functions. Most of the tools relate to the graphical grating design interface. The toolbars can be customized by adding and removing buttons, and grouping them as desired. These toolbar buttons are described below.

The Tool Customization dialog is activated by clicking on the menu item Tools→Customize.

Use the toolbar Customize dialog to turn on and off any toolbar, and use the Command page of the toolbar Customize dialog to add or remove buttons from any toolbar. Command buttons may be dragged from one toolbar to another. To remove a button from a toolbar simply drag it from the toolbar to the Command button palette.

Toolbars are docking enabled.

2.6.1 Menu bar

The File menu item includes the commands for saving and loading saved gs5 (GSolver V5.1) grating files. It also hosts the printing commands. The print commands will be active for any form that supports printing.

Use the Import GS4 command to attempt to import a Version 4.20 grating file. This command is active for the Editor tab form. To import a gs4 file, start from a new GSolverV50 window. Click the Editor tab and then click the import command on the File menu. GSolver V5.1 will import the file, assigning constant materials for all of the grating regions. If a required constant material is not found, a new constant material is created. There may be problems importing gs4 gratings that have non-constant materials (see the known bugs section).

The Edit menu command list includes numerous actions that apply to the grid data structures in the Listing/RUN form, the GA form and the Results form. The bottom section of the Edit menu contains a group of commands that apply to the graphical Editor form. Although most of these commands are self explanatory, notes for particular commands are presented below:

Edit→Components – This command activates the Components dialog. Each object on the Editor canvas is identified with a default name. This dialog helps navigate a grating construct with numerous objects. It also provides an alternative way to call up the properties dialog for any particular object.

Edit→Properties – The Properties dialog can be used to define the properties of the selected Editor drawing object. The essential property is the Material, which defines the index of refraction for the object. Other properties exist for convenience, and include the object name, edit flags (indicating whether a property can be altered) the thickness of the boundary line, and the color. By default the color is tied to the index of refraction (see the Editor Form chapter). However, the color can also be set independently of the assigned index of refraction for display purposes

only, since the display color has no effect on the assigned material property. **Note** that the boundary line is generally not used in creating the piecewise constant approximation of the canvas objects. However if the boundary line is made thick enough, and intersects a grid point, it may be included and assigned default superstrate properties by the piecewise constant algorithm.

Edit→Default Properties – The Default Properties are used when a new graphical object is created. **Note** the material property does not take a default value but is set according to the substrate material property.

Edit→Measurements and Size – This dialog controls that canvas viewport units and display scheme. It is recommended that the default settings be used. See the Editor form chapter for more details.

Edit→Canvas Properties – This dialog allows control of the relative canvas size (number of canvas units to 1 period). See the Editor form chapter for more details.

Edit→Color Map – This Dialog controls the color look-up table for the real and imaginary parts of the index of refraction. See the Refractive Index Color Map Dialog for more details.

Edit→Material – This command brings up the Materials editor dialog. See the Materials Editor dialog for more details.

The Format and Grid menu items all apply to the data grids on the various forms. As will be noted, it is possible, separately from the grating, to save as a text file the data on any grid. Thus, several different parameter runs may be saved (and reloaded) for a single grating configuration. The grid data only is saved and loaded with this feature, not the internal piecewise constant data structure. Several commands apply only if a grid item is selected. If a command does not apply it is grayed out (disabled).

The Formulas menu item group applies to the Listing/RUN and GA grid formula engine which is detailed in the Grid Formula Engine chapter.

2.6.2 Main

The default Main command button bar contains the following commands:

New – start a new GSolver window

Load – load a saved (*.gs5) grating structure

Save – a grating structure

Cut, copy and **paste**, apply to graphical as well as to data items

Print

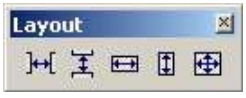
2.6.3 Drawing

The default Drawing command button bar contains commands to generate various graphical items. Included on this command bar are additional buttons to instantiate the Materials Editor, and the Color Map dialogs. Other drawing commands – line, polyline, text fields, bitmaps, and ports – are included for convenient grating design annotation and markups, and are not otherwise used for actual grating structures.

2.6.4 Rotate

These commands are used to rotate graphical objects. The default canvas properties include a snap to grid (allows only discrete moves based on grid spacing) and angle snap (discrete angles based on grid spacing). These snap properties may be toggled on or off.

2.6.5 Layout



The Layout commands are used to size multiple selected drawing objects to each other. Use the shift key in concert with mouse button to select multiple objects.

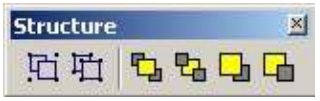
2.6.6 Align

The Align commands are used to align multiple selected drawing objects with each other.

2.6.7 Nudge

The Nudge commands move the selected object a small distance in the indicated direction, but do not allow moving past canvas boundaries.

2.6.8 Structure



The Structure command buttons can be used to alter the z-order (which object is on top) of overlapping objects. When creating the piecewise constant approximation of the grating, the top-most object is used at each grid sample point to define which material property to use.

2.6.9 Zoom

The zoom and pan commands affect only the canvas view; they have no effect on the internal object dimensions which are sized to units of the grating period.

2.6.10 Canvas

The Canvas command buttons include the undo and redo commands (also accessible with control-z and control-y) as well as the grid and canvas property dialogs.

2.7 Index of Refraction

Each enclosed region in the model is assigned a material property from which an index of refraction is calculated. The default is for each material to use the substrate property as assigned on the Parameters form.

GSolver comes with a number of predefined material properties in each model class. This list is not exhaustive and it is expected that materials will be added as needed by the user. This can be done directly editing the Gsolver.ini file with a text editor (such as Notepad). Or it can be done from within GSolver using the Material Editor.

NOTE: It is recommended that new materials in any model class be added to the end of the list. When grating structures are stored, the material property is stored as an index into the material list. When a saved grating is loaded, materials are loaded by index, not by name. Therefore if materials are rearranged by editing the INI file, this might effect the properties of a saved grating. If needed, multiple copies of the material (INI) file can be used. Copy the needed file into the root directory (where the exe is located) before starting GSolver. GSolver reads the INI from the

root directory. If one is not found there a new one is created with minimal entries.

The material model parameters are stored in the GSolver.ini file detailed in the GSolver.ini section. This ASCII file can be edited with a text editor such as Notepad. Described below are the various material models, their parameterizations and representation within GSolver.

2.7.1 Models

GSolver currently has six index of refraction models: Constant, Drude, Sellmeier, Herzberger, Schott, Polynomial, and Table. Of these models, the Constant, Drude, Polynomial, and Table give complex indices of refraction; the others are real valued. The Table model offers the most flexibility as the entries may be made with a wavelength resolution as fine as desired.

Each model has approximate validity over a continuous, finite range of wavelengths. The user must assure that the wavelength values remain within the valid range throughout the diffraction calculations as GSolver makes no check on 'index of refraction validity.'

2.7.2 Constant

The Constant material property returns a fixed index of refraction for any wavelength setting. A Constant material property is specified with a name and real and imaginary indices of refraction. In the INI file these appear as

name: real value, imaginary value

The colon after the name serves as a text (name) delimiter.

2.7.3 Drude

The Drude model is a well-known, simple analytic index of refraction model based on a simplified physical model of the material. A two-parameter model, it is not expected to give accurate results at any wavelength, particularly above the first model resonance.

A Drude model material is entered as

name: p1, p2

Where p1 and p2 are the two real model parameters. The relation between the parameters and the model index of refraction is as follows:

$$n + ik = \sqrt{e_1 + ie_2}$$

$$e_1 = \frac{p_2^2}{\lambda'^2 + p_1^2}$$

$$e_2 = \frac{p_2^2 p_1}{\lambda'(\lambda'^2 + p_1^2)}$$

$$\lambda' = \frac{10000}{\lambda}$$

where λ is the *wavelength in microns*. The square root branch is taken so that *n* and *k* are positive quantities. (All *n* and *k* in GSolver are treated as non-negative quantities.) Typically a Drude model might be used to estimate indices of refraction for metals in the infrared region.

2.7.4 Sellmeier

There are several Sellmeier models in the literature, and GSolver's 12-parameter Sellmeier model comprehends several of them. A Sellmeier material is entered as a name followed by 12 comma-delimited parameters. For example,

> BK7: 0.5, 1, 1.03961, 0.231792, 1.01147, 0, 0, 0.0060007, 0.0200179, 103.561, 0, 0

gives one Sellmeier formulation for the common glass BK7. The index of refraction is calculated according to the following formula

$$n = \left[c_3 + \sum_{i=0}^{4} \frac{c_{4+i}\lambda^2}{\lambda^2 - c_{9+i}} \right]^{c_2}$$

where the *c*'s are the various model parameters, and λ is wavelength in *microns*. (The internal GSolver representation of wavelength is in microns, as are all quantities with length units.)

This model is purely real. Since it does not estimate the imaginary part of the index of refraction, *k* is set to 0 (transparent) for Sellmeier materials.

2.7.5 Herzberger

GSolver's Herzberger model is a 20-parameter real index of refraction model. A typical INI file entry for a material of Herzberger type is shown:

> MgO(IRTR-5): 1, -0.00309946, -9.61396e-006, 1.72005, 0, 0.00561194, 0, 0, 0, 0, 0.028, 0, 0, 0, 0, -1.09862e-005

where the name, Mg0(IRTR-5) in this example, is followed by the 20 comma-delimited model parameters.

The index of refraction is calculated according to

$$n = \left[c_3\lambda^2 + c_5 + c_4\lambda^4 + \frac{c_6}{\lambda^2} + \sum_{i=0}^{4} \frac{c_{7+i}}{\lambda^2 - c_{12+i}} + \frac{c_{17}}{\lambda^2 - 0.0028} \right]^{c_2}$$

There is no parameter labeled c_1 so the first list entry starts with c_2.

This is a real index of refraction model; the imaginary part of Herzberger models are set to 0.

2.7.6 Schott

GSolver incorporates a six-parameter Schott index of refraction model. A Schott material entry example is shown below:

> BK7: 2.27189, -0.0101081, 0.0105925, 0.00020817, -7.64725e-006, 4.24099e-007

This is the Schott model for the glass BK7.

The index of refraction for the Schott model is calculated according to the following formula:

$$n = \left[c_2 + c_3\lambda^2 + \frac{c_4}{\lambda^2} + \frac{c_5}{\lambda^4} + \frac{c_6}{\lambda^6} + \frac{c_7}{\lambda^8} \right]^{1/2}$$

where λ *is in microns* and the six parameters are labeled c_2 through c_7. The Schott material model is real so materials of type Schott return $k = 0$.

2.7.7 Polynomial

The Polynomial model allows for tenth-order polynomials to define both the real and imaginary parts of an index of refraction. This requires 20 real parameters to define a material model of type Polynomial. The basic INI gives a few hypothetical materials. For example

> type2: 1.5, 0. 2, 0, 0, 0, 0, 0, 0, 0, 0, -0.1, 0.095, -0.1, 0, 0, 0, 0, 0, 0, 0, 0

defines a polynomial mode of name type2. The 20 comma-delimited parameters are used to calculate real and imaginary indices of refraction according to the following formulas:

$$n = \left| \sum_{i=0}^{9} c_i \lambda^i \right|$$

$$k = \left| \sum_{i=0}^{9} c_{i+10} \lambda^i \right|$$

where the absolute value signs assure that n and k are both non-negative.

2.7.8 Table

The Table model is the most general material model. It consists of a material name followed by a list of entries. Each line in the list consists of three numbers: wavelength, n, and k. The *wavelength is in microns*.

If a wavelength evaluation is done at a wavelength that is not in the table, GSolver linearly interpolates the table. For example, the following is a partial entry for silver (AG):

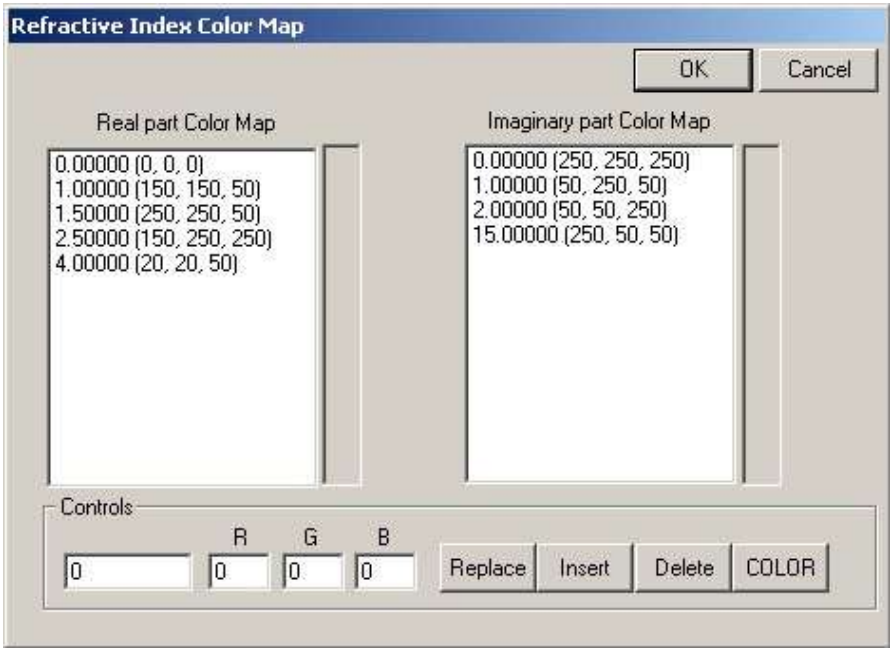
> AG:
> 0.186412 0.995 1.13
> 0.187836 1.00425 1.14938
> 0.189282 1.012 1.16

0.19075 1.0195 1.16813
0.192242 1.028 1.18
0.193757 1.0375 1.19438
0.195296 1.048 1.21
0.196859 1.05963 1.22563
0.198448 1.072 1.24
0.200063 1.08481 1.25125
0.201704 1.098 1.26
0.203373 1.11163 1.26563
0.205069 1.125 1.27
0.206793 1.13719 1.275
0.208547 1.149 1.28
0.210331 1.16144 1.28531
0.212146 1.173 1.29
0.213992 1.18188 1.29281
0.215871 1.19 1.295

For a wavelength selection of 0.20, for example, the table value entries at 0.198448 and 0.200063 would be linearly interpolated. This is a common method of tabulating indices of refraction, and users are encouraged to use the Table model.

2.7.9 Color Map

Indices of refraction, both real and imaginary parts, are represented by colors on the Editor canvas. The two colors are given as a background and a cross-hatching pattern. Assigning of the colors is through a user-definable color map interpolation scheme.



The Color map has two components, lists of piecewise-linear breakpoints through RGB space for both the real and imaginary components of the index of refraction. Break points may be added and deleted from the list.

For example, given n, as the real part of the index of refraction, a search is made through the real breakpoint list to find the two break points that bracket n. These two points define two RGB coordinates. The color of the given n lies along the line between these two points in RGB space as a linear interpolant. The same goes for the k value with the list of imaginary component break points.

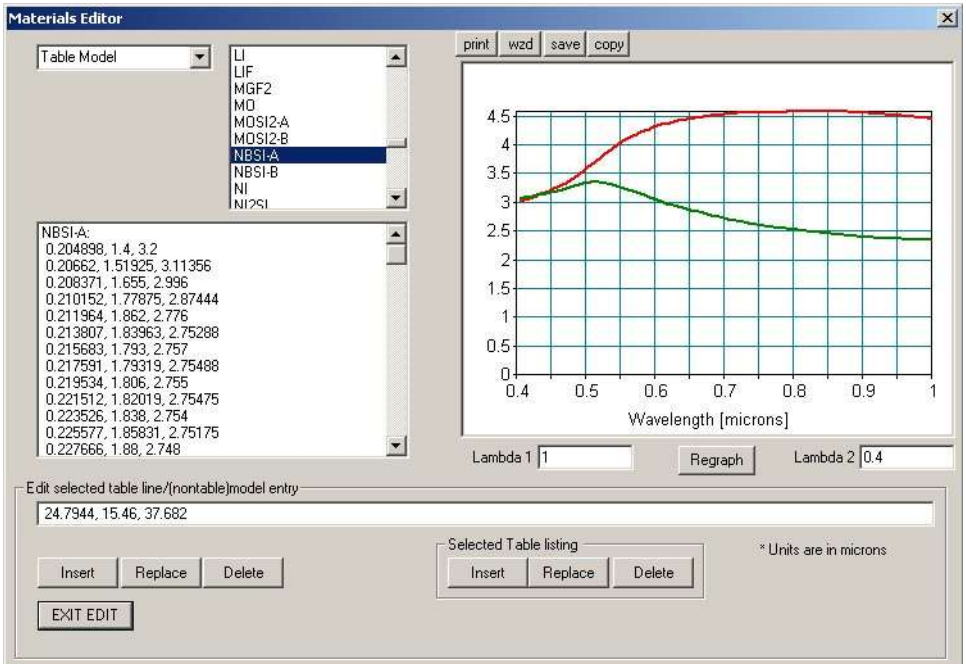
This scheme allows for fairly general color assignments to the real and imaginary parts of the index of refraction. The representation of the colors is done with a two-color fill pattern made up of a cross hatch against a solid background.

Changes to the default color map are stored with the grating in the gs5 file. Therefore, when starting GSolver, each new grating has the default values.

To use modified values simply save a simple grating as a gs5 file. Loading that file will change the color map to the saved settings.

2.8 Materials Editor

The Materials Editor Dialog, as shown in the figure, provides a graphical editing tool for the material catalog items. Any changes made using the Materials Editor do not get written to the GSolver.ini disk file until the current version of GSolver is closed. However, the internal materials tables that are created, by reading the GSolver.ini file when GSolver starts, are modified, and any changes are available for immediate application.



There are two sets of edit buttons on the bottom of the dialog (Insert, Replace, and Delete). The first set applies to all materials. The second apply to the table entries themselves in a line-by-line fashion.

The first step in editing a material is to select a model from the drop down list box; the next is to select a specific material. The selected material

properties are then loaded in the large list box (for Table Models) or in the Edit box for the other materials.

Make any modifications to the material parameters in the edit box and select the edit operation desired: Insert to add it to the model list; Replace the current material selection; Delete to remove the current selection.

For the Table Model materials, the second set of buttons are used to edit the list, and the first set of buttons are used to update the Table material object in the Table catalog.

The Chart provides a graph of the currently-selected material and any changes. The graph has a number of interactive properties, including the ability to drag data points with the mouse (see the chapter on graphing).

2.9 Types of Saved Data

There are three types of data files that are created, saved, and loaded within GSolver: First there is the grating definition file with all of the related data structures and parameters. This is a binary file of type gs5.

The second type of data files contains the saved contents of the various grids: Listing/Run, GA, and Results. The grid contents are saved as ASCII and can be viewed and manipulated by any text editor. The contents of the grids can be saved and loaded, allowing for archiving various data runs based on a single grating definition. They can also be loaded into other programs for further analysis.

The third type of file supports saving the graphs. The graphs are generated with the SoftwareFX client.server graphics interface (including the Microsoft GDI libraries for optimal display device interaction). These graphs can be saved in a variety of formats (*.cfx, *.bmp, and *.emf). All graphic images can be copied to the clipboard and pasted into other applications (control-c, control-v).

2.10 Known 'Bugs'

2.10.1 Inversion of OLE Coordinates

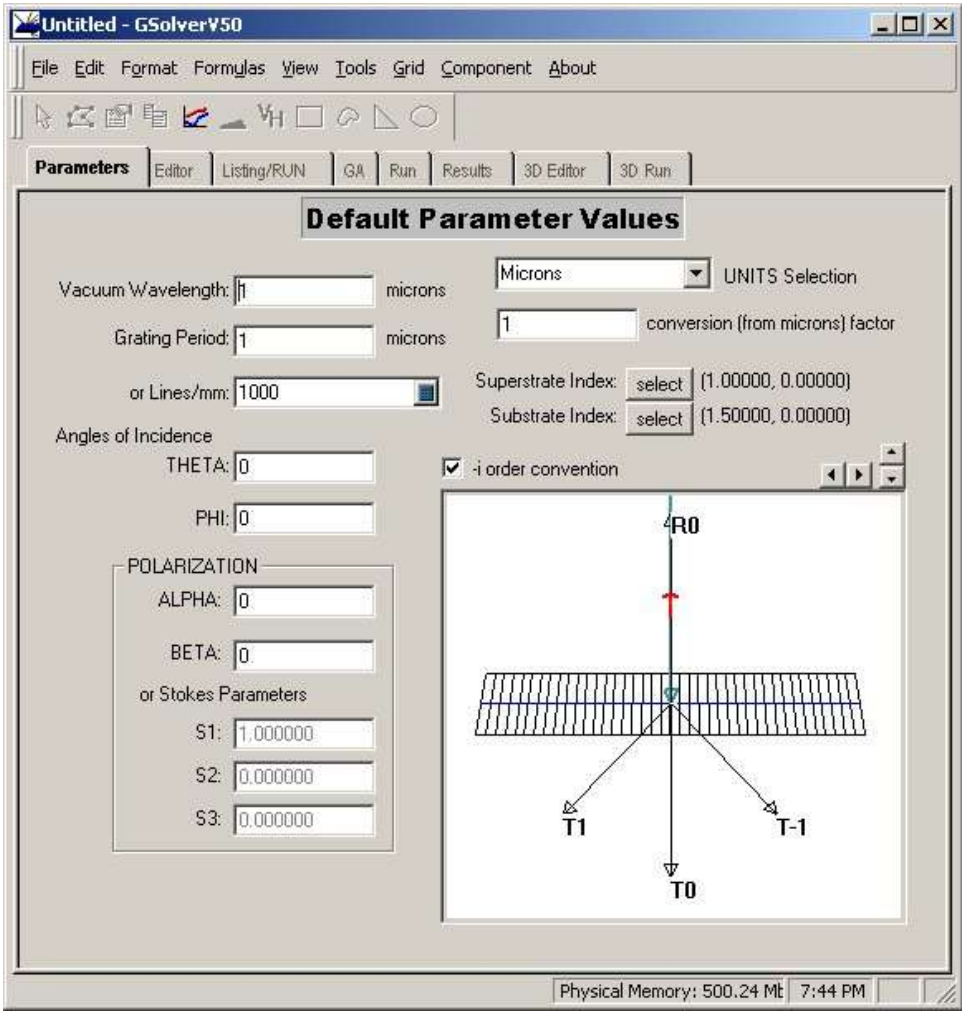
The Editor Graphics are created in a normal Cartesian coordinate system with the origin in the lower left-hand corner of the canvas viewport. The conventional coordinate system for windows objects has the origin in the upper left-hand corner of the window with the y-axis increasing down. Thus, when graphical objects are dragged into other OLE objects, including print objects, the figures are upside down. Since this issue touches a lot of code it is difficult to change, but is being addressed.

2.10.2 V4.20c Data Import Crash

There is an unfortunate bug that can creep into V4.20c binary data files (*.gs4) owing to the existence of two 4.20 binary schemas. In V4.20 an additional data field was created to attempt saving the V4.20 links list as well as any assigned material properties with the grating data. This required adding data fields to the binary schema with a flag to identify which type of file was being loaded. The logic that was used is not sufficiently robust to correctly align the binary data in every case. This causes an unrecoverable read error when a file containing catalog data is read by a different GSolver 4.20 version. This problem is being addressed. The current work-around is to eliminate material catalog links in 4.20 data before importing it to V5.1. This problem can also manifest itself between different installs of V4.20c.

3 Parameters Tab

This chapter describes the various data fields and controls on the Parameters tab form which is shown in the following figure.



The figure in the lower right depicts the grating, showing the illumination k-vector (plane wave), along with the various diffracted orders.

The various Parameter entries are discussed in subsequent sections.

3.1 Units Selection

The internal representations of wavelength and grating period are in units of *microns*. For display, different units may be chosen for these quantities. Several common length units are available for selection from the Units drop down list box. Selecting one of these defines the units conversion factor for the display. The bottom selection in the list is 'User units'. This allows configuring the conversion for units not in the drop down box. Select this item, and then enter the conversion factor in the related text entry box.

The two quantities that have units in a grating calculation are the wavelength and the period. The absolute wavelength is needed for the index of refraction calculation. Otherwise, all calculations are normalized to the grating period. This implied length scaling is permitted since Maxwell's equations are linear.

NOTE: With file version 5.1.1.1 a more consistent use of units has been implemented, with a bug fix. All forms now expect input in the selected units. The parameters with units are

- *Wavelength*
- *Period*
- *Layer thickness*

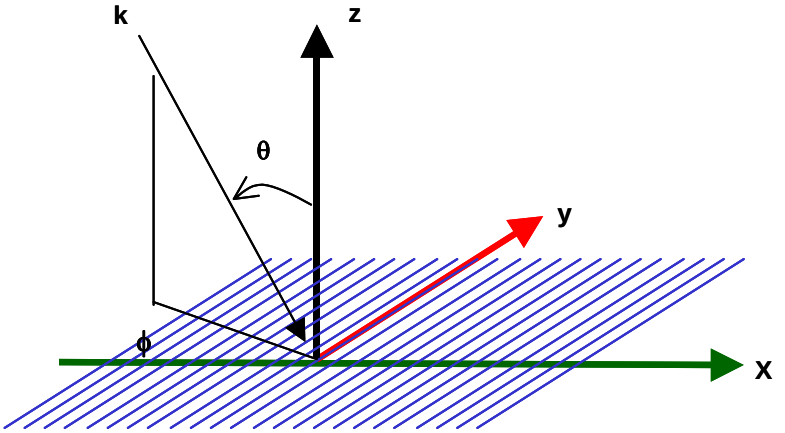
The refractive index transitions within a layer are relative to a Period and so are within the range 0 to 1.

3.2 Angles

All angles are entered as degrees. On the Parameters form are four angle entries that describe the incident plane wave direction and polarization.

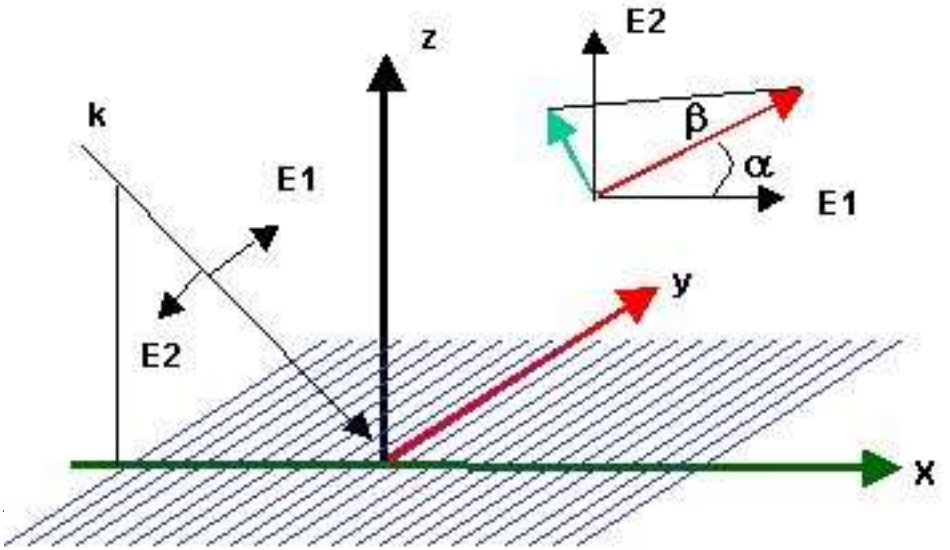
Polar angles θ (theta) and ϕ (phi) are defined as shown in the figure below:

θ is positive for deviation away from the +**z** axis towards the **x** axis. ϕ is



positive for counterclockwise rotation around the **z** axis from the –**x** axis. This convention is for the incident plane wave (**k** vector) illumination. For the reflected components the +**x** axis is used as a reference.

The two angles α (alpha) and β (beta) are used to define the polarization state. If β = 0 the illumination is linearly polarized. For transverse electric (TE) polarization, the principal E-field is normal to the plane of incidence defined by **k** and the **z**-axis. For transverse magnetic (TM) polarization, the principal E-field is in the plane of incidence.



α is the angular deviation of the principle E-field direction away from TE towards TM; $\alpha = 0$ for pure TE, and $\alpha = 90$ for pure TM.

β determines the magnitude of the secondary E-field which is perpendicular to the principal E-field and **k,** and 90 degrees out of phase in time. If the principal and secondary E-fields have equal magnitude, the wave is circularly polarized.

In general $-45 \leq \beta \leq 45$. Labeling the principle E-field as E1, and the secondary E-field as E2, β is the angle shown in upper right in the figure.

3.3 Stokes Definition

The polarization state is also defined by the Stokes vector. Since there is a well-defined plane wave, the Stokes vector has three relevant components {S1, S2, S3}. They are calculated as follows:

E1 = cos(α)
E2 = sin(α), [these are the magnitudes of E1 and E2]
S1 = E1*E1 – E2*E2
S2 = 2*E1*E1*cos(β)
S3 = 2*E1*E1*sin(β)

These components are shown on the Parameters form as read only.

3.4 Order Convention

Different coordinate conventions lead to a different numbering of the diffracted orders. These various schemes arise from choice of the definition of the plane wave vector propagation (± k, ± ω, and ± i). To accommodate the European convention, GSolver includes a sign convention check box on the Parameters form just above the orders display. This check box only changes the sign of the orders. It has no effect on the calculation, or the internal representation of the diffraction orders. The orders are labeled as shown on the Parameters form.

3.5 Substrate/Superstrate

In line with V5.1 convention, all regions of the grating must be assigned a material property. The superstrate and substrate material properties are

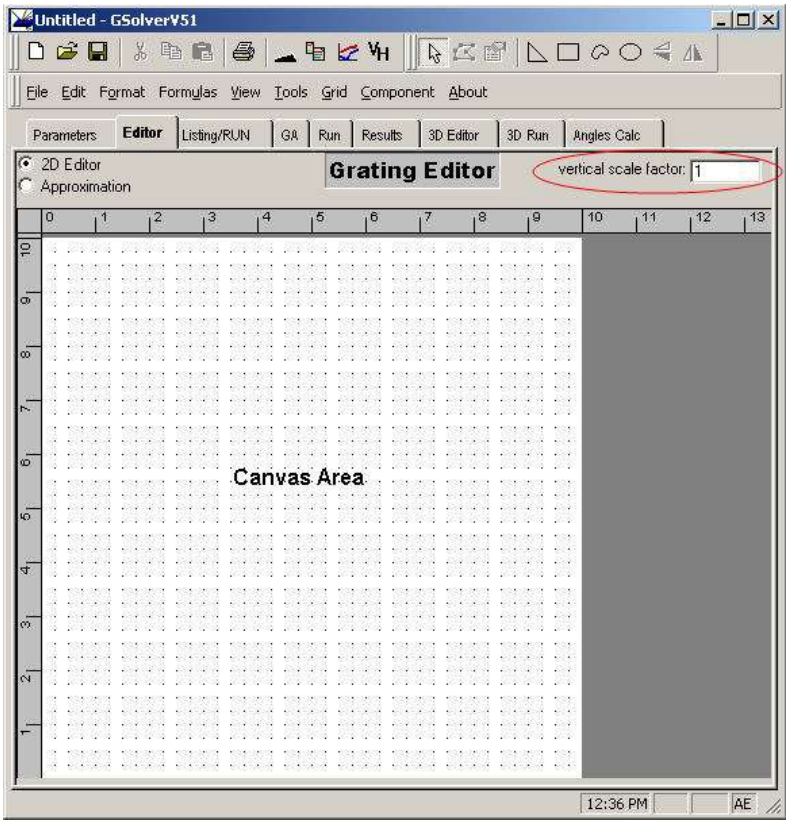
assigned from the Parameters page using the two labeled buttons. The button command creates a Material Property Dialog where a material type and entry may be selected.

3.6 Saving

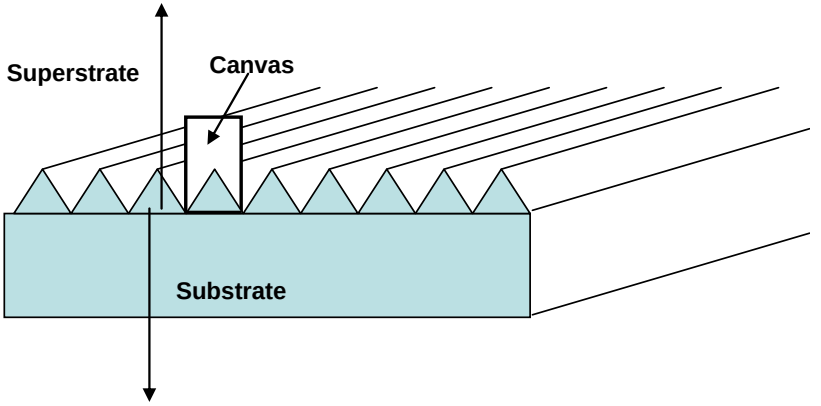
To Save the current grating use the File→Save menu command. A grating file always has a *.gs5 type. If the Listing, Results, or GA form data grid contents need to be saved, use the Grid→Save Grid menu command. Data from grids are saved as ASCII text (*.txt) files.

4 Graphical Editor (Editor Tab)

The graphical grating editor, as shown below, is the primary tool for defining a linear grating structure. **Note** that crossed gratings are handled separately for both editing and calculation, and are discussed in the 3DEditor and 3DRun chapters.



The main area is called the ‘canvas’ where all drawing takes place. The canvas represents an edge-on view of the grating. The substrate exists in the region below the canvas. The area above the substrate is the superstrate. The canvas is the ‘modulation region’ where the grating exists. This is illustrated in the following figure.



Once a figure is drawn, using the primitive shapes and automatic profile tools, a click on the 'Approximation' radio button in the upper left corner invokes the piecewise constant approximation routine. This routine examines the canvas at the each of the canvas grid points and creates a piecewise constant approximation, the internal representation GSolver uses for diffraction calculations.

If drawing objects overlap, the object on 'top' determines the index of refraction for that region. If several objects are grouped, the grouped object is treated as a single object with the 'first' object in the group setting the material property for the group.

New to version 5.1.18 is the Vertical Scale Factor (in the upper righthand corner of Editor form. The scale factor multiples the vertical dimension when the 'Approximation' function is called. GSolver assumes that all horizontal dimensions are relative to a grating period (defined on the Parameters tab). The vertical dimensions are absolute. However it is often convenient to construct a grating with a predetermined number of layers with a certain total thickness. The Vertical Scale Facter multiples the vertical scale (scale factor > 0.) by the desired quantity. In short, the canvas vertical scale is relative to the Vertical Scale Factor.

The Editor tools and operating principles are discussed below.

4.1 Coordinate System

The canvas width is equal to 1 grating period for all unit settings (ie. 10 units on the ruler).

The canvas origin is the lower left-hand corner. The two rulers that span the canvas, on the left and top, represent units relative to the canvas view. The substrate lies in the region <0 on the vertical scale, and is not accessible from the canvas. (The substrate and superstrate material properties are assigned on the Parameters form.) All drawing must be done on the canvas.

There are two dialogs that hold the definitions of how the canvas is displayed. They are the 'Canvas properties. . .' and 'Measurements and size. . .' dialogs. Although the canvas width always maps to 1 grating period, this unit length can also be mapped to some number of pixels on the screen. This is done in the following manner:

GSolver sets the default coordinate mapping style to MM_LOMETRIC which is interpreted as one logical unit equals 0.1 mm (on the monitor). The actual dimensions depend on the type of monitor used. The other screen modes are as follows:

MM_HIENGLISH – one logical unit is 0.001 inch
MM_HIMETIRIC – one logical unit is 0.01mm
MM_ISOTROPIC – one logical unit is 1 pixel in both x and y
MM_LOENGLISH – one logical unit is 0.01 inch
MM_TEXT – one logical unit is one pixel
MM_TWIPS – one logical unit is 1/1440 inch.

While it is possible to change the mapping mode for printing purposes, it is generally recommended that the *mapping mode not be altered*.

On the Measurements and Size dialog, together with the mapping mode, are entries to determine the relation between logical and physical extents (for viewing and printing).

The canvas Drawing scale should usually be set to the drawing units (default is centimeters).

The canvas area can also be modified from the Canvas Properties dialog. This dialog simply assumes that the canvas width and height are some number times the grating period. The grating period is taken as arbitrary for viewing purposes.

The Default canvas size, shown on the Size and Units tab of the Measurements and Size dialog, is 10 cm by 10 cm. Thus the default viewing scale is 10 cm = 1 grating period.

If the canvas width is set to 2 (=2x) on the Canvas Properties dialog, while all other settings remain at default values, the canvas will be drawn with a 20 cm width, which would then represent one grating period. The canvas width and height scales may be set independently.

If the width of the canvas is resized, to increase the grid sampling resolution for example, the various components can be selected and stretched to the new width. Recall that the canvas width is 1 grating period independent of how the viewport of the canvas is configured. If the canvas is resized smaller, any grid objects that now are off the canvas must be resized to the new canvas size.

4.2 Canvas Grid

The grid spacing is set in the Canvas Properties dialog and the grid represents the resolution of GSolver's piecewise constant approximation. There is a minimum grid spacing determined by the monitor resolution together with the mapping modes settings. The easy way to increase resolution is to simply set the canvas size to some larger value, putting more monitor pixels at disposal.

On the other hand, there is a point beyond which increased resolution has no benefit or effect on the outcome of the calculation. This will be grating specific and depends on the relative changes in the material properties. A rule of thumb is design to $\lambda/10$.

The 'snap to grid' feature may be turned on/off from the Canvas Properties dialog. This feature attempts to size all components so that boundaries are on grid points. This is often convenient for sizing components, but can be inconvenient if components have incommensurate

dimensions with respect to the grid spacing. In this case the snap to grid can be turned off. **Note** that the better place for fine tuning dimensions is on the piecewise constant representation of the grating structure, accessible on the Listing/RUN tab.

4.2.1 Accelerator Keys

To delete a region, select it and then key shift-del.

To copy a region, select it and, while holding down the control key, drag the object with the mouse. Objects can be dragged from one grating canvas to another for multiple concurrent GSolver objects.

To copy an object for pasting into another canvas, or any OLE enabled application, right click the object and select copy. To paste, right click the canvas and select paste.

4.3 Tools

Several tools available for drawing grating profiles are discussed in the following sections.

When any region is selected, the boundary is augmented with handles (small gray squares) that can be dragged to resize the object.

4.3.1 Rectangle

The Rectangle tool icon is used to add a uniform layer (thin film). A uniform layer is a rectangle that spans the width of the canvas. Or, it may be used to add a binary transition region.

4.3.2 Piecewise Linear (poly-line)

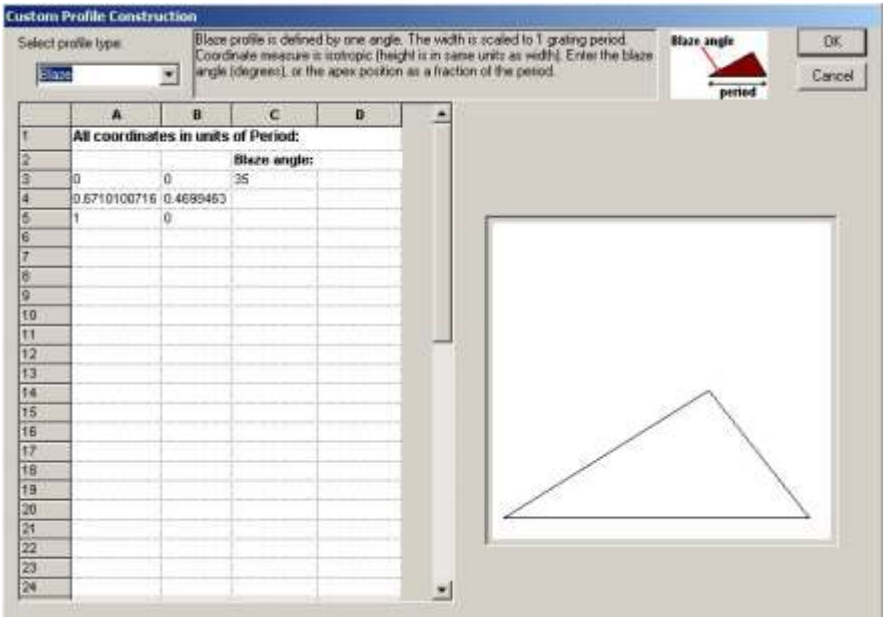
The poly-line tool icon is a triangle. A linear poly-line region is defined by a starting point, defined by clicking the canvas after the tool selection, moving the mouse to a new point and clicking again, and repeating. Each click generates a boundary line from the prior click location to the current click. Double clicking will complete the region.

4.3.3 Spline Curve and Ellipse

The spline curve icon is the kidney shaped command icon. The operation is similar to the poly-line tool, however the shape is smoothed by a cubic spline estimation through each set of 3 points. Double click to complete the figure.

4.3.4 Classical Form Generation

This tool invokes a dialog whose tools generate Blaze, Triangle, Sinusoidal, General Poly-line and General Spline curves. The tool icon for the classical form (custom profile) tool is a black blaze profile (triangle).



Use the list box to select among the several predefined profile types.

Blaze – A blaze profile is defined by a single parameter, the blaze angle. Enter the blaze angle in grid location C3 in the dialog. After the profile is updated, clicking the dialog OK button will insert the profile onto the canvas. The canvas size is increased automatically if needed.

General Sawtooth – A sawtooth profile is defined by two sub-ninety degree angles. Enter the angles to define the profile in grid locations C3 and D3.

Sinusoid (poly) – This profile is a generalized sinusoid constructed by a piecewise-linear approximation. The number of line segments that define the boundary may be set to any reasonable number. The default is 15. Enter the number of line segments in grid location D2.

There are two columns of coefficients, labeled A and B in the equation below, with A entries in grid locations C4-13, and B entries in grid locations D4-13. The general sinusoid profile is defined by the following formula, where A0 is in grid location C3, A1 and B1 are in grid locations C4 and D4, and so forth.

$$y = A_0 + \sum_{i=1,N} A_i \cos(x) + B_i \sin(x)$$

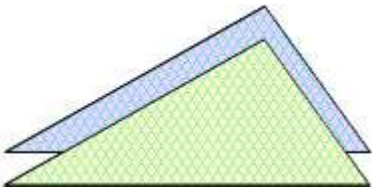
Any desired number of coefficients may be used. The table may be extended simply by entering nonzero values in grid locations Cn where n>13 and so forth.

General poly-line – This form provides a method for constructing an arbitrary poly-line approximation to a general profile. Enter the coordinates of the poly-line end points as an (X,Y) pair in grid locations An, Bn starting with n=2. All x-coordinate entries must be in the range 0<=x<=1, where 1 represents one grating period unit. y-coordinate values should be in the range y>=0. y is absolute, 0≤x≤1 (x is scaled by Period).

General cubic spline – This tool is very similar in operation to the General poly-line. The difference is that every 3 consecutive points are taken as a cubic spline definition. Thus, the number of points entered in the table should be a multiple of 3.

These two tools allow for precise point location for both a poly-line and spline profile definition.

4.3.5 Conformal Coats



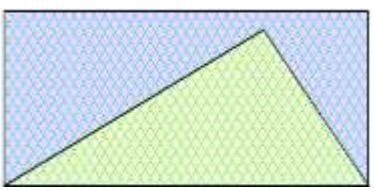
Conformal coats are created by selecting the profile group or object, copying it, and shifting the copy vertically. The copy properties are then set, and the new object is sent to the bottom of the z-stack, or the original object is brought to the front. This procedure is illustrated with the following example.

Conformal coat on a blaze profile:

1. Start a new canvas by clicking on File→New
2. Click on the custom tool icon; select the blaze profile tool (default), and click OK. This puts a blaze profile on the canvas.
3. Right click the blaze profile object and set the material property
4. While holding down the control key, click on the blaze profile object and drag it up (towards the top of the canvas). This makes a copy of the profile object so there are now two on the canvas.
5. Right click on the new copy and set the material properties to the coating material.
6. Move the copy so that the peak of the copy is a few grid units above the original; most of the copy will overlap the original.
7. Right click on the new copy again and then click on the Order option and then Send to back.
8. You may want to turn off the 'snap to grid' property of the canvas
9. To fill in the small areas at the base of the coating use the rectangle tool to create two small rectangles to fill in the area remaining. Use the order property to put the new objects behind the original.

The grating listing generated by the piecewise constant approximation, which is the internal representation of the grating for purposes of calculation, can be edited for precise thicknesses. This is discussed in Chapter 5.

4.3.6 Uniform (fill) Coats



Uniform (fill) coats are made in a similar manner to the conformal coats discussed

above. Simply select the rectangle tool, set its properties and size (width as wide as the canvas), and then put it at the bottom off the z-order. All other objects will be on top, and any canvas space is now covered by the fill material defined by the rectangle object.

4.3.7 Text and Lines

For convenience GSolver contains text and line tools that can be used to annotate grating structures on the canvas. Text and line tools do not have a material property, and should not be used as part of the grating approximation. They do have a color property, but this is not tied to any particular material.

However if it happens that a line or text object intersects a grid point, it is possible that the piecewise constant approximation algorithm will assign some (undefined) property to that location. Therefore the text and grid lines should be used for annotation only; if they affect the piecewise constant approximation algorithm they should be either temporarily covered (sent behind something), moved slightly, or not used.

4.4 Automatic Piecewise Approximation

Once the grating profile is drawn it is necessary to run the piecewise-constant approximation algorithm on the grating objects. This is accomplished by clicking on the ‘Approximation’ radio button in the upper left-hand corner of the canvas area. The approximation is recalculated each time this button is clicked.

The algorithm begins operation by scanning through all of the grid points on the canvas, filling an array with the material properties of any object it finds, always using the top-most object for overlapped regions. If there is no object found it fills the sampling array with the superstrate property.

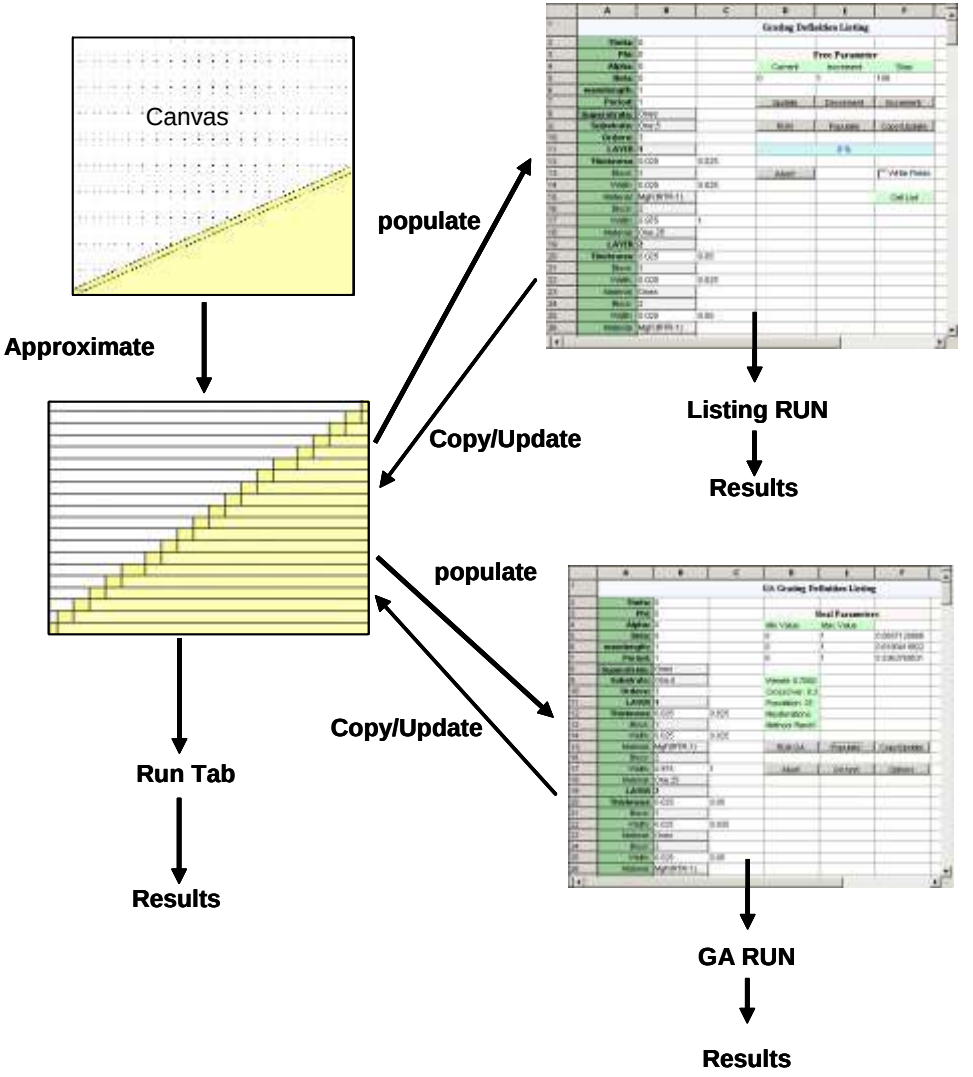
In the case of grouped objects, the material property that gets assigned is the first object in the group list. Thus, it is important to keep track of which objects are grouped, and it is good practice to only group objects of like material property.

Once the sampling array is filled it is then parsed. The array is scanned by columns and rows to find the maximum rectangle (grouped sampling points) that satisfies the piecewise constant approximation. For example, if every grid point happened to have a material property different from any nearest neighbor, then the result would be a maximal set of squares centered on each grid point. If adjacent grid cells in a single row have the same material properties, then the boundaries between them are removed. Columns are scanned before rows. Any adjacent rows that are identical are combined into one row of twice the thickness.

Since the sampling is done at the grid spacing, it is convenient to leave the snap to grid property turned on. It takes a little discipline not to attempt to create finer detail. Some experimentation with a grating structure will indicate what feature size is required for accurately estimating the diffraction efficiency.

4.4.1 Grating Representations

There are four internal representations of the grating structure. The following is an overview of their interrelationship, and indications of which representation is sent to the solver routines to calculate the diffraction efficiency. [See sec 1.2 figure for additional detail]



The Canvas (on the Editor Tab) contains a list of geometric primitives, and represent the grating structure (within a single period). No diffraction efficiency calculations are done using the list of geometric primitives.

Whenever the Approximate button is clicked, the list of geometric primitives are converted to a piecewise constant approximation. This internal representation is the basic grating description which is passed to the solver routines. For example, working from the Run tab, clicking the RUN button will invoke the solver routines with the grating structure which results from the Approximate function.

Two other grating representations are also created for the Listing/RUN tab and the GA tab. In both cases the Populate function *copies* the results of the Approximate function representation to the respective grids.

When the RUN (Listing/RUN tab) and RUN GA (GA tab) buttons are pressed, the solver routines are invoked with the grating definition given on their respective grid.

To copy any modifcations from the Listing/RUN grid (or the GA grid) to the grating definition generated by the Approximate function simple click the Copy/Update button on the grid.

If you make modifications to the grating on (say) the Listing/RUN grid, and then want to use those modification to do a GA run, you will need to first Copy/Update the Listing/RUN grid (to update the Approximate data structure) and then Populate the GA grid.

4.5 Holographic Tool, V_H, S_H

New to Version 5.1.22 is an additional holographic tool. VH is used to generate volume holograms with fringes close to the normal direction to the grating. SH is used to generate a fringe pattern parallel to the grating (a Bragg reflector). SH creates a series a thin film slabs, in the piecewise approximation, whose index of refraction varies periodically.

The **V_H** tool (button **V_H**) assumes that some material (base index) has some density modulation. The modulation is defined by a sinusoidal variation. The index of refraction is given by

$$n(x,y,z) = n_{base} + n_{\mathrm{mod}} \sum_{j=0} A_j \sin(2j\pi + sz\tan(\varphi)) + B_j \cos(2j\pi + sz\tan(\varphi))$$

where n_{base} the base index of refraction, and n_{mod} the modulation index. The period is normalized (one grating period), and s=2π/thickness. φ is the so-called slant angle and causes modulation in the z-direction. When $\varphi = 0$ only one layer is needed.

The general index is then descretized into a number of layers and number of steps within each layer. This a piecewise approximation to the index variation. It is convenient to choose a step size (number of blocks) that is commensurate with the grid.

The **S_H** tool (button **S_H**) is used to generate a fringe pattern that is parallel to the substrate. The index of refraction is given by

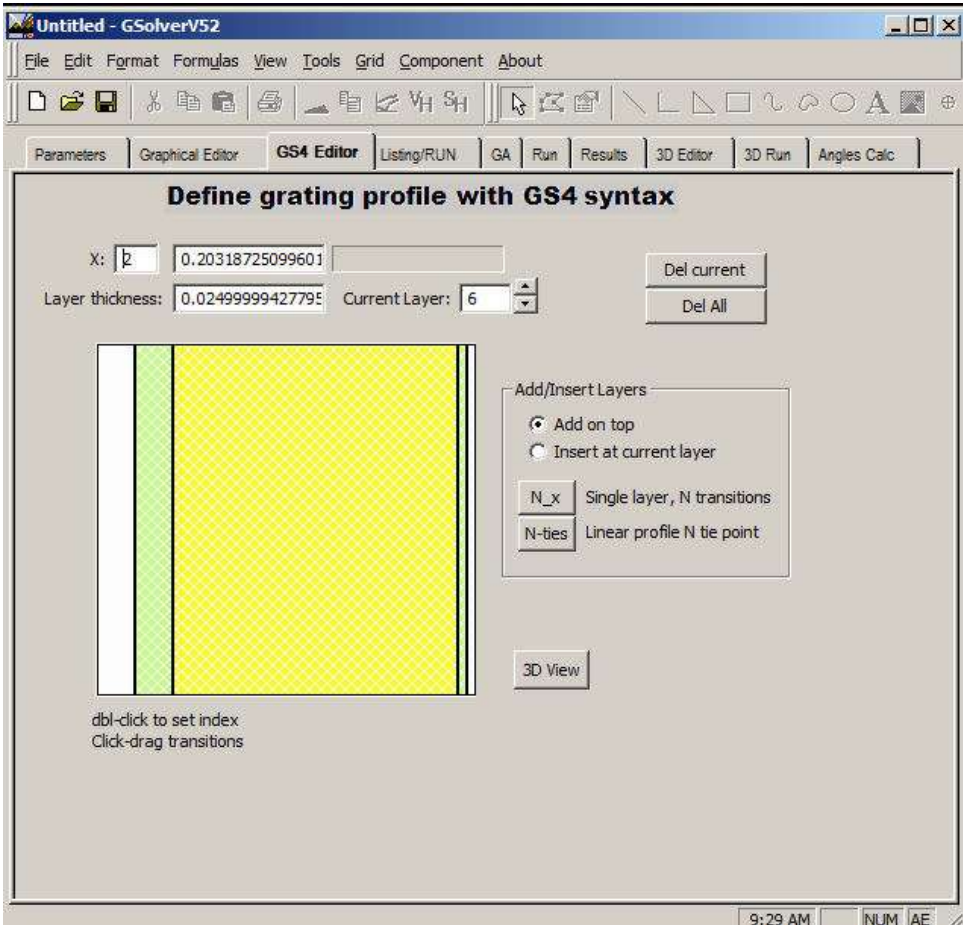
$$n(z) = n_{base} + n_{\mathrm{mod}} \sum_{j=0} A_j \sin\left(2j\pi \frac{z}{T}\right) + B_j \cos\left(2j\pi \frac{z}{T}\right)$$

where n(z) varies in the normal direction only and T is the layer thickness.

Since GSolver is material oriented, the various constant regions within a holographic layer are assigned the ‘constant’ material property, independent of wavelength. The material catalog is augmented with as many constant material regions as called for. When invoked, GSolver first looks through the Constant material list to see if a material already exists with the required index of refraction. If one is not found a new material is created and appended to the list. When GSolver is exited, the GSolver.ini material catalog file is rewritten with the new materials.

5 GS4 Editor

The GS4 Editor is new to GSolver V5.2, it includes editing syntax of V4.20 and is a layer-by-layer graphical editor. A representation of the editor is shown in the following figure.



This editor operates directly on the internal discrete approximation, and each layer in the grating can be displayed in the graphic window on the left. A layer consists of various regions which each region identified by a

width (relative to a period) and an index of refraction. Each ‘block’ in the layer can be directly edited by clicking on and dragging the boundary lines (or after selecting a boundary line by clicking and dragging it, simply entering the relative location in the text box).

Boundary lines are numbered from left to right. Each boundary is limited by the position of the boundary on the immediate left and immediate right. Thus a boundary may not be dragged past an adjoining boundary.

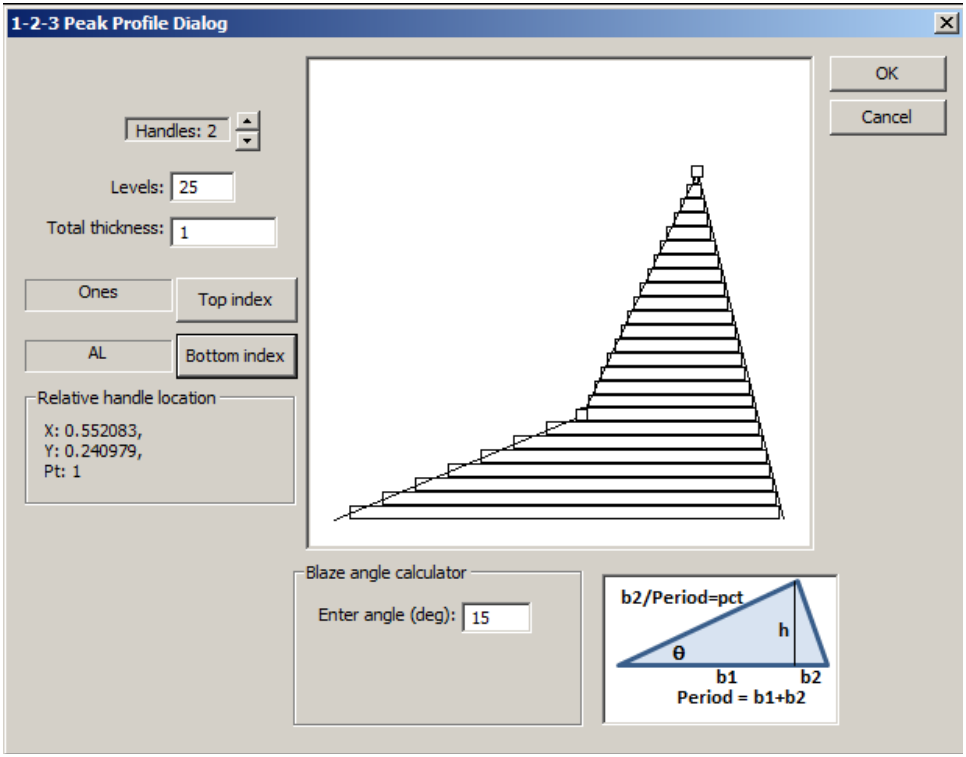
To edit the material, simply double click the region to bring up the material selection dialog.

There are two layer delete options: Del current, removes the current layer from the grating, and Del All removes all grating layers.

The layer thickness is also indicated and may be edited directly (absolute units).

There are two tools to insert grating layers. To insert a single layer, use the N_x button, which inserts a layer with N transitions. To insert a grating profile (such as triangle, blaze, or some sort of linear profile) use the N-ties button. The ‘ties’ refers to the number of piecewise linear parts there are to the profile ($1 \leq ties \leq 3$).

5.1 N-ties Profile Tool

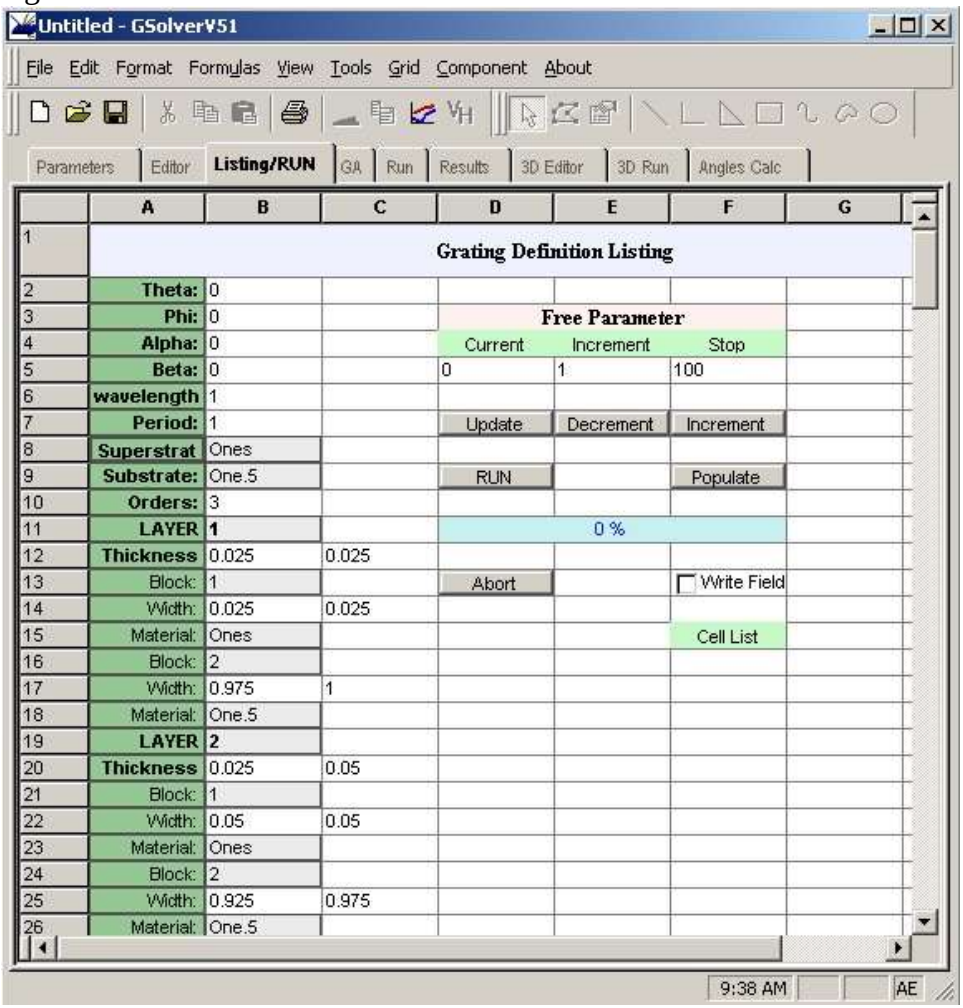


The profile tool is shown in the figure above. Essentially a linear profile may be defined (up to three linear sections) by clicking and dragging the tie points. The relative location of the tie points are shown in the location region. Note that the width is relative to the Period, and the vertical dimension is relative to the Total thickness entry. **That is the the maximum vertical position drawn in the figure is set to Total thickness**.

The linear profile represents a partition between two regions defined by the ‘top’ and ‘bottom’ index of refractions.

6 Listing/Run Tab

The Listing/RUN tab form is the main interface to the solver routines. The internal piecewise constant grating approximation is listed on the grid, and the various entries can be modified and constrained with user defined algebraic constraints.



Click on the Listing/RUN tab to activate the listing view. The grating structure is found in column B together with the grating parameters. Column A is used to label the column B entries. On the right of the grid are a group of controls used for setting the free parameter. Column C displays the cumulative thickness at each layer, for information purposes.

Layer 1 is the first layer of the grating structure and interfaces to the substrate. Each subsequent layer lies on top of the previous layer.

The first thing to do is to populate the grid with the grating definition structure created on the Editor using the Approximation function.

Any empty grid cell can be used to hold intermediate results. The grid supports split views for both vertical and horizontal splitting.

Grid-specific menu items are grouped under Format, Formulas, View and Grid. Many of the controls operate on specific elements of the grid. In those cases, the element must be selected before the controls are activated.

6.1.1 Make Grid Current

Make grid current option copies the current piecewise grating structure (including parameters) as represented on the grid to the internal grating storage array. It has no effect on the Canvas (graphic representation) of the grating. This allows for any updates/changes to the grating structure to be used between the Grating Listing tab, the GA tab, and the RUN tab. For example, after a GA run, the resulting grating structure can be copied into the general grating storage array, after which a RUN will use the results of the GA run.

6.2 Parameter Control

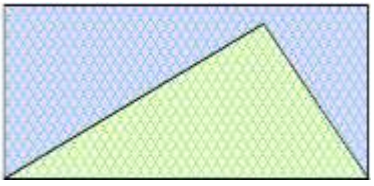
The Listing/RUN grid is equipped with a single parameter which is located in cell D5. This cell can be incremented and decremented, by the increment value in cell E5, using the button controls in F7 and E7.

When the RUN button is clicked, the parameter in D5 is incremented by the amount in E5 until it equals or exceeds the stop value set in F5.

The order of operation of GSolver when the RUN button is clicked is to first increment the D5 parameter from its current value, update all formulas, and continue through to the Stop condition. All formula dependencies are calculated, but error checking is minimal. D5 is then reset to the starting value the parameter loops through its range again, this time taking the Listing values in column B, and running the related diffraction calculation for each step.

The following example assumes that a grating structure has been defined and populated on the listing grid, such as the coated blazed grating example given in 4.3.5.

6.2.1 Using Listing/RUN to find the diffraction efficiency as a function of incident angle (theta) example.



1. Populate the grid by clicking the Populate button
2. Enter the following formula into cell B2: =D5/100
3. Enter 0 into cell D5, 1 into cell E5, and 80 int cell F5
4. This formula and set up will change the value of the theta parameter from 0 to 80 in steps of 0.01 degrees.
5. Click RUN

The D5 parameter runs through its range, updating cell B2, and then is reset to the starting value. The loop is repeated, this time running the diffraction calculation. The progress bar estimates the time to completion.

At the end of the calculation the results tab is activated automatically. The results grid is configured to hold the results during the first run through of the parameter loop. The user can, therefore, click over to the Results tab and watch the table being filled. At the end of the calculation GSolver eliminates zero-value columns.

6.2.2 Abort Button

It is possible to set up grating structures that take a very long time to both allocate memory and run the defined calculation. The Abort button attempts to stop the loop. However the calculation only responds to the

abort message at certain convenient places. For example, if the operating system is off trying to allocate sufficient RAM the abort will not happen until the OS returns from that activity.

6.2.3 Example of varying the thickness of the grating

1. Populate the grid by clicking the Populate button (assumes you have defined a grating with the Editor)
2. Select the Thickness Formula tool using menu item Grid→ Thickness Formula
3. On the Thickness formula dialog click on the All button. This tells GSolver that the formula should be entered in every layer thickness cell on the grid. If you only want to vary the thickness of some of the layers, then click to deselect other layers from the list. A selected layer is indicated with a '+' sign.
4. Enter the following into the entry text box on the dialog
   =D5/100
5. Click OK. The grid layer cells should now be populated with the formula D5/100. To check the result increment or decrement the parameter in D5 or simply have the Grid show all the cell formula entries using menu item Formulas→Formula Expressions.
6. Enter 0 in D5, 10 in D6, and 200 in D7
7. Click RUN. The total grating thickness is varied from 0 to 2.

6.2.4 Example of Littrow constraint

The Littrow condition constrains the incident angle (Theta) by the wavelength-to-period ratio. One way to implement this constraint is

Theta = asin(lambda / 2*Period)

Additional checking should be done to ensure that the argument of the asin is correct, and that |Theta|<90. The example below shows one way to implement a Littrow condition constraint using the wavelength as the free parameter (fixing the Period). If this example is worked following the previous example, clear the layer thickness formulas by using the dialog tool to enter the formula =0.1 in all the layer cells.

1. Populate the grid (if needed)
2. In cell B6 (the wavelength parameter) enter
   =D5/100+1

3. In cell B2 (Theta cell) enter
   = degrees(asin(if(abs(B6/(2*B7))<1,B6/(2*B7),0.)))
4. Enter 0 in D5, 1 in D6 and 99 in D7. This will change the wavelength from 1 to 1.99 microns.
5. Click RUN
6. Another way to constrain this formula is as follows:
   =degrees(asin(if(abs(B6/(2*B7))<1,B6/(2*B7),0.))); #>=0 && #<90

Note there are a variety of ways to enter this constraint (see section 5.2.1.2). The appendix contains a listing of all the functions available in the grid formula engine as well as formula syntax.

6.3 Cell List

Cell F15 contains the label 'Cell List'. Any cell designation (such as B2, C12, G23, etc.) that is entered in the column below F15 will be included on the Results List.

For example, assume that you want to include a listing of the contents of cell B2 (theta, which may be the results of a formula calculation) on the Results listing. Simply enter

B2

in column F below the 'Cell List' label. During a Run cycle, GSolver scans down column F (starting at row 16) for a list of cell designations. Then for each parameter update it records those current cell contents in the Results listing. This provides a way to include any grating definition results in the Results listing for additional analysis.

6.4 Formula Engine

Any cell entry that begins with an equals sign (=) is interpreted as a formula. Each formula is evaluated immediately and the results are shown in the same cell. To expose the formula scripts of a cell, select it and use the menu item Formulas→Formula Expression.

Formulas are limited to 512 characters. Formula recursion is not supported. That is, a formula cannot depend, either directly or indirectly, on its own output value.

All calculations are done in double precision. Calculations with logical operators (!, &&, ||, ?:) consider a non-zero value as TRUE and a zero value as FALSE.

Integer operators (~, &, |, ^, %) convert their argument(s) to integer first.

The maximum number of grid columns is 4096. The maximum number of grid rows is one million.

Entries that begin with the apostrophe character are treated as text.

Covered cells cannot be altered. This feature is used on any cell that contains labeling information.

Do not use commas or spaces to delimit pure numbers. Scientific notation (E convention) is supported.

A range of cells can be referenced absolutely such as A2..A10. Cells may also have relative references.

6.4.1 Syntax

In general a formula will have the following syntax

=expression; constraint expression // comment

where *expression* defines the calculations, *constraint expression* places limits on acceptable values or circumstances under which the calculation should take place, and *comment* may be any text. It is recommended that constraints be entered using the if(. .) function, otherwise the grid will generate an information dialog each time a constraint is violated.

6.4.1.1 Expressions

Expressions are algebraic formulas comprised of values and operators that define the relationships between values. They adhere to the following:

- A formula must begin with an equal sign

- The grid automatically assumes you are typing a formula if you begin with any of the following characters

  0 1 2 3 4 5 6 7 8 9 . - @ = +
- Spaces are ignored but count against the 512 byte limit
- Ranges look like B12..G29, A1..D5

Operators (order of precedence)

% 14	Unary percent
**13	Exponentiation
+12	Unary plus
-12	Unary minus
~12	Bitwise complement (integer)
!12	Logical not
*12	Multiplication
/11	Division
%11	Remainder (integer mod)
+10	Addition
-10	Subtraction
<<9	Shift left (bit shift on integer)
>>9	Shift right (bit shift on integer)
<8	Less than
>8	Greater than
<=8	Less than or equal
>=8	Greater than or equal
==7	Equal
!=7	Not equal
&6	Bitwise And or string concatenation
^5	Bitwise XOR (integer)
|4	Bitwise Or
&&3	Logical And
||2	Logical Or
?:1	Conditional (like the C language conditional)

In formulas with more than one operator, the grid formula evaluates operators in the order of precedence presented above, with highest precedence first. That is, AND/OR/NOT operators are evaluated after inequality operators in a logical expression, and multiplication/division operations are performed before subtraction/addition operations in an arithmetic expression. Operators at the same precedence level are evaluated from left to right.

Indirect Reference

An indirect cell reference specifies a row, column offset from the current cell location with the follow syntax:

#{column offset, row offset}

- If one value is included, the grid formula assumes that it is a column offset. For example, the offset reference #{-1} tells the grid formula to look to the column just left of the current cell.
- Offset values may be constants or expressions

Examples:

- #{0,-1} refers to the cell above the current cell
- #{-2} refers to the cell two columns to the left of the current cell
- #{1} refers to the cell to the right of the current cell
- #{0,1} refers to the cell below the current cell
- @CSUM(C4..C100, #{-1} == "Joe") calculates the sum of all the values in the range C4..C100 for which the cell in the column to the left contains the string "Joe".
- @CCOUNT(C4..C100, # #{0,-1}) counts all the cells in the range C4..C100 whose value is greater than the contents of the cell immediately above.
- /verb/#-1+2/ adds 2 to the cell value from the cell to the left.

6.4.1.2 Constraint Expressions

Constraints are limitations or conditions placed on the variables in the gird. They are expressed as algebraic statements appended to formulas. A

constraint expression can be attached to any formula, by typing a semicolon (;) and the constraint conditions after the formula.

Constraint expressions establish either conditions under which a formula operates, or boundaries for valid results of the formula. Constraint expressions can be simple equality/inequality relationships, or arbitrary formulas. Any valid grid expression that returns a numeric value is a valid constraint expression. However, unlike the expression that defines a cell value, a constraint expression can reference the cell in which it resides, by using the symbol #. For example, the formula =A1 + A2 ; #>2 && #<=B5 || #==C7 means: the value of the current cell is the sum of cells A1 and A2, and that value must be either greater than 2 and less than or equal to the value of cell B5, or equal to the value of cell C7. The benefit of constraint expressions is maximized when combined with current cell reference support (#) as indicated in the above example.

Constraint violation generates an error dialog box, and so can be inconvenient in loops. An alternative is to us the if(*,*1,*2) function. This function returns *1 if the condition in the first slot is true, otherwise it returns the result in *2. For example

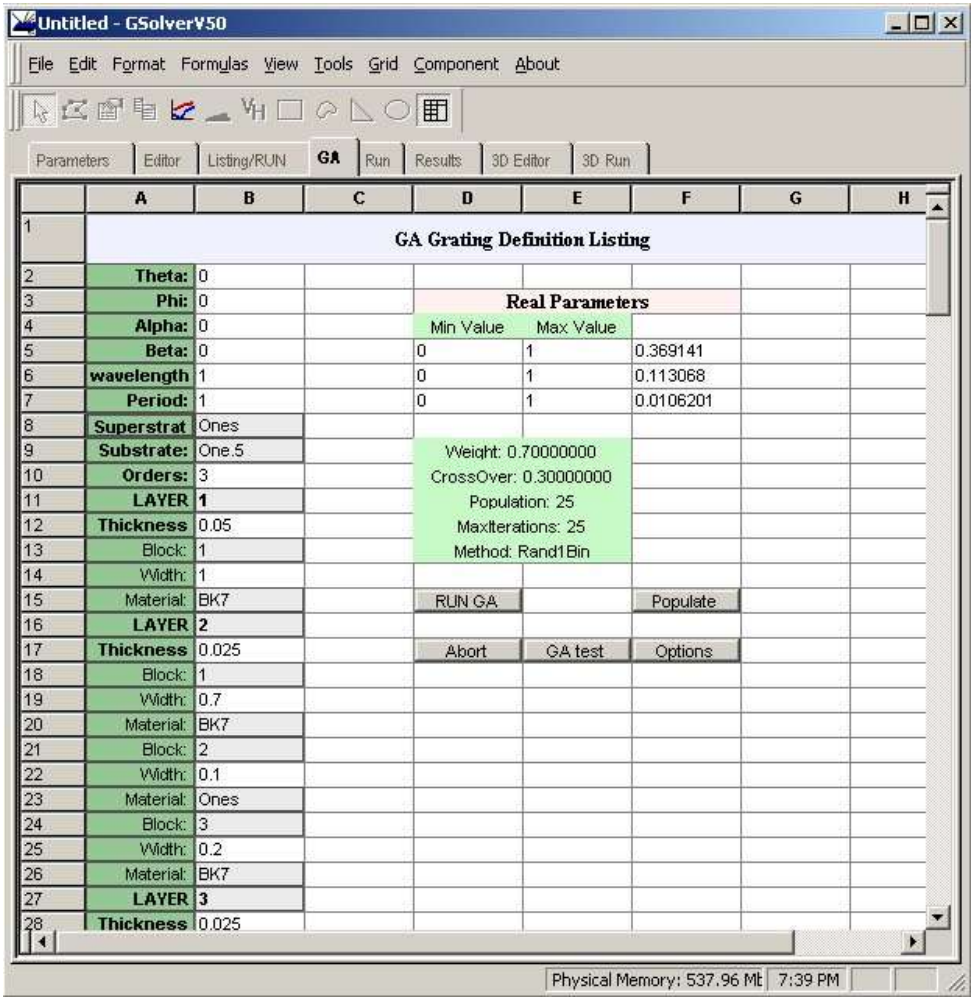
=if(d5/100>-90 && d5/100<90,d5,0)

will return the value d5/100 if it is between -90 and 90, otherwise the function returns 0.

7 Genetic Algorithm (GA Tab)

The GSolverV5.1 genetic algorithm has been significantly enhanced. It is based on Differential Evolution (DE), a class of genetic algorithms for which there is a large literature . The Differential Evolution home page is

http://www.icsi.berkeley.edu/~storn/code.html



The GSolver DE implementation allows for an arbitrary number of real parameters, and all of the popular evolution strategies. However some care and skill are required to find any particular grating efficiency solution. If the solution constraints are too far afield of any physical solution, the algorithm is likely to simply wander around in parameter space and never produce a satisfactory result. However the application of DE to grating design is a very powerful tool in optimization.

This chapter explains DE and how it applies to grating design.

NOTE: I file version 5.1.1.1 an additional menu item as been added to the Menu/Grid menu called 'Make grid current'. This option will copy the current piecewise grating structure (including parameters) to the internal grating storage array. It has no effect on the Canvas (graphic representation) of the grating. This allows for any updates/changes to the grating structure to be used between the Grating Listing tab, the GA tab, and the RUN tab. For example, after a GA run, the resulting grating structure can be copied into the general grating storage array, after which a RUN will use the results of the GA run. Previously the only way to update the internal grating array was directly from the 2D Editor 'Approximation' function

7.1 Overview of Differential Evolution

DE parameterizes optimization problems. A specific set of parameters (a vector) is associated with a merit function whose extremum is to be found. A set of parameter vectors is a population. The algorithm will alter various population member entries with other entries, as well as creating new entries from random distributions. Population members with 'good' merit functions are chosen more often than others to serve as a source of parameters. New vectors are made up with these 'good' parameters as well as new random members and the entire set is iterated until some stopping criterion is reached. See the web page above for tutorial information.

7.2 Guiding Principles

Applying DE to the grating problem creates some difficulties. For example, most parameterizations of the grating problem require careful

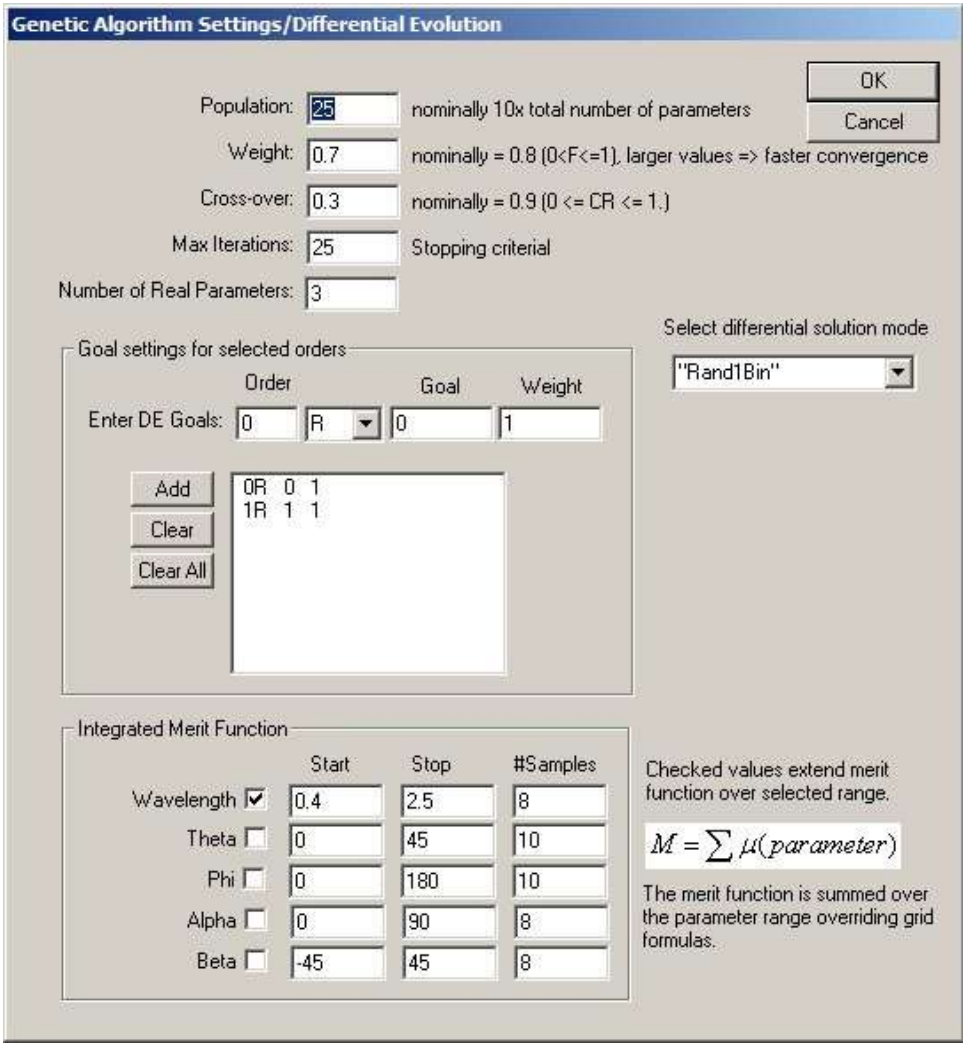
attention to physical constraints to produce meaningful solutions. The piecewise-constant approximation suggests a direct parameterization based on the geometric constraints (cell thickness and width). However, the cells that make up the grating are constrained in the following ways: all cells in a layer must have the same thickness; the sum of the widths of the cells in a row must equal 1 since the unit canvas width is one period.

In addition to the grating geometry parameters, the global parameters may also be used. These include grating period, wavelength, and the angles that define the illumination plane wave.

The actual material properties in any particular cell are problematic. Since GSolver ties all indices of refraction to an actual material in a catalog, it is difficult to allow arbitrary changes in these indices. However a limited solution is to create specialized materials that cover the range of the index of refraction (the search space) at known, specific wavelengths. Then, using those materials, the wavelength can be allowed to vary over the discrete space of wavelengths so that different index of refractions are selected in a controlled manner.

7.3 Setting GA Options

The DE options are set in a dialog, shown below, which is invoked by clicking the Options button (cell F17 on the default GA grid).



The Population, Weight, Cross-over, and Max Iterations control the operation of the DE run. The number of real parameters (must be at least 1) is also entered on this dialog. Select the solution mode from the drop down list box.

The Goal settings area of the dialog contains controls for generating input to the DE metric function which will be minimized. The DE merit function is as follows:

$$merit = \sum w_i \left(DE_{calc} - DE_{goal} \right)_i^2$$

where the sum is over the diffraction efficiency (DE) by orders given in the Goal settings. Each term in the sum includes a weight factor, which is also entered in the Goals Setting box.

Enter the goals in the dialog by entering an order (R and T for reflection and transmission) together with a weight and goal and add the selection to the list. Usually a merit function consists of one or two DE goals. The object of the DE algorithm is to find parameters that minimize the merit function (a perfect match is at merit = 0).

With file version 5.1.1.1 the merit function has been expanded to allow for the optimization over a range of angles and/or wavelengths. If a parameter in the Integrated Merit Function area is selected the diffraction efficiency is solved for the range of parameters selected and the above merit function is accumulated. The parameter range is uniformly sampled from the Start to Stop range with #Sample samples. The resulting merit function is used by the GA.

Note: By using this feature, the calculation of the merit function can be significantly increased. It is recommended that the number of samples be set to a small number initially to gauge the CPU time.

The GA grid contains the same functionality (formula engine) as the Listing/RUN grid. The formula engine is described Section 5.2.

7.4 Applying Constraints

The GA parameters are selected from a uniform random population, given by Min Value and Max Value, for each parameter in the list. *It is very important to remember that DE makes algebraic combinations of current parameters to use as new parameters. Therefore actual parameters are not constrained to the Min and Max bounds*.

Each formula should also have a constraint on the chosen parameter so that the result gives a physically-realizable value. For example, if a cell width is to be altered, you must enter a constraint on the other cells in that

grating layer so that that total width (sum of all the cells in a layer) sums to 1. The order of operation is illustrated in the following examples.

7.4.1 GA Design of a Thin Film AR Coating

In this example the optimal AR (antireflection) coating thickness is sought for MgF2 on an Al2O3 substrate in air at normal incidence at 0.5 μm wavelength.

1. Start a new grating editor
2. Change the wavelength to 0.5 μm on the Parameter tab
3. Change the Substrate material to Table: Al2O3
4. Using the Rectangle tool in the Editor tab, create a thin film coating with width of the canvas and of arbitrary thickness.
5. Set the material property to Table: MgF2
6. Click the Approximation button which creates the piecewise grating data structure
7. On the GA tab click Populate
8. On the GA Options dialog, click the Options button, enter the following goal
   0 R 0 1 (click Add)
9. This indicates that the specular reflection has 0 energy–the AR condition. Click OK.
10. In cell B12 enter the following formula
    =if(F5>0&&F5<0.2,F5,0)
11. Change E5 to 0.4
12. Click the GA test button to exercise the parameter selection and verify that the thickness is being updated, and constrained (non-negative and <0.2)
13. Click RUN GA
14. The merit function (Best Energy) is updated each time a new minimum is found. The final result is updated to the listing. The result should be somewhere around 0.09.
15. Increasing the maximum constraint may cause the region of multiple minima to be reached. If so, multiple ‘optimal’ solutions may be found by executing the GA algorithm multiple times.

While the GA is running, the current generation and best merit function are displayed. A merit function value of 0 indicates that an optimal solution has been found based on the goals given.

Upon completion the GA loads the values of the best parameters to the grid and creates a table of all the diffraction orders (-Orders to +Orders for T & R).

This example is easily extendable to include multiple thin film layers. Simply add the materials in the Editor tab and use a separate parameter for each layer thickness.

7.4.2 GA Design Example 2

This example considers a sawtooth profile, such as might be cut by a DPT (diamond point turning) machine, in ZnSe. The problem is to find the optimal sawtooth profile (depth and period) to maximize transmission in the -1T order (-i order convention box on Parameters tab unchecked) for 3 μm wavelength, TE polarization, and for 30° incident light.

1. Start a new grating
2. Change the wavelength to 3 and the substrate material to Herzberger: ZnSe(IRTR-4) and check the Lambda change update box. (This tells GSolver to update the index of refraction if the wavelength changes.)
3. Change Theta to 30
4. From the Editor tab, change the canvas properties (Edit→Canvas Properties) so that Canvas height is 2. This allows for grating structures that are 2x the grating period, creating an approximation with a large number of layers for finer resolution.
5. On the Editor tab, select the Custom Profile tool (black triangle)
6. Select the General Sawtooth form, and change the angles to 35 and 90. Click OK.
7. Select the newly created object and set its properties to Herzberger:ZnSe(IRTR-4). This should be the default if the substrate material was set.

8. Select the shape and assure it is moved all the way to the bottom of the canvas. Then grab the top, center handle and stretch the shape so that it's height is 19 units (this equals 1.9*4 = 7.6 μm)
9. Click the Approximation button
10. Click the GA tab and Populate the grid
11. Click the Options button and enter the goal as -1T 1 1 (-1T order, DE of 1, weight of 1). Click Add, then click OK.
12. In cell B7 enter the following formula
    =if(f5>2&&f5<5,f5,4)
13. This constrains the DE algorithm to only allow periods between 2 and 5 microns, and uses 4 microns as the default.
14. Change D5 to 2 and E5 to 5
15. Click the menu item Grid→Thickness Formula, select All and enter the formula
    =if(f6>0&&f6<.2,f6,.1)
16. This allows for a maximum thickness of 8 and a minimum of 0. **Note** there are 40 layers in the approximation.
17. Set B10 (orders retained) to 8
18. Set D6 to 0 and E6 to .2
19. Click RUN GA

While the GA is running, the current generation is displayed together with the best merit function value. A value of 0 indicates that the goals were met perfectly.

For this example, a period of around 2.0, a total thickness of about 7.6, and an -1T order with approximately 96.9% efficiency are typical.

Change the mode settings under GA Options to examine the behavior of different DE evaluation schedules.

Following is a modification to the above example to find the best grating for simultaneously maximizing transmission, in the 1T and –1T, for thickness, period and angle of incidence. The best such configuration will have 1T = -1T = 0.5.

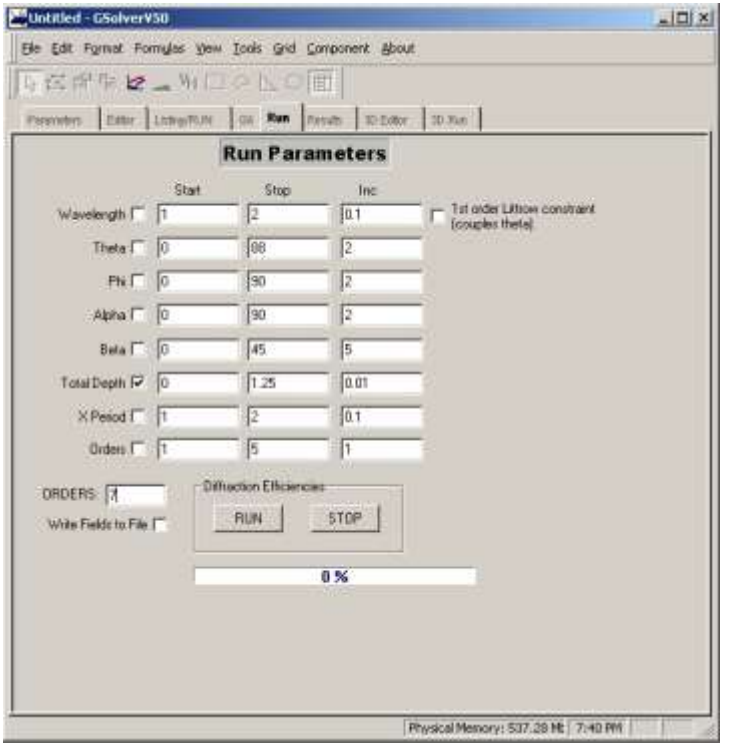
1. Enter the following in B2
   =if(F7>0&&F7<80,F7,40)
2. Enter 0 in D7 and 80 in E7

3. Change the goals on the Options dialog to
   1T 0.5 1 and -1T 0.5 1
4. Click RUN GA

A typical run may result in Theta = 2., Period = 2.7 and thickness = 2.7 with 1T = 42.% and –1T = 47%.

8 Execution (RUN Tab)

Just as in previous versions of GSolver, the RUN tab provides immediate access to several key grating parameters.



8.1.1 Run Constraints

The RUN tab parameters that are checked define a loop over which the selected parameters vary.

Select a parameter and enter the start, increment, and stop values for it. Click on RUN to start the calculation. The STOP button puts a message in the queue to terminate the loop. The loop will stop at the first convenient break point. When the RUN is finished the Results tab is activated with results written to the Results grid as they are computed.

8.1.2 1st order Littrow

The 1st order Littrow check box invokes a simple Littrow condition. As the wavelength changes, Theta is altered so that the first-order Littrow condition (in reflection) is satisfied. A Littrow constraint is generally run as a function of wavelength only.

8.1.3 Write Fields to File

The Write Fields to File command directs GSolver to record the computed complex E-fields as an ASCII text file. Clicking on this control activates a file save dialog; enter the name of the file into which to record the complex E-fields. The data can be saved to a new or existing file. If the file already exists the results will be appended to its end.

The Complex E-fields are the field amplitudes of every order retained in the calculation at the top interface of the grating (reflected fields) and at the bottom interface (transmitted fields). In general, all orders have non-zero magnitude. However they may not be propagating. For a field in some order to propagate, the related k-vector z-component must have a real component. Grating structures can support large amplitude evanescent fields, which can be visualized as standing waves. These fields are essential in the solution of the boundary conditions which explains why some gratings require a large number of orders, beyond the number of real propagating orders, be retained to get 'convergence' or physically meaningful results. This is particularly true for gratings that contain materials where relative differences in complex index of refraction are large, and the field is in TM mode.

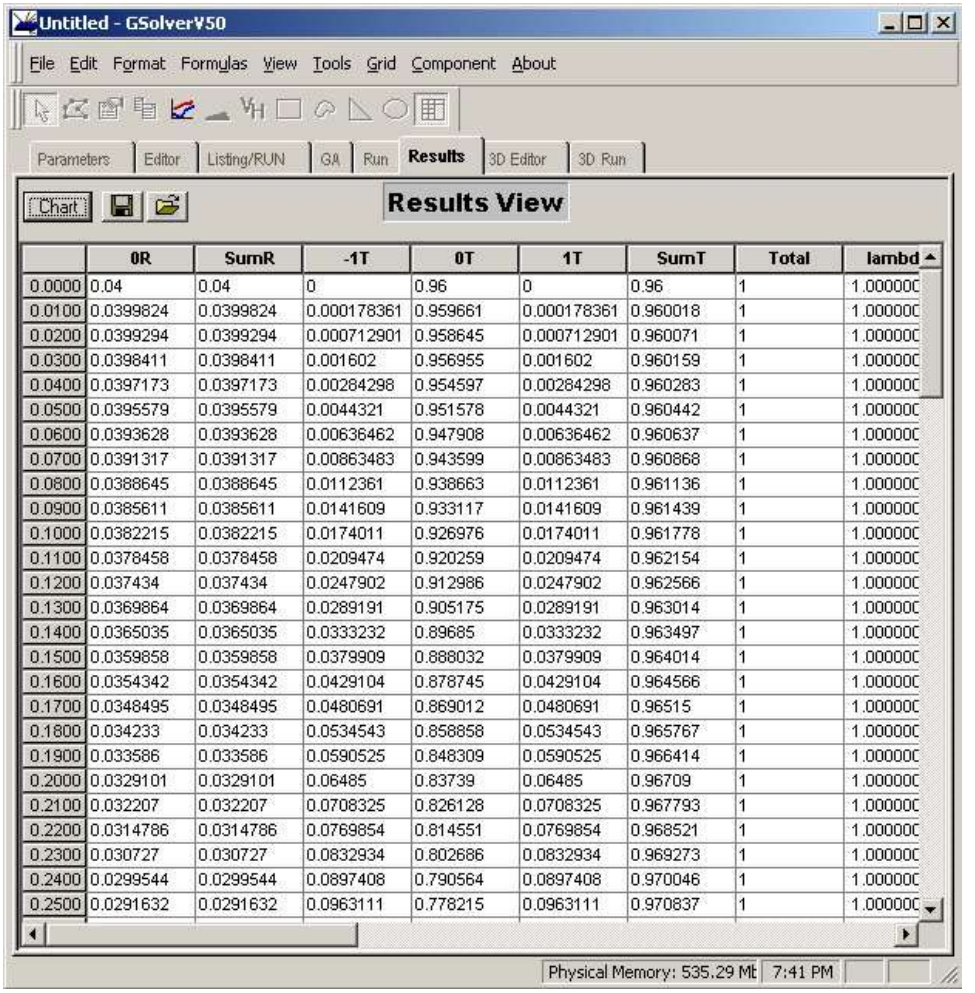
8.1.4 Run/Stop

The RUN button executes a loop defined by the selected parameters. There is always at least one calculation in a RUN, which represents the current version of all the parameters, even if no parameters are selected.

The STOP button simply posts a message to the GSolver message queue to halt the current calculation. This is a non-deterministic action and GSolver will respond to the STOP command at a convenient point.

9 Results Tab

The Results tab holds the grid where the calculated diffraction efficiencies are posted. Reintroduced in GSolver 5.1 is a simple phase calculation which is also listed.



	0R	SumR	-1T	0T	1T	SumT	Total	lambd
0.0000	0.04	0.04	0	0.96	0	0.96	1	1.00000
0.0100	0.0399824	0.0399824	0.000178361	0.959661	0.000178361	0.960018	1	1.00000
0.0200	0.0399294	0.0399294	0.000712901	0.958645	0.000712901	0.960071	1	1.00000
0.0300	0.0398411	0.0398411	0.001602	0.956955	0.001602	0.960159	1	1.00000
0.0400	0.0397173	0.0397173	0.00284298	0.954597	0.00284298	0.960283	1	1.00000
0.0500	0.0395579	0.0395579	0.0044321	0.951578	0.0044321	0.960442	1	1.00000
0.0600	0.0393628	0.0393628	0.00636462	0.947908	0.00636462	0.960637	1	1.00000
0.0700	0.0391317	0.0391317	0.00863483	0.943599	0.00863483	0.960868	1	1.00000
0.0800	0.0388645	0.0388645	0.0112361	0.938663	0.0112361	0.961136	1	1.00000
0.0900	0.0385611	0.0385611	0.0141609	0.933117	0.0141609	0.961439	1	1.00000
0.1000	0.0382215	0.0382215	0.0174011	0.926976	0.0174011	0.961778	1	1.00000
0.1100	0.0378458	0.0378458	0.0209474	0.920259	0.0209474	0.962154	1	1.00000
0.1200	0.037434	0.037434	0.0247902	0.912986	0.0247902	0.962566	1	1.00000
0.1300	0.0369864	0.0369864	0.0289191	0.905175	0.0289191	0.963014	1	1.00000
0.1400	0.0365035	0.0365035	0.0333232	0.89685	0.0333232	0.963497	1	1.00000
0.1500	0.0359858	0.0359858	0.0379909	0.888032	0.0379909	0.964014	1	1.00000
0.1600	0.0354342	0.0354342	0.0429104	0.878745	0.0429104	0.964566	1	1.00000
0.1700	0.0348495	0.0348495	0.0480691	0.869012	0.0480691	0.96515	1	1.00000
0.1800	0.034233	0.034233	0.0534543	0.858858	0.0534543	0.965767	1	1.00000
0.1900	0.033586	0.033586	0.0590525	0.848309	0.0590525	0.966414	1	1.00000
0.2000	0.0329101	0.0329101	0.06485	0.83739	0.06485	0.96709	1	1.00000
0.2100	0.032207	0.032207	0.0708325	0.826128	0.0708325	0.967793	1	1.00000
0.2200	0.0314786	0.0314786	0.0769854	0.814551	0.0769854	0.968521	1	1.00000
0.2300	0.030727	0.030727	0.0832934	0.802686	0.0832934	0.969273	1	1.00000
0.2400	0.0299544	0.0299544	0.0897408	0.790564	0.0897408	0.970046	1	1.00000
0.2500	0.0291632	0.0291632	0.0963111	0.778215	0.0963111	0.970837	1	1.00000

The first line of the results grid contain headers that identify each column. The general format is #R and #T for diffraction efficiencies where # is the

order number. On the far right are columns labeled #r and #t. These are the phase data (in degrees). Between the diffraction efficiencies and the phase data are several columns that list the values of the global parameters.

If the RUN tab is used to generate the results, the first column is a list of the current value of the first parameter checked. Thus, if multiple parameters are checked, the first column will run through its values, and then repeat as often as required by the loop.

If the Listing/RUN tool is used to generate the results, then the first column represents the value of the parameter in cell D5 (see the Listing/RUN chapter).

9.1 Diffraction Efficiency

The diffraction efficiency is defined as follows:

$$DE_k = \left[\left(E_x conj(E_x) \right)_k + \left(E_y conj(E_y) \right)_k + \left(E_z conj(E_z) \right)_k \right] * re(k_{zRk}) / k_{zinc}$$

where subscript k = diffraction order, k_{zRk} is the z-component of the kth diffraction order (as defined by the grating equation), and R is reflection. R gets changed to T for the transmitted orders. Since all orders are represented as plane waves, if the z-component of the diffracted k-vector is 0 (or pure imaginary), then DE is identically 0 for that order.

9.2 Phases

Phase for each order is defined as follows: given the complex E-field for the nth order equal $\mathbf{E_n}$, first calculate

$$sz = sign(re(\mathbf{E_n}) \times im(\mathbf{E_n}))$$

the sign of the z-component of the usual vector cross product. Next compute

$$\varphi = \pm sz \times \arccos\left(\frac{re(\mathbf{E}_n) \cdot im(\mathbf{E}_n)}{|re(\mathbf{E}_n)||im(\mathbf{E}_n)|} \right)$$

on the range $-\pi < \phi < \pi$. The + sign (of the ± operation) is used for the transmitted orders, and the – sign for the reflected orders. This defines the complex angle between the real and imaginary components of the complex E-field vector. The dot in the above formula is the usual vector dot product. No attempt has been made to do phase unwrapping.

This is a relative phase calculation in the sense that it computes phases that are relative to each other for the set of reflected and transmitted orders. At each stage of the internal calculation fields are normalized by the largest (complex) eigenvalue in the related algebraic eigenvalue problem, as defined by the Fourier components of the layer permitivities (and impermitivities) and Maxwell's equations. This normalization improves numerical stability. The absolute magnitudes of the *internal* fields are calculated only up to some constant (complex) multiplier.

The system of equations is configured so that this normalization has no effect on the calculation of the external fields. That is, the system of equations is ordered so that the external fields come first, and back substitution is used to solve only for those fields.

9.3 Graphing

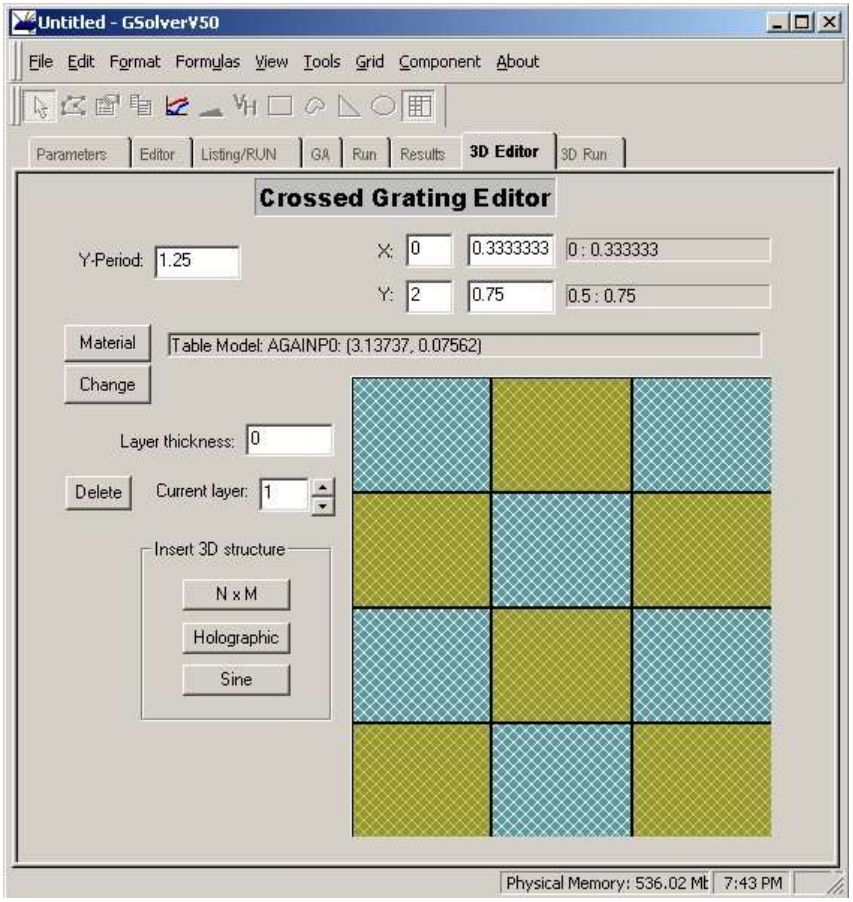
Select the columns to graph; multiple columns can be selected using the shift and control keys along with the mouse. Click the chart button.

The initial chart uses defaults on all settings. To alter any feature of the graph, click on the various tools. Clicking on most items invokes a properties dialog for that item. For example to change x-axis properties such as display, limits, and numerical format, simply right-click on one of the x-axis tic-mark labels and select properties.

GSolver's graphing tool is very powerful, and includes a large number of display and customization options. More information is given in the graphing chapter.

10 3D Editor Tab

Some crossed grating (3D) structures can be solved with GSolver. The 3D Editor is the interface for defining these structures and is essentially the same as in prior versions of GSolver.



NOTE: with file version 5.1.1.1, the 3D Editor Tab must have units set to Microns. And all entries with units are interpreted in Microns.

10.1 Limits on Solving 3D Structures

The coupled wave solution is based on solving the truncated infinite set of Maxwell's equations by the well-known algebraic eigensystem method. This implies that for each layer of the grating regions a full complex eigensystem is solved, followed by a boundary conditions solver. This process is iterated through each layer, from the substrate to the superstrate. The behavior and solvability of general complex eigensystems has been thoroughly studied for decades.

The size of the eigensystem, including auxiliary memory arrays for holding intermediate results (using 64bit floating point structures), is roughly estimated as

$$bytes = 1760(2 * orders + 1)^2 + 560(2 * orders + 1) + 8224$$

For crossed gratings it is

$$bytes = 1760(2 * orders + 1)^4 + 560(2 * orders + 1)^2 + 8224$$

Notice that for crossed gratings the size of the memory requirements grows as orders retained to the fourth power. In addition, both the eigensystem solver, and the boundary system solver, which operate in a manner similar to matrix inversion, require computer operations that grow roughly as the cube of the size of the arrays. With just a few orders retained on a crossed grating, a significantly large eigensystem problem must be solved (for each grating layer). In computer terms there are a huge number of multiply-accumulate operations needed for finding each eigenvector and eigenvalue, and for matching boundary conditions. Considering that the basic floating point formation on a typical Intel® processor is limited to 64 bits (80 bit internal), difficulties with round off error are to be expected.

Since GSolver is a full vector implementation and a 3D structure is a natural subset of the problem space, the 3D structure solver is included. However, due to symmetry issues, the 3D structures generally do not lend themselves to the several convergence and numerical acceleration 'tricks' employed in the normal (linear) grating solver routines. There are, in fact,

four solver routines in GSolver: a TE solver, a TM solver, a general linear grating solver, and a full crossed grating solver. The first three take advantage of the various known methods for stabilizing and accelerating the coupled wave problem solution.

The 3D solution is retained in GSolver primarily for backward compatibility. For those aware of the limitations imposed by the 64-bit floating point hardware on the numerical algorithms, the algorithm allows investigation of a fairly large crossed grating problem space.

Problems that need only a few retained orders (such as all orders being evanescent) are usually readily solved. It is generally recommended that there be no more than a few real propagating orders and that materials with large phase shifts, such as metals, be avoided. The convergence behavior of all 3D grating structures should be investigated, since the general approach to convergence often has an oscillatory component.

10.2 Defining a 3D Grating

GSolver handles all gratings as piecewise-linear approximations. For a 3D grating this approximation consists of a unit cell with periodic boundaries. This cell has a width of one grating X-period and a length of one grating Y-period. The thickness is arbitrary and cells may be stacked as desired.

Each unit cell may be divided into any desired number of ‘checkerboard’ regions. Each region is then assigned a material property, which gives it an index of refraction.

The basic tool for defining a 3D unit cell is the NxM tool. This tool creates an NxM checkerboard with two materials.

For any layer, any region of the unit cell can be altered by simply clicking on it. A new material may then be assigned to that region by clicking on the Material button and selecting a new material.

The boundary lines between regions of a cell can be moved by dragging with the mouse, or altered by entering new values in the X: and Y: text boxes at the top of the form.

The 3D layer structure is numbered starting with the first layer which lies on the substrate, and then increasing for each layer above.

The Holographic tool and the Sine tool automate two popular 3D grating profiles. The basic 3D grating parameters are entered on the Parameters Tab as usual; the additional Y-period is entered on the 3DEditor tab.

10.2.1 Holographic Tool

A holographic grating may require 1 or many layers depending on whether the modulation of the photoresist has density variation in the z-direction or simply in the x-, and y-directions. The tool handles either situation.

The tool assumes that some material (base index) has some density modulation. The modulation is defined by a sinusoidal variation of up to 10^{th} order. The index of refraction is given by

$$n(x, y, z) = n_1 + n_2 \sum A_j \sin(\, j\mathbf{K}.\mathbf{x} + sz \tan(\varphi))$$

where n_1 is the base index of refraction, and n_2 is the modulation index. **K** is the in-plane (spatial) k-vector ($2\pi/\Lambda_x$, $2\pi/\Lambda_y$), and s=2π/thickness. φ is the so-called slant angle and causes modulation in the z-direction. When φ = 0 only one layer is needed.

The general index is then descretized into a number of layers and number of steps within each layer; the steps are taken equally in the x- and y-directions. This creates a checkerboard layer approximation.

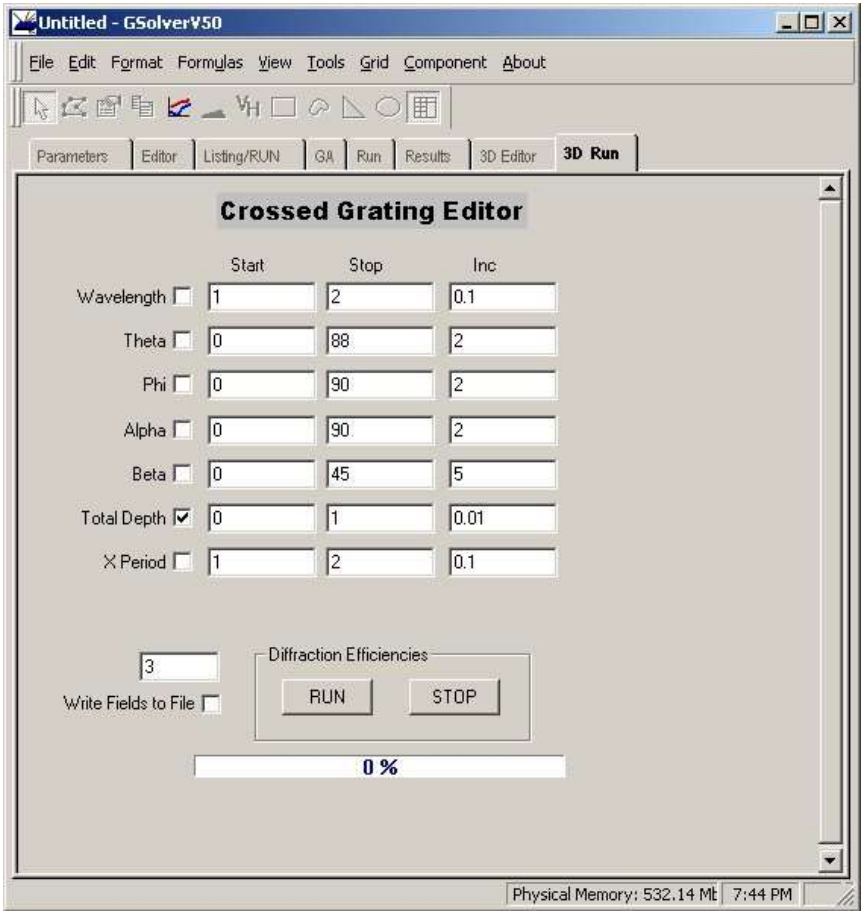
Since GSolver is material oriented, the various constant regions within a holographic layer are assigned the ‘constant’ material property, independent of wavelength. The material catalog is augmented with as many constant material regions as called for. When invoked, GSolver first looks through the Constant material list to see if a material already exists with the required index of refraction. If one is not found a new material is created and appended to the list. When GSolver is exited, the GSolver.ini material catalog file is rewritten with the new materials.

10.3 Sine Tool

The Sine Tool is used to create a crossed sinusoidal ‘height’ boundary between the superstrate and the substrate. The boundary is between the top and bottom regions. These top and bottom regions do not have to have the same material properties as the super- and substrates.

11 3D RUN Tab

The 3D RUN tab is the only user interface to the full vector crossed grating solver routine.

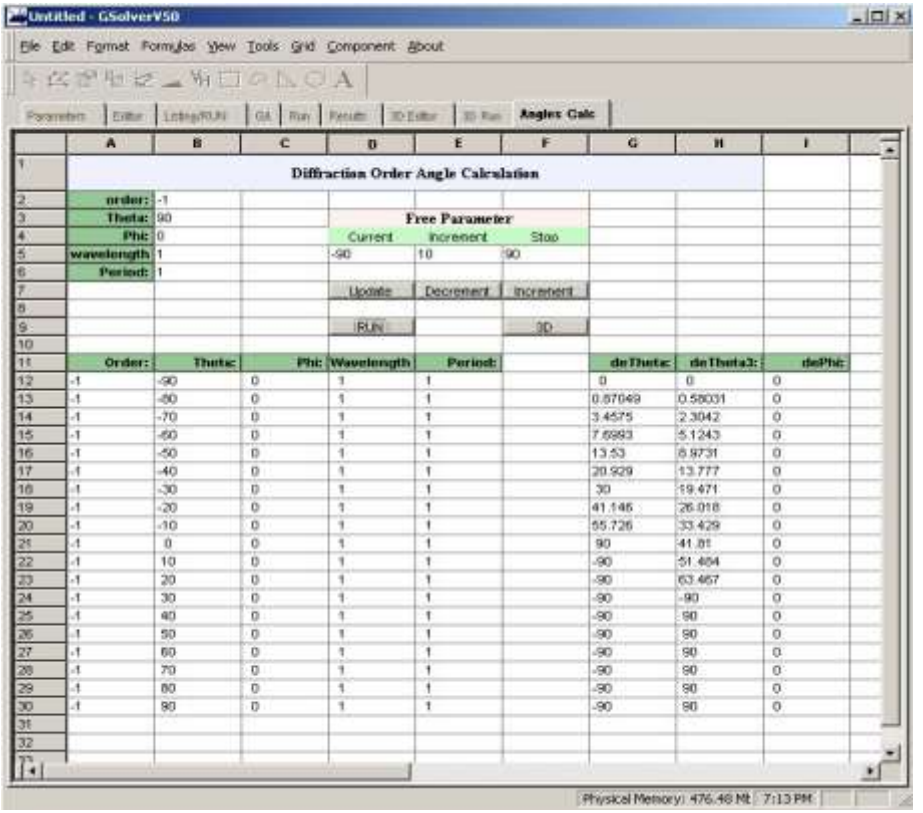


Selected parameters generate a loop structure within which the solver routine is repeatedly called. As the solutions are found, they are written to the Results tab in the normal way.

Diffraction efficiencies and phases are just as in the case of linear gratings. Please refer to the RUN tab chapter for more information.

12 Angles Calc

Angles Calc is a tool to calculate the diffraction order angles. The propagating directions of the orders are determined by the wavelength, period, incident k-vector, and the super- and substrate indices of refraction, and do not depend on the details of the grating structure. The grating structure determines the magnitude of energy in each order.



The basic layout of the Angles Calculation tool follows the general format of the Listing/RUN and GA forms. There is a free parameter, cell D5, that varies from the Current entry to the Stop value in increments of the value in cell E5. Formulas are used to set up a particular order calculation.

Refer to Chapter 5 for a description of the use of formulas in a grid.

12.1 Example DE Angle Calc

This example creates a table of the -1 order angles as a function of the incident angle (assuming the substrate is type Constant One.5 and the superstrate is type Constant Ones).

1. Click on the Angles Calc tab
2. Enter a -1 in cell B2
3. In cell B3 enter the following
   =D5
4. Click the RUN button (cell D9)

The table displays values in degrees for the diffracted angle for the -1R order (labeled deTheta), the -1T order (labeled deTheta3) and the relevant Phi angle.

Formulas can be used to alter any of the parameters in cells B2 through B6. For crossed (3D) gratings, click on the 3D button. The table is now augmented with an additional order, since orders are then defined in the x- and y-directions.

12.2 Definition of the Angle Calc

The Angle Calculation for the diffraction order is defined as follows, where λ = wavelength, and Λ are the X- and Y-periods define:

$$dx = \lambda / \Lambda_x$$
$$dy = \lambda / \Lambda_y$$

For normal gratings Y$\rightarrow \infty$, $dy = 0$.

Set N_{sup} = superstrate index of refraction, and N_{sub} = (N3, K3) = complex substrate index of refraction. Now calculate:

$$k_x = N1\sin(\theta)\cos(\phi) + m_x dx \quad \text{and} \quad k1_z = \sqrt{N_{\sup}{}^2 - k_x^2 - k_y^2}$$
$$k_y = N1\sin(\theta)\sin(\phi) + m_y dy \qquad\qquad k3_z = \sqrt{N_{sub}{}^2 - k_x^2 - k_y^2}$$

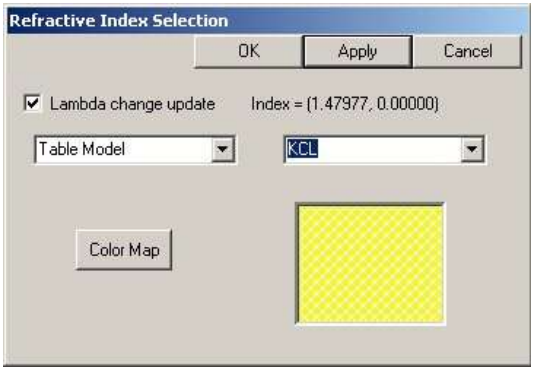
These are the vector components of the k-vector in the superstrate (region 1) and the substrate (region 3) for order (m_x,m_y). The x- and y- kvector components are the same in the super- and substrates due to boundary

conditions. The diffraction order angles are then calculated in the usual way from these components.

13 Dialogs

13.1 Refractive Index Selection Dialog

The superstrate and substrate materials properties are set with the following dialog which is similar to the material selection property page used to set material properties for the Editor canvas objects:



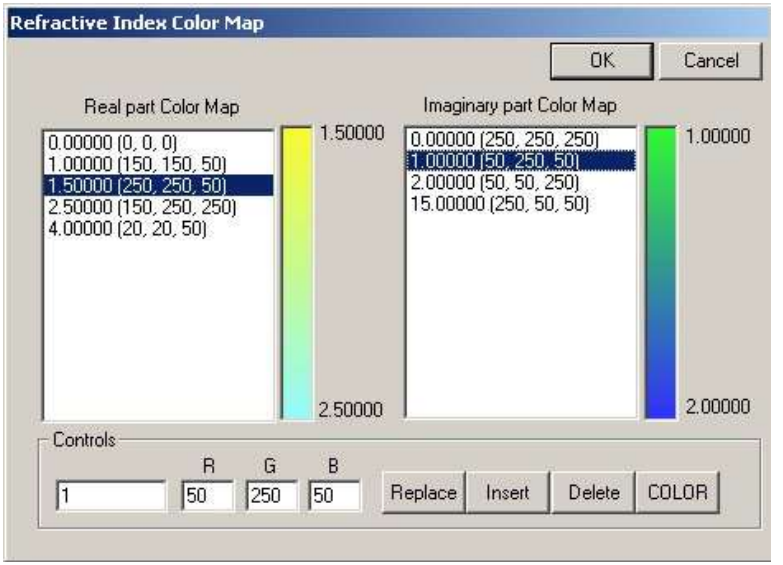
The superstrate and substrate are not represented on the Editor canvas, so the color assignments are not relevant.

13.2 Refractive Index Color Map Dialog

Every material property has two colors that represent the real and imaginary parts of the index of refraction. The mapping between a color and the value of the index of refraction is set using the Color Map dialog.

The dialog contain two lists that represent the range for the real (n) and imaginary (k) parts of that index of refraction. Each list is comprised of a number of entries, in increasing order, together with a color defined in RGB space (8-bit coordinates). Numbers in the list are called break points.

The algorithm that identifies a color with an index of refraction entry is identical for both the real and the imaginary pars. Following is a description of the algorithm for the real part (n).



Given a value n, find the two entries in the appropriate list that bracket it such that

$$n_1 \le n \le n_2$$

where n_1 and n_2 are consecutive members of the list.

Then draw a line in RGB space from the n_1 RGB coordinate to the n_2 RGB coordinate, and find the RGB coordinate for the linear interpolant given by n between n_1 and n_2. The resulting color is used for the n value.

The Color Map may be altered as needed; break points may be added, removed, and changed. The COLOR button may be used to find a specific COLOR RGB coordinate.

Use the Replace, Insert, and Delete buttons, together with the Control entries (n, R, G, B) to modify the list.

The color lookup list is stored with the grating in the gs5 file. When GSolver is started it creates a new color lookup table based on default values. To use a custom lookup table, simply save a grating file with the desired lookup table. Then, after starting GSolver, open the grating file (gs5) containing the desired lookup table and save it to a new filename.

14 Material File GSolver.ini

The materials file, GSolver.ini, format is similar to previous versions. New to version 5.1 is a constant material class. The various classes are

[CONSTANT]	[HERZBERGER]
[DRUDE]	[SCHOTT]
[SELLMEIER]	[TABLE]

The analytic forms for each of these models is given in section 2.6. Following is a description of the ini file.

The ini file has seven sections, the 6 material class sections and the [GSOLVER V5.1] section for comments.

Each material section begins with one of the material class names (in brackets). Following the class name is a line that gives the number of members of the class which will be read in. It has the following format:

total = x

where x is the number of materials. The ini file may be edited with a text editor. However, it is important to update the 'total =' line if materials are added or deleted.

Each time GSolver starts, it reads the ini file found in the GsolverV50 directory. If it does not find an ini file it creates a list of default materials for each class.

When GSolver exits, it re-creates the ini file. Thus if any material editing is done within GSolver, the changes are only written out to disk when GSolver exits.

In general no checking is done on the material parameter entries other than $n>0$ and $k\geq 0$.

The recommend material class is the Table model. Table models are the most general, and easily extensible. Also most index of refraction data is recorded in tabular form.

15 Grid Formula Engine

Quick-Reference Guide to Built-in Functions

15.1 Mathematical Functions

The following lists the supported mathematical functions.

Function Description

ABS(X) The absolute value of X.
ACOS(X) The arc cosine of X.
ASIN(X) The arc sine of X.
ATAN(X) The 2-quadrant arc tangent of X.
ATAN2(X, Y) The 4-quadrant arc tangent of Y/X.
CEIL(X) The smallest integer greater than or equal to X.
COS(X) The cosine of X.
COSH(X) The hyperbolic cosine of X.
DEGREES(X) Converts the angle expressed in radians to degrees.
DET(M) The determinant of the square matrix range M.
DOT(R1, R2) The dot product of the vectors R1 and R2.
EXP(X) e raised to the X power.
FACT(N) The value of N!.
FLOOR(X) The largest integer less than or equal to X.
FRAC(X) The fractional portion of X.
GAMMA(X) The value of the gamma function evaluated at X.
GRAND( ) A 12th-degree binomial approximation to a Gaussian random number with zero mean and unit variance.
INT(X) The integer portion of X.
LN(X) The log base e (natural log) of X.
LNGAMMA(X) The log base e of the gamma function evaluated at X.
LOG(X) The log base 10 of X.
LOG10(X) The log base 10 of X.
LOG2(X) The log base 2 of X.
MOD(X, Y) The remainder of X/Y.
MODULUS(X, Y) The modulus of X/Y.

@PI The value of pi.
POLY(X, ...) The value of an Nth-degree polynomial in X.
PRODUCT(X, ...) The product of all numeric values in the argument list.
RADIANS(X) Converts the angle expressed in degrees to radians.
RAND( ) A uniform random number on the interval (0,1).
ROUND(X, n) X rounded to n number of decimal places (0 to 15).
SIGMOID(X) The value of the sigmoid function.
SIN(X) The sine of X.
SINH(X) The hyperbolic sine of X.
SQRT(X) The positive square root of X.
SUMPRODUCT(R1, R2) The dot product of the vectors R1 and R2.

15.2 Statistical Functions

The following lists supported statistical functions.

TAN(X) The tangent of X.
TANH(X) The hyperbolic tangent of X.
TRANSPOSE(M) The transpose of matrix M.
VECLEN(...) The square root of the sum of squares of the arguments.
AVG(...) The average (arithmetic mean) of the arguments.
CORR(R1, R2) Pearson's product-moment correlation coefficient for the paired data in ranges R1 and R2.
COUNT(...) A count of the non-blank arguments.
F(M, N, F) The integral of Snedecor's F-distribution with M and N degrees of freedom from -∞ to F.
ERF(L[, U]) Error function integrated between 0 and L; if U is specified, then between L and U.
ERFC(L) Complementary error function integrated between L and ∞.
FORECAST(...) Predicted Y values for given X.
FTEST(R1, R2) The significance level of the two-sided F-test on the variances of the data specified by ranges R1 and R2.
GMEAN(...) The geometric mean of the arguments.
HMEAN(...) The harmonic mean of the arguments.
LARGE(R, N) The N^{th} largest value in range R.
MAX(...) The maximum of the arguments.

MEDIAN(...) The median (middle value) of the range R1.
MIN(...) The minimum the arguments.
MODE(...) The mode or most frequently occurring value.
MSQ(...) The mean of the squares of the arguments.
PERCENTILE(R, N) The value from the range R that is at the N^{th} percentile in R.
PERCENTRANK(R, N) The percentile rank of the number N among the values in range R.
PERMUT(S, T) The number of T objects that can be chosen from the set S, where order is significant.
PTTEST(R1, R2) The significance level of the two-sided T-test for the paired samples contained in ranges R1 and R2.
QUARTILE(R, Q) The quartile Q of the data in range R.
RANK(E, R[, O]) The rank of a numeric argument E in the range R.
SSQ(...) The sum of squares of the arguments.
RMS(...) The root of the mean of squares of the arguments.
SMALL(R, N) The N^{th} smallest number in range R.
SSE(...) The sum squared error of the arguments.
STD(...) The population standard deviation (N weighting) the arguments.
STDS(...) The sample standard deviation (N-1 weighting).
SUM(...) The sum of the arguments.
T(N, T) The integral of Student's T-distribution with N degrees of freedom from $-\infty$ to T.
TTEST(R, X) The significance level of the two-sided single population T-test for the population samples contained in range R.
TTEST2EV(R1, R2) The significance level of the two-sided dual population T-test for ranges R1 and R2, where the population variances are equal.

15.3 Conditional Statistical Functions

The following lists supported conditional statistical functions.

TTEST2UV(R1, R2) The significance level of the two-sided dual population T-test for ranges R1 and R2, where the population variances are not equal.

VAR(...) The sample variance (N weighting) of the arguments.
VARS(...) The sample variance (N-1 weighting) of the arguments.
VSUM(...) The visual sum of the arguments, using precision and rounding of formatted cell values.
CAVG(..., C) Conditional average.
CCOUN(..., C) Conditional count.
CMAX(..., C) Conditional maximum.
CMIN(..., C) Conditional minimum.
CSTD(..., C) Conditional sample standard deviation (N weighting).
CSTDS(..., C) Conditional sample standard deviation (N-1 weighting).
CSUM(..., C) Conditional sum.
CVAR(..., C) Conditional population variance (N weighting).
CVARS(..., C) Conditional population variance (N-1 weighting).

15.4 String Functions

The following lists supported string functions.

CHAR(N) The character represented by the code N.
CLEAN(S) The string formed by removing all non-printing characters from the string S.
CODE(S) The ASCII code for the first character in string S.
EXACT(S1, S2) 1 if string S1 matches string S2, otherwise 0.
FIND(S1, S2, N) The index of the first occurrence of S1 in S2.
HEXTONUM(S) The numeric value for the hexadecimal value S.
LEFT(S, N) The string composed of the leftmost N characters of S.
LENGTH(S) The number of characters in S.
LOWER(S) S converted to lower case.
MID(S, N1, N2) The string of length N2 that starts at position N1 in S.
NUMTOHEX(X) Hexadecimal representation of the integer portion of X.
PROPER(S) The string S with the first letter of each word capitalized.
REGEX(S1, S2) 1 if string S1 exactly matches string S2; otherwise 0. Allows "wildcard"' comparisons treating S1 as regular expression.
REPEAT(S, N) The string S repeated N times.
REPLACE(S1, N1, N2, S2) The string formed by replacing the N2 characters starting at position N1 in S1 with string S2.

RIGHT(S, N) The string composed of the rightmost N characters of S.
STRCAT(...) The concatenation of all the arguments.

15.5 Logic Functions

The following lists the supported logic functions.

STRING(X, N) Numeric value of X as a string to N decimal places.
STRLEN(...) The total length of all strings in the arguments.
TRIM(S) The string formed by removing spaces from the string S.
UPPER(S) The string S converted to upper case.
VALUE(S) Numeric value of S as a string; 0 for non-numeric S.
FALSE The logical value 0.
FILEEXISTS(S) 1 if file S can be opened for reading; otherwise 0.
IF(X, T, F) The value of T if X evaluates to 1, or F if X evaluates to 0.
ISERROR(X) Returns 1 if X "contains" an error, otherwise 0.
ISNUMBER(X) 1 if X is a numeric value; otherwise 0.
ISSTRING(X) 1 if X is a string value; otherwise 0.
TRUE The logical value 1.
AND(...) 0 if any argument is 0; 1 if all arguments are 1; otherwise -1.
NAND(...) 0 if all arguments are 1; 1 if any argument is 0; otherwise -1.
NOR(...) 0 if any argument is 1; 1 if all arguments are 0; otherwise -1.
NOT(X) 0 if X=1; 1 if X=0; otherwise -1.
OR(...) 0 if all arguments are 0; 1 if any argument is 1; otherwise -1.
XOR(...) -1 if any argument is not 0 or 1; otherwise 0 if the number of arguments valued 1 is even; 1 if the number of arguments valued 1 is odd.

15.6 Date and Time Functions

The following lists the supported date and time functions.

DATE(Y, M, D) The date value for year Y, month M, and day D.
DATEVALUE(S) The corresponding date value for a given string S.
DAYS360(S, E) The number of days between two dates, based on a 30/360 day count system.
DAY(DT) The day number in the date/time value DT.
EDATE(S, M) The date/time value representing number of months (M)

before or after start date (S).

EOMONTH(S, M) The date/time value of the last day of the month M months after S, for M +, or M months before if M is -.

HOUR(DT) The hour value (0-23) of date/time value DT.

MINUTE(DT) The minute value (0-59) of date/time value DT.

MONTH(DT) The number of the month in date/time value DT.

NETWORKDAYS(S, E[, H]) Number of working days between S and E.

NOW The date/time value of the current system date and time.

SECOND(DT) The seconds value (0-59) of the date/time value DT.

TIME(H, M, S) The time value for hour H, minute M, and second S.

TIMEVALUE(S) The corresponding time value for a given string value S.

TODAY The date value of the current system date.

WEEKDAY(D) Integer representing the day of the week on which day D falls. 1 is Sunday, 7 is Saturday.

YEAR(DT) The year value of date/time value DT.

YEARFRAC(S, E[, B]) The portion of the year represented by the number of days between start date S and end date E.

15.7 Miscellaneous Functions

The following lists miscellaneous supported functions.

CELLREF(N1,N2) A reference to the cell in column N1 and row N2.

CHOOSE(N, ...) The N^{th} argument from the list.

COL(C) The column address of the cell referenced by C.

COLS(R) The number of columns in the specified range R.

HLOOKUP(X, S,R) The cell in range S that is R rows beneath X.

INIT(X1, X2) The first argument on the first recalculation pass and the second argument on all subsequent recalculation passes when Grid is performing iterative calculations.

INTERP2D(R1,R2, N) The interpolation value for a 2-dimensional vector.

INTERP3D(R, X,Y)The interpolation value for a 3-dimensional vector.

MATCH(V, R[,T]) The relative position in range R of value V based on positioning criteria T.

N(R) The numeric value of the top left cell in range R.

RANGEREF(N1, N2, N3, N4) A reference to the range defined by

coordinates N1 through N4.

ROW(C) The row address of the cell referenced by C.

ROWS(R) The number of rows in the specified range R.

S(R) The string value of the top left cell in range R.

VLOOKUP(X, S,C) The cell in range S that is C columns right of X.

DFT(R) The Discrete Fourier Transform of the range R.

EIGEN(M) The eigenvalues of the matrix M.

FFT(R) The Discrete Fourier Transform of the range R using a fast Fourier Transform algorithm.

FREQUENCY(R, B) F frequency distribution for R with intervals B.

INVDFT(R) The inverse of the Discrete Fourier Transform of the range R.

INVERT(M) The inverse of matrix M.

INVFFT(R) The inverse of the Discrete Fourier Transform of the range R using a fast Fourier Transform algorithm.

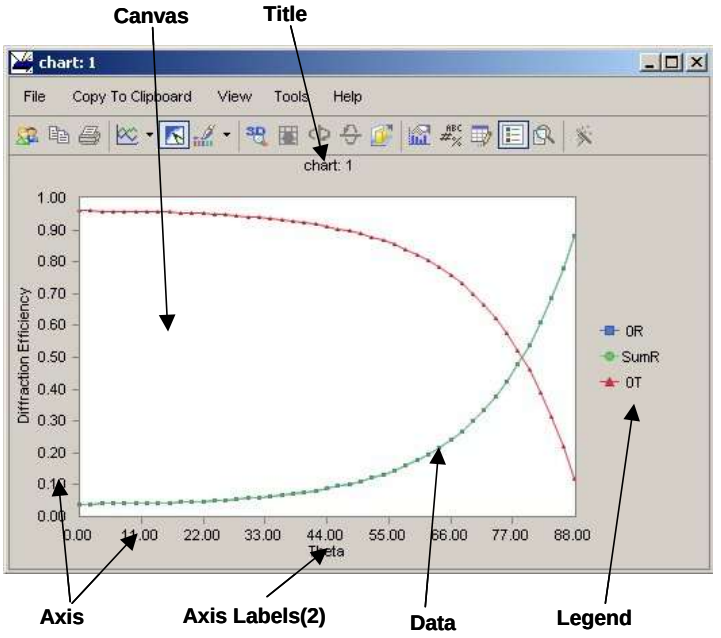
LINFIT(X, Y) The straight line least squares fit.

16 Graphing Options

The graphing engine uses ChartFX.ClientServer.Core.dll, the ChartFX® core graphing engine, which provides general chart object options.

Charts are created from the Results tab, and from the Materials Editor.

The general chart has eight regions that can be customized. Customization is accomplished by right clicking on a region to create a menu list, and then selecting the options to modify. The eight regions are identified in the figure shown below. The Axis properties menu is activated by clicking on one of the tick mark labels for the desired axis.



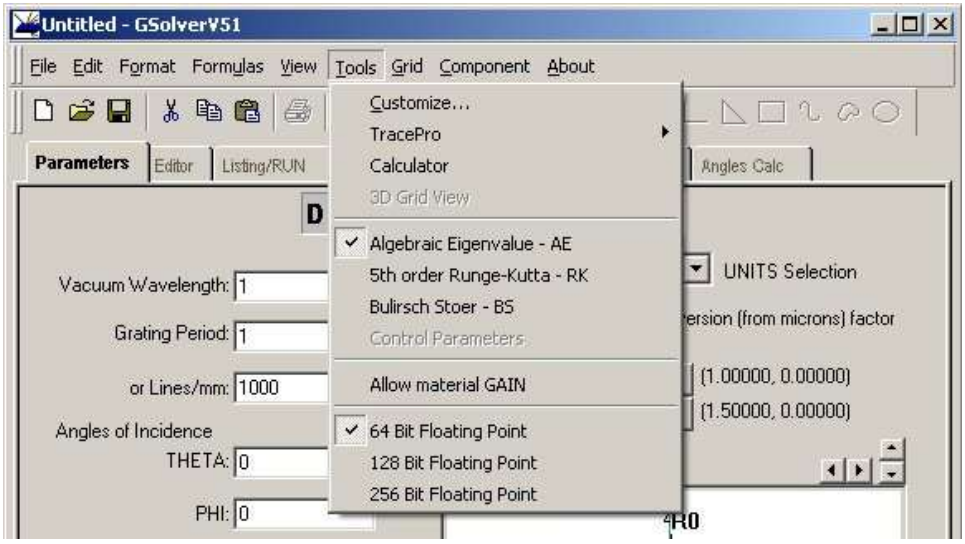
In addition to the region-specific menus, a number of general properties are accessible for modification from the chart tool bar and menu items.

The chart object includes a data editor. Data is copied from the source when the chart is created. Changing any data items by using the chart data editor has no effect on the original data source.

17 Algorithm Selection

GSolver has three distinct algorithms for solving the inter-layer set of coupled differential equations determined by Maxwell's equations, and the Fourier expansion of the permitivity (and impermitivity) of the layer. The three solution methods are the Algebraic Eigensystem solution (traditional method for GSolver), a 5th order Runge-Kutta method, and a Bulirsch-Stoer method with Richardson extrapolation and rational approximation.

The algorithm of choice is selected from the Tools menu.



The current Algorithm selection is shown on the status bar in the lower right hand corner.

In the piecewise constant grating approximation, each layer defines constant regions of (complex) index of refraction that are independent of depth. Using periodic boundary conditions (in the transverse directions), a

Fourier expansions of the index of refraction, and Maxwell's equations that relate the transverse electric field (**E**), and transverse magnetic field (**H**), leads to a general coupled differential equation of the form

$$\frac{d}{dz}\begin{pmatrix} E_{x,i} \\ E_{y,i} \\ H_{x,i} \\ H_{y,i} \end{pmatrix} = M \begin{pmatrix} E_{x,i} \\ E_{y,i} \\ H_{x,i} \\ H_{y,i} \end{pmatrix}$$

where the z coordinate is normal to the layer. M is a constant matrix (independent of z in the piecewise constant approximation) and is a function of the Fourier coefficients of the permitivity (and impermitivity), and of the propagation constants defined by the Rayleigh basis for the grating.

17.1.1 Algebraic Eigensystem Solution (AE)

Much effort has been given to the stable numerical solution of this differential equation system using the algebraic eigensystem method of solution. In particular all growing exponential solutions may be avoided with proper renormalization of the eigenvalues, or ordering of the solution space. GSolver also takes advantage of the intra-layer field normalizations (which are never actually evaluated absolutely). The internal fields are scaled to eliminate any growing exponential. The remaining numerical stability issue is in the calculation of the eigensystem of M, and limitations due to finite (round off) precision arithmetic (see Chapter 17).

GSolver incorporates an exact truncated Fourier series inversion (the impermitivity is the inverse of the permitivity independent of truncation order), matrix balancing, reduction to Hessian form, and QR decomposition to solve the eigensystem. However for large eigensystems (lots of orders retained in the Fourier representation of the permitivity), and for slow convergence of the Fourier system, numerical round off error can propagate through the eigensystem solution leading to meaningless

results. In that case additional numerical precision can often stabilize the solution.

There are no user modifiable parameters associated with the Algebraic Eigensystem (AE) method of solution. The numerical formulation of the solution is generally stable for arbitrary grating layer thickness and for arbitrary polarization. This method is recommended.

17.1.2 5th Order Runge-Kutta (RK)

New to GSolver V5.1 is the addition of a 5th order Runge-Kutta solution method for solving the set of coupled constant coefficient differential grating equations. This method includes adaptive step size control accurate to 5th order.

The implementation of the Runge-Kutta follows standard practice. There are two user definable parameters associated with the RK method. They are the maximum integration depth, and a relative error.

Any grating layer may have an arbitrary thickness. Any particular layer may be subdivided into m layers, and the RK solution method is then applied to each sub layer. In this case, the boundary condition solver propagates the fields through the m sub-layers. At issue is the numerical stability of the RK integrator through a thick layer with potential exponentially growing solutions. There is also a trade between layer subdivision and speed of solution. The GSolver boundary condition solver (S-matrix methods) are numerically stable. Experience shows that a RK numerical integration may become unstable for thick grating layers, with complex index of refraction in TM and conical mount illumination. By subdividing a thick layer into thinner sublayers, the solution can be made numerically stable.

A heuristic layer subdivision parameter (maximum layer thickness) of 0.75 ($=2\pi z/\lambda$ where z is the thickness, and λ is the vacuum wavelength) controls maximum layer thickness. If a layer is thicker than this, it is automatically subdivided, and the fields are propagated through the sublayers using the solution of the Maxwell's equations common to each sublayer.

The other parameter is a relative error term, which is used to halt the RK adaptive step size algorithm at some minimum estimated relative error in the solution. The default for this value is 0.001. It is tempting to make the relative error very small, in the hope of getting more numerical precision. While this is true in principle, it is seldom practical. Care should be exercised in setting the relative error, and generally the default setting results in numerical solutions that are much better than 0.001 (remember it is a maximum error estimate, the actual error may be much smaller).

RK may also benefit from greater numerical precision.

17.1.3 Bulirsch-Stoer Method (BS)

Most of the comments made about the RK method apply to the Bulirsch-Stoer method. The two user adjustable parameters of the RK method have the same function in the BS method. This method is distinguished from the RK method by subdividing the interval into many steps, propagating the function (through a midpoint method) and applying rational function approximations. There is a large literature on both the RK and BS differential equation solver methods.

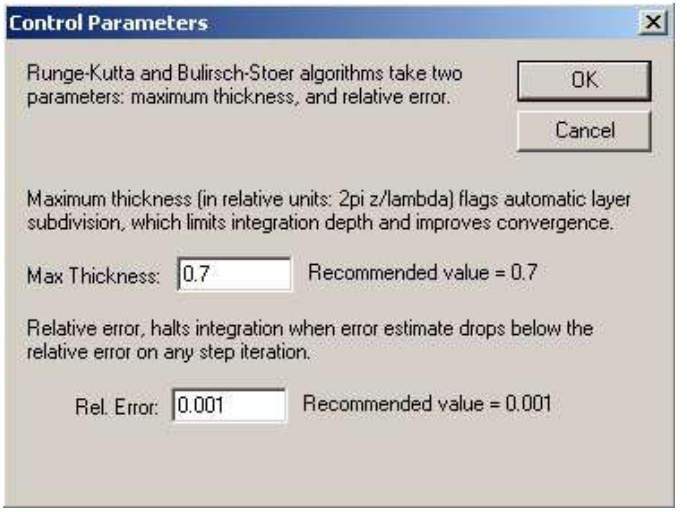
17.1.4 General Method Comments

Limited experimentation have demonstrated that the AE method is the fastest. I have not found any situations where the AE method failed while the RK or BS method succeeded. However I've only made cursory experimentation.

I've also found that BS generally takes the longest time and takes more computer resources to give similar numerical accuracy as AE. These comments are only meant as anecdotal, and based on the class of grating designs I generally work with.

17.1.5 Setting Algorithm Choice

The algorithm setting is determined from the Tools menu. The two user definable parameters are set by clicking on Tools→Control Parameters menu item.



Max Thickness is the (normalized) maximum layer thickness allowed. If a layer is thicker than Max Thickness, it is automatically subdivided.

Rel. Error is the relative error stopping criteria in the Runge-Kutta and Bulirsch-Stoer integration routines.

The current algorithm choice (AE, RK, BS) is indicated on the status bar, and is used for any calculation RUN (grating listing tab, genetic algorithm tab, run tab, 3Drun tab).

In general I find that AE remains the algorithm of choice in terms of speed and accuracy. There may be situations where the RK algorithm offers superior results (for example when AE fails).

17.1.6 GAIN

The GAIN setting on the Tools menu item is also new to GSolver V5.1. It flags the materials index of refraction evaluation routines to permit negative index of refraction for the Polynomial and Table models. In essences, a negative imaginary part of the index of refraction implies that energy is gained as the wave propagates through the material. This may happen, for example in optically pumped laser gain media.

To use a ‘gain’ medium, you will need to either edit the GSOLVER.INI file, or use the GSolver materials editor. Add a table model (for example) and enter negative values for the imaginary part of the index of refraction over some wavelength range. Then use this new material with the GAIN flag (from the Tools menu item) set (checked).

18 Precision Double Double and Quad Double

GSolver includes optimized extended precision arithmetic including floating point and complex data types. Double Double refers to 128 bit floating point made out of two 64 bit floating point words (106 bit mantissa, 21 bit exponent for approximately 32 decimal digit precision). And Quad Double refers to 256 bit floating point implementations (212 bit mantissa, 43 bit exponent for about 64 decimal digit precision). These numeric types are implemented in software using optimized calls to emulate a full IEEE complient operation including optimized routines for function calls (exponentiation, trig functions, and so forth).

Since operations with these data types are implemented in software the corresponding run times will increase dramatically. Having run simple test on a series of multiply-accumulates (assuming that there is no dedicated 64bit floating point multiply accumulate hardware instruction), I find that Double Double multiply-accumulate takes about 125 times a Double, and a Quad Double takes about 1000 times as a Double. These numbers are given only as very rough estimates. I have not taken into account any memory fetch optimizations, nor compiler optimizations.

The purpose for adding this option to GSolver is to provide a mechanism for increasing the bit depth for the eigensystem solution. Often (but not always) increasing the numerical precision will stabilize the solution. If on of the extended precision options is selected it is applied to whichever solution algorithm is selected.

Selection of the numerical precision is made from the tools menu. The three choices are

64 bit Floating Point - normal hardware implementation
128 bit Floating Point – Double double precision
256 bit Floating Point – Quad double precision

The selection is valid from the **Run** tab, **3D Run** tab, and the **Listing/Run** and **GA** tabs when an item in the respective grids are selected.

The numerical precision selection applies regardless of which solution algorithm is selected (see Chapter 16). Generally the Algebraic Eigenvalue method should be used. It solves the system of differential equations simultaneously.

18.1.1 Example Calculation

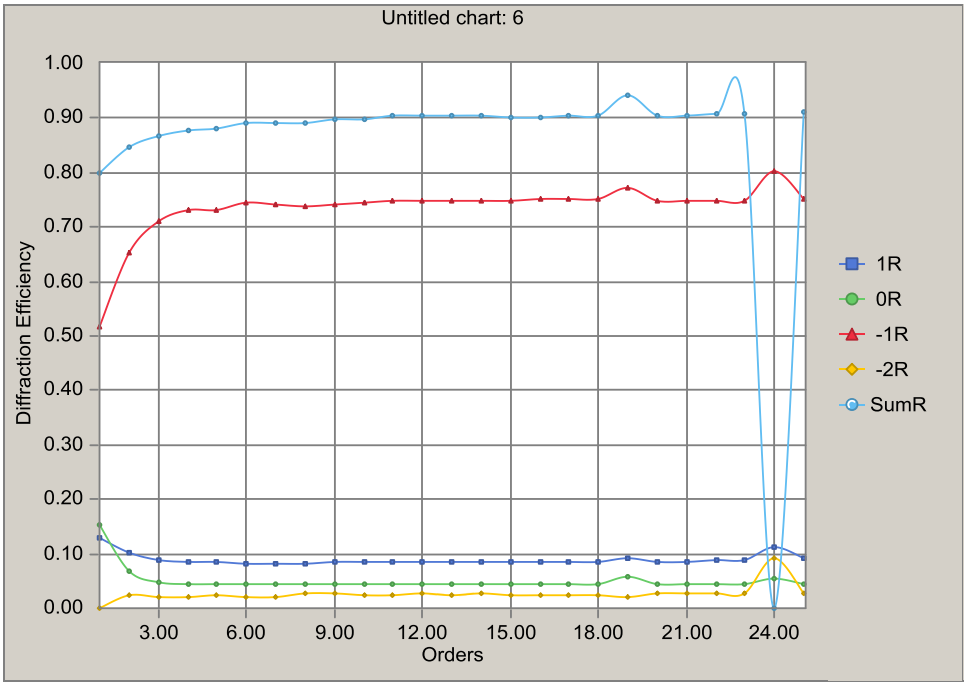
This example illustrates the value of increased precision. The following Blaze grating in conical mount with elliptic polarization is used.

Start GSolver. From the **Parameters** tab:
Change the substrate to Table model and AL
Change the Lines/mm to 1200
Change the wavelength to 0.5 microns
Change THETA to 17.5 degrees
Change PHI to 10 degrees
Change BETA to 10 degrees

From the **Editor** Tab
Selecte the Custom Profile Tool [menu→Component→Special Profile tool]
Select Blaze (default) and set the blaze angle to 17.5 (cell C3). Select OK
Verify that the material is Table→AL (right click the figure and check materials property)
Select the 'Approximation' button to load up the piecewise constant approximation.

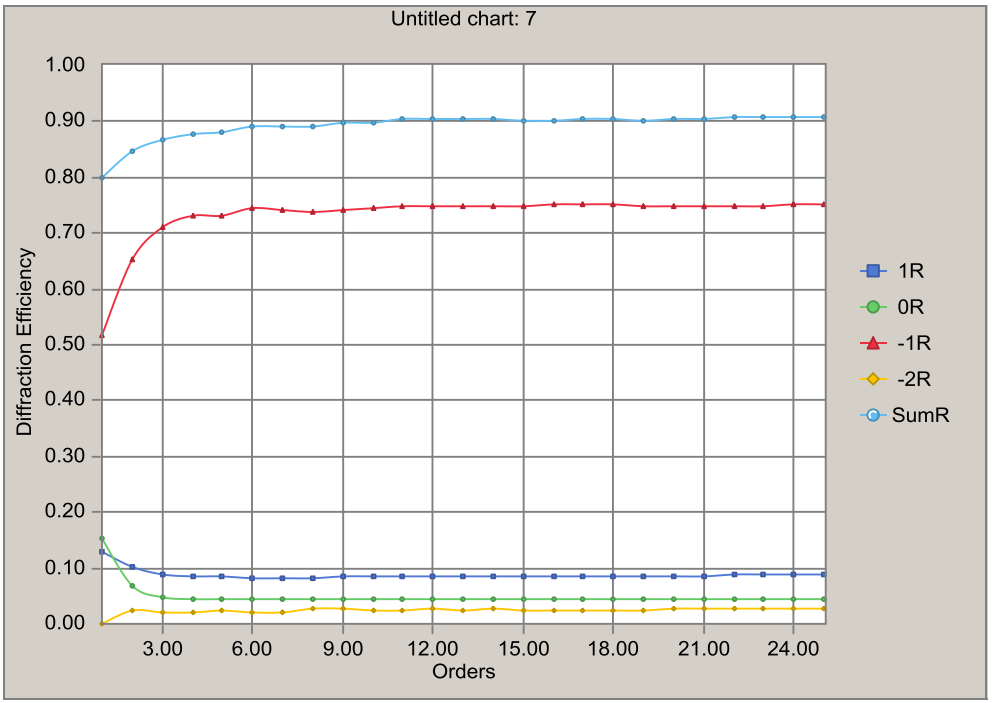
From the **Run** Tab
Select Orders with Start = 1 and Stop = 25.
Click RUN.

When the calculation is finished plot the 1R through the SumR columns. You should see something like the following



Notice that at order 19 and 24 the calculation appears to become unstable (the SumR result for order 24 is NAN indicating a problem).

Return to the Run tab and select the menu item Tools→128 Bit Floating Point and then click on RUN again (the calculation will take several times longer to run). When complete the plot now looks like



Examination of the Results table values indicate that the calculations at 19 and 24 orders appears better behaved.

19 Diffraction Solution Implementation

This chapter contains a general description of the theory used by GSolver to solve the grating equations. After a review of the general ideas behind the grating structure, the formulation for Maxwell equations and various solution techniques are discussed.

19.1 The Grating

A general periodic grating structure is defined to exist at the interface of two semi-infinite homogeneous, isotropic media called the superstrate, and the substrate. In GSolver the superstrate is characterized by a single real index of refraction making it a lossless dielectric. This permits the definition of the normalized incident plane-wave anywhere in the medium. The substrate is characterized by a single complex number. The transmitted energy, or rather complex E-field, is calculated at the top, or entrance into the substrate. If the substrate is lossy, then the fields will decay away exponentially, depending on the size of the imaginary component of the index of refraction.

The grating region, which may also be thought of as a modulation region, naturally divides itself into three categories depending on the number of geometric degrees of freedom. In GSolver these have been termed 1-, 2- or 3-dimensional gratings. The same code is used for 1- and 2-dimensional gratings. Three-dimensional, or crossed gratings, mix or couple the x- and y-dimension layer Fourier coefficients, which complicates the convergence optimizations used elsewhere.

19.1.1 Stratified Grating Approximation

All gratings are constructed as piecewise constant lamellar stacks. This is described in detail in the following paragraphs.

19.1.2 1-Dimensional Gratings

A one-dimensional grating or modulation region has a single degree of freedom. A stack of uniform, isotropic thin films is an example of a one-

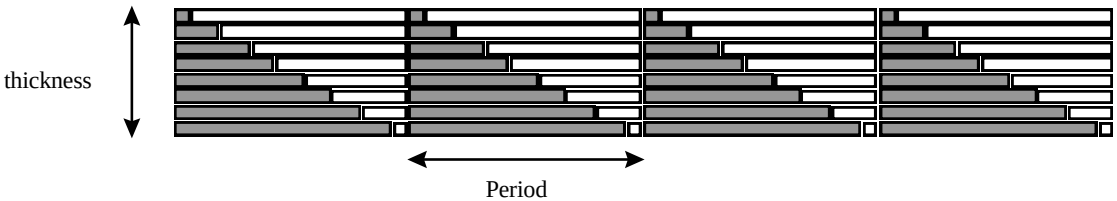
dimensional modulation region. The only geometric degree of freedom is the thickness of each layer, along the z-direction.

19.1.3 2-Dimensional Gratings

Two-dimensional gratings consist of a stack of layers, each consisting of a periodic array, or stripes of homogeneous materials. The orientation from layer to layer must be the same. In GSolver the uniform dimension is taken as the y-direction, the periodic dimension is the x-direction, and the thickness of the layer is the z-direction.

There are no restrictions on the number of layers, or the number of materials within each period in each layer. However, the more complex the grating structure, the more Fourier coefficients are needed to describe it sufficiently. Experience has shown that, generally, the number of terms needed is a strong function of the period-to-wavelength ratio, and not so much as the wavelength-to-grating *feature* ratio.

All classical diffraction gratings fall into the 2-dimensional category. Most of these gratings may be defined as a surface height relief of the substrate.



The figure illustrates an example of a lamellar approximation to a sawtooth grating profile. Only a single period needs to be defined. Simple surface relief gratings such as blaze, sinusoidal, triangular, and binary are constructed by a thin-layer stack approximation. Each layer consists of some number of index transitions (1 for the present example) where the index transition point is placed at the appropriate location so that the stack approximates the surface relief desired. Any degree of accuracy may be imposed by increasing the number of layers. However, once the individual layer thickness becomes significantly smaller than a wavelength (less than a few percent), little change is noted in the solution. More complicated grating structures might require several index transitions per layer.

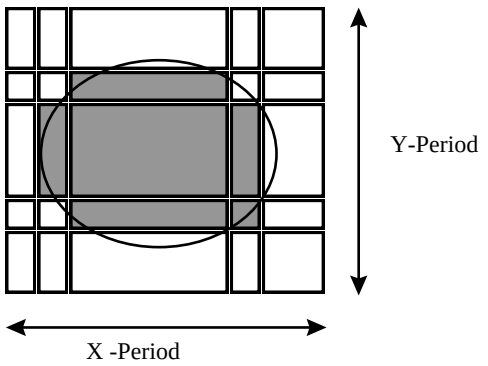
Any complex number may be entered as an index of refraction. The GSolver code enforces correct sign conventions so that no material exhibits gain. The n and k values are entered as positive real numbers with n strictly greater than 0. The solver makes k → |k| → -k, which indicates absorption with the sign convention used.

Use of the lamellar approximation permits arbitrarily complex grating structures to be analyzed.

19.1.4 3-Dimensional Gratings

Three-dimensional gratings are crossed gratings – periodic diffraction structures etched along both the x- and y-dimensions. GSolver uses the same 3D solver that was used in versions 1.0 through 4.0 This means that the TM convergence is not accelerated. The reason is that the fundamental theorem of algebra does not apply to polynomials in more than one variable. However, there remains an expectation that, in time, the problem can be significantly mitigated using the ideas that have satisfactorily solved the two-dimensional convergence problems. Some recent progress in this area has been made if the grating as appropriate symmetries. However, since these ideas only apply to a certain class of gratings they cannot be used for the general case.

As an example, suppose that a dimpled surface is to be analyzed. The following figure illustrates how an elliptical mesa, in a unit cell of the crossed periodic structure, might be approximated.



In the figure, note that the x- and y-periods are independent, and that the number and placement of the index transition regions are also independent. Shown is an oval shaped dimple being approximated with 4 index boundaries (points where the index may change) in the x-direction, and 4 index boundaries in the y-direction. The white-colored squares are assigned one material index value, and the gray-colored squares are assigned a second material index value. The grid may be made as fine as deemed necessary.

Using this simple example as a guide, arbitrarily complex structures may be built by stacking layers. Each layer is independent of the ones above and below, so that some layers may have fine structure with numerous index transitions, while other layers might be uniform.

19.1.5 Relation of Index of Refraction to Permittivity

All material indices are entered as n and k values. This formulation is used so that the GSolver sign convention for permittivity need not become a source of confusion. The index (n + ik), are entered as two real numbers with $n>0$ and $k\geq 0$. GSolver then forms the permittivity as $\varepsilon=(|n|-i|k|)^2 = |n|^2-|k|^2 - 2i|n||k|$. The permittivity is used in the grating description vector, not the index of refraction. **The wavelength specified in GSolver is the vacuum wavelength.**

19.1.6 Solution Routines

There are four routines that perform all the calculations for the internal fields, and boundary condition matching. SolveTE handles the special case of TE mode polarization for one- and two-dimensional gratings; SolveTM handles TM polarization for one- and two-dimensional gratings; and Solve handles general polarization for one- and two-dimensional gratings. Solve3D handles all polarizations for three-dimensional gratings. The reason that TE and TM polarization modes have their own routines is that, in each, certain vector components are known to be identically 0, and therefore can be deleted from the general vector formulation. SolveTE, SolveTM and Solve use a so called stack matrix method to solve for the boundary conditions, as well as using certain Toeplitz matrix inversion methods to ‘stabilize’ the Fourier coefficient representation of the

permittivity and impermitivity for each grating layer. Solve3D uses Gaussian elimination with partial pivoting to solve for the boundary conditions. It is less numerically stable and slower than the stack methods.

All routines solve for the fields, internal to each layer of the modulation region, by solving an algebraic eigensystem. Symmetry is used to reduce the order of the problem by a factor of 2 for an acceleration by a factor of 8. Some authors have shown that additional symmetry considerations exist for the special case of TE and TM, at the added expense of greater problem complexity and memory requirements. These alternate methods are not used in GSolver.

After solving for fields internal to each layer, and matching all internal boundary conditions, a final boundary condition matching is performed between the input and output (superstrate and substrate).

19.2 Theory

This section contains a presentation of the theory of the solution of the diffraction problem. The grating is defined as a piecewise-constant, periodic, lamellar structure at the boundary between the semi-infinite superstrate and substrate regions.

The grating is illuminated by an incident plane wave determined by five parameters, a wavelength and four angles. Two angles determine direction of travel from the superstrate to the substrate, and two angles determine the state of polarization. The incident E-field has unit magnitude. The only dimensioned measures in the problem are the wavelength and the grating period(s). Since these lengths enter as ratios, their units are not important as long as they are the same (such as microns).

GSolver computes the fields internal to each layer, and explicitly at the boundaries. These fields are complex **inhomogeneous plane waves**. The reflected diffracted fields and transmitted diffracted fields are computed by eliminating all internal fields and solving for the fields at the top and bottom interface. The diffraction efficiency is defined to be

$$DE_{ij} = -\left\|\mathbf{R}_{ij}\right\| \mathrm{Re}(k1_{zij} / kz)$$

$$DE_{ij} = \left\|\mathbf{T}_{ij}\right\| \mathrm{Re}(k3_{zij} / kz)$$

where ||.|| is the norm (sum of the magnitude squared of the vector components), and the subscripts *ij* refer to the ijth diffracted field, and R_{ij}, T_{ij} are the complex vector E-field magnitudes. For i=j=0 the specular fields are obtained (in the case of no diffraction these are the Fresnel fields). When $k1z_{ij}$ or $k3z_{ij}$ become purely imaginary, the related DE is identically 0. This happens for evanescent waves, which can be thought of as standing waves at the boundary surface since the grating is being illuminated by an infinite-extent plane wave.

The fields internal to each grating layer are found by solving Maxwell's equations with the permittivity expanded as a Fourier series. This leads to the solution of the field equations with a number of unknown amplitude coefficients. These are found by application of the boundary conditions for the tangential components of the E and H fields. By ordering the equations properly all internal fields may be eliminated from the calculation, greatly simplifying the solution and allowing it to proceed in an iterated manner, reusing the same work arrays. The final boundary condition call results in the incident (reflected) and transmitted fields.

19.2.1 Maxwell's Equations

The solution of the field equations within each layer, and the region of the problem, is found by solving the first-order Maxwell.

19.2.1.1 Superstrate and Substrate Solutions

The superstrate and substrate are semi-infinite, homogeneous media. It is common knowledge that a traveling wave solution to Maxwell's equations, in terms of the E-field, may be written as

$$\mathbf{E}_1 = \mathbf{E}_{inc} + \sum_{ij} \mathbf{R}_{ij} \exp(-I\mathbf{k}1_{ij} \cdot \mathbf{r})$$

$$\mathbf{E}_3 = \sum_{ij} \mathbf{T}_{ij} \exp(-I\mathbf{k}3_{ij} \cdot (\mathbf{r} - d\hat{z})$$

where **E** is a vector with complex coefficients (to account for polarization), $\mathbf{R}_{ij}$ are reflected (diffracted) complex-valued E-field amplitudes, and $\mathbf{T}_{ij}$ are the transmitted (diffracted) complex valued E-field amplitudes. $\mathbf{k}_{ij}$ are the wave vectors for the superstrate (1) and substrate (3) regions. *I* is the square root of -1.

The $\mathbf{k}_{ij}$ vectors are known in regions (1) and (3), as well as $\mathbf{E}_{\text{inc}}$. Orienting the coordinate system so that z points from the superstrate to the substrate

$$\mathbf{k}_1 = k1(\sin(\theta)\cos(\varphi)\hat{x} + \sin(\theta)\sin(\varphi)\hat{y} + \cos(\theta)\hat{z})$$

$$k1 = \frac{2\pi n_{\text{sup}}}{\lambda},$$

$$\mathbf{E}_{inc} = \mathbf{u}\exp(-I\mathbf{k}_1 \cdot \mathbf{r})$$

$$\mathbf{u} = (\sin(\tau)\cos(\theta)\cos(\varphi) - \cos(\tau)\sin(\varphi))\hat{x} +$$
$$(\sin(\tau)\cos(\theta)\sin(\varphi) + \cos(\tau)\cos(\varphi))\hat{y} -$$
$$\sin(\tau)\sin(\theta)\hat{z}$$

where cos(τ) and sin(τ) are complex numbers, such that $||u||=|u_x|+|u_y|+|u_z|=1$. Explicitly

$$\sin(\tau) = Complex(\sin(\alpha)\cos(\beta), \cos(\alpha)\sin(\beta))$$

$$\cos(\tau) = Complex(\cos(\alpha)\cos(\beta), \sin(\alpha)\sin(\beta))$$

where Complex(.,.) is a complex number a+ib.

Obvious changes in sign need to be made for coordinates systems where the z-axis points from the substrate to the superstrate.

In each layer the k_x and k_y components of the k vector are identical because of continuity of transverse field components. Knowing the values of the magnitude of the **k** vector in regions (1) and (3) leads to the following equations:

$$\mathbf{k}1_{ij} = k1((\sin(\theta)\cos(\varphi) - iK_x)\hat{x} + (\sin(\theta)\sin(\varphi) - jK_y)\hat{y} + \sqrt{k1 - k_{xi}^2 - k_{yj}^2}\hat{z}$$

$$\mathbf{k}3_{ij} = k3((\sin(\theta)\cos(\varphi) - iK_x)\hat{x} + (\sin(\theta)\sin(\varphi) - jK_y)\hat{y} + \sqrt{k3 - k_{xi}^2 - k_{yj}^2}\hat{z}$$

$$K_x = \frac{\lambda}{\Lambda_x}, \qquad K_y = \frac{\lambda}{\Lambda_y}, \qquad k_{xij} = k1(\sin(\theta)\cos(\varphi) - iK_x),$$

$$k_{yij} = k1(\sin(\theta)\sin(\varphi) - jK_y)$$

where *i* and *j* are integer indices (ranging from –s to +s, where s is the number of orders retained). **k1** and **k3** are the magnitudes of the **k** vectors in the superstrate (1) and substrate (3) regions, as given previously. For one- and two-dimensional gratings *j*=0, and the K_y term is irrelevant. Λ_x and Λ_y are the grating period dimensions in the x and y directions.

All **k** vectors and fields have now been defined for the superstrate and substrate regions. The fields in each layer are found by application of Maxwell's equations, and expansion of the permittivity in a Fourier series. This results in a set of coupled wave equations that are solved with algebraic methods, resulting in a set of inhomogeneous plane waves.

19.2.1.2 Inhomogeneous Plane Wave Intra-layer Solutions

Considering the n^{th} grating layer, assuming the standard time harmonic formulation, and working in Rationalized MKSA units where $\mathbf{B}=\mu_0\mathbf{H}$, $\mathbf{D}=\varepsilon\varepsilon_0\mathbf{E}$, the curl equations are as follows:

$$\nabla \times \mathbf{E} = -\dot{\mathbf{B}} = -\mu\dot{\mathbf{H}} = -I\omega\mu_0\mathbf{H} = -Ik\sqrt{\frac{\mu_0}{\varepsilon_0}}\mathbf{H}$$

$$\nabla \times \mathbf{H} = \dot{\mathbf{D}} = \varepsilon\varepsilon_0\dot{\mathbf{E}} = I\omega\varepsilon\varepsilon_0\mathbf{E} = Ik\sqrt{\frac{\varepsilon_0\varepsilon}{\mu_0}}\mathbf{E}$$

Note that extensions to anisotropic media requires that $\varepsilon \rightarrow \boldsymbol{\varepsilon}$ a 3x3 matrix, and for magnetic media $\mu_0 \rightarrow \mu_0\mu$. The permittivity of free space may be substituted as $Z_0=(\varepsilon_0/\mu_0)^{1/2}$; the fact that $c=1/(\varepsilon_0\mu_0)^{1/2}$ and the vacuum dispersion relation have been used.

The electric and magnetic fields are represented as

$$\mathbf{E} = \sum_{ij} \mathbf{S}_{ij}(z) \exp(-I\mathbf{k}_{nij} \cdot \mathbf{r})$$

$$\mathbf{H} = \sum_{ij} \mathbf{U}_{ij}(z) \exp(-I\mathbf{k}_{nij} \cdot \mathbf{r})$$

where **S** and **U** are unknown complex-valued vector field functions.

The key to the coupled wave expansion within each layer is to replace ε with a truncated Fourier series representation. Both ε (the permittivity) and the inverse of ε (impermitivity) are required. The permittivity within each layer is a function of x and y only (for the general three-dimensional grating case) but not of z. These are periodic functions in Λ_x and Λ_y.

$$\varepsilon(x,y) = \sum_{gh} \widehat{\varepsilon}_{gh} \exp(IK_x gx + IK_y hy)$$

$$\varepsilon(x,y)^{-1} = \sum_{gh} \widehat{\xi}_{gh} \exp(IK_x gx + IK_y hy)$$

where the Fourier coefficients are constants. ε and ε^{-1} are only strictly inverses when gh ranges from -∞ to +∞. When the series are truncated they may no longer be inverses. This is the origin of some of the convergence problem generally, and manifested principally in the TM polarization case. By properly adjusting the coefficients of the truncated series so that the permittivity and impermitivity are inverses for any truncation order, convergence is greatly facilitated. For one- and two-dimensional gratings, the permittivity and impermitivity are functions of a single variable and it is fairly straightforward to enforce the proper relationships. The one- and two-dimensional code calculates the Fourier coefficients of the permittivity (eh), the impermitivity (ah), and the inverses of each of these (eh1, ah1).

For the general three-dimensional case, the coefficients are coupled (between x and y). The Fourier coefficients of the permittivity and impermitivity are directly computed and used. The inverses of these two matrices could also be calculated and similar use could be made of them. Inter-layer Solution, Inhomogeneous Plane Wave Expansion

19.2.1.3 Formulation of Eigensystem Solution

Applying the curl equations to the assumed form of the fields within the n^{th} layer, and eliminating the z terms, four coupled equations remain:

$$\frac{dS_{xij}}{dz} = Ik_{nz}S_{xij} - IkU_{yij} + I\frac{k_{xij}}{k}\sum_{pq}\hat{\xi}_{gh}(k_{xpq}U_{ypq} - k_{ypq}U_{xpq})$$

$$\frac{dS_{yij}}{dz} = Ik_{nz}S_{yij} + IkU_{xij} + I\frac{k_{yij}}{k}\sum_{pq}\hat{\xi}_{gh}(k_{xpq}U_{ypq} - k_{ypq}U_{xpq})$$

$$\frac{dU_{xij}}{dz} = Ik_{nz}U_{xij} + Ik\sum_{pq}\hat{\varepsilon}_{gh}S_{ypq} + I\frac{k_{xij}}{k}(k_{yij}S_{xij} - k_{xij}S_{yij})$$

$$\frac{dU_{yij}}{dz} = Ik_{nz}U_{yij} - Ik\sum_{pq}\hat{\varepsilon}_{gh}S_{xpq} + I\frac{k_{yij}}{k}(k_{yij}S_{xij} - k_{xij}S_{yij})$$

where $p=i-g$, and $q=j-h$. This represents a set of coupled first-order differential equations that are solved by standard eigenvector techniques. S_x, S_y, U_x, and U_y are functions of z only and their functional values are needed at the top and bottom of each layer. They turn out to be the sums over terms of the eigenvector times $\exp(\lambda_{ij} z)$, where λ_{ij} is the appropriate eigenvalue and z is either 0 (top of layer) or t_n, the n^{th} layer thickness.

All solvers (SolveTE, SolveTM, Solve, Solve3D) use the same eigensystem solver. The coefficient matrix is formed, the matrix is balanced, the Hessian is found, and the system is solved with LR decomposition. The fields are then calculated at the top and bottom of the layer (z=0 and z=d, the thickness of the n^{th} layer).

The E-fields are unnormalized, and may be multiplied by any quantity without affecting the computation of the resultant diffraction efficiencies. This fact is used to 'normalize' the internal fields so that no exponential is ever taken with a positive real (exponentially growing) argument. Without this precaution, there would be exponentially growing solutions that cause instabilities for 'deep' gratings.

The full coefficient matrix system that needs to be solved is of order s, where $s = 2m+1$, and m is the number of orders retained. GSolver uses a

symmetric order calculation so that the calculated orders range from $-m$ to $+m$. This enhances convergence by producing a balanced Fourier sum. Examination of the coefficient matrix reveals certain symmetries that permit a reduced system to be solved, and the remaining eigenvectors and eigenvalues are related with simple algebraic expressions to reduce the system solutions. This is an important step, as the solution of the eigensystem in each layer is a principal component of the solution time budget, the other component being the boundary condition solver.

19.2.1.4 Eigensystem Order Reduction

GSolver solves a reduced eigensystem due to the following structure:

$$\begin{bmatrix} \mathbf{0} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{bmatrix} = \begin{bmatrix} \Omega_{11} & \Omega_{12} \\ \Omega_{21} & \Omega_{22} \end{bmatrix} \begin{bmatrix} \Lambda_{11} & \mathbf{0} \\ \mathbf{0} & \Lambda_{22} \end{bmatrix}$$

where the **B** matrix is the coefficient matrix, Ω are the eigenvectors, and Λ is a diagonal eigenvalue matrix. The coefficient matrix is reduced to this form through the equivalence of a field normalization that removes the constant diagonal term. Multiplying the matrices leads to the following:

$$\mathbf{B}_{12}\mathbf{B}_{21}\Omega_{11} = \Omega_{11}\Lambda_{11}\Lambda_{11}$$
$$\mathbf{B}_{12}\mathbf{B}_{21}\Omega_{12} = \Omega_{12}\Lambda_{22}\Lambda_{22}$$

hence

$$\Omega_{12} = \Omega_{11}$$
$$\Lambda_{22} = -\Lambda_{11}$$
$$\Omega_{21} = \mathbf{B}_{21}\Omega_{11}\Lambda_{11}^{-1}$$
$$\Omega_{22} = -\Omega_{21}$$

These relations are used to reduce the overall eigensystem computational effort by about a factor of 8.

19.2.1.5 Permittivity and Impermitivity

For infinite orders, the permittivity and impermitivity are strictly inverses of each other. For finite orders, this relation no longer holds. This is the origin of the convergence issues with coupled wave expansions. In GSolver, both the Fourier coefficients of the impermitivity and

permittivity are computed, and the inverses are also computed. The Fourier coefficients enter into the coefficient matrix calculation as a Toeplitz matrix, so the inversion can be done much faster than if it were a general matrix inverse calculation. The inverse of a Toeplitz matrix is generally not a Toeplitz matrix.

The question remains as to where to substitute the Toeplitz impermitivity matrix with the inverse of the permittivity Toeplitz matrix. eh and ah are the permittivity and impermitivity Toeplitz matrices (stored as vectors to reduce memory). eh1 and ah1 are the coefficient matrices computed as the inverses of eh and ah. They are not Toeplitz, and enter as two-dimensional arrays. By pairing ah with eh1, and eh with ah1, convergence of the TM and general polarization is greatly accelerated. Indeed, for one- and two-dimensional gratings, only a few evanescent orders are needed to converge to better than the 1% level for dielectrics. For larger phase shift materials, such as metals, three to eight evanescent orders are generally sufficient. Some experimentation with the number of orders retained is recommended to demonstrate convergence. The diffraction efficiency may not converge monotonically, but could have an exponentially damped sinusoid component.

19.2.2 Intra-layer Solutions, Boundary Conditions

The fields in each region are readily solved. To complete the problem, the tangential electric and magnetic fields must be made continuous across each interface. The general problem can be set up as a series of matrix manipulations that include finding at least one inverse per boundary. The internal layers required to track only the x- and y-components of the E and H fields and are, therefore, 4s x 4s dimensional (where s=2*orders+1). The superstrate and substrate require calculation of the x-, y- and z-components of E and H and are 6s x 6s dimensional. The Stack matrix methods of solving the boundary conditions are significantly different than the Gaussian elimination method. Both are described below. The first step in either case is to reorder the equations so that the final matrix inversion connects the superstrate with the substrate. The Gaussian system used in the Solve3D/Fnlmat3D code is conceptually easier and is described first, followed by the Stack matrix methods.

19.2.2.1 Gaussian Elimination

At the first boundary, going from the superstrate down, the equivalence of the tangential E and H fields require that

$$u_x \delta_{ij00} + R_{xij} = S^1_{xij}(0)$$
$$u_y \delta_{ij00} + R_{yij} = S^1_{yij}(0)$$
$$\delta_{ij00}[k_y u_z - k_z u_y] + k_{yij} R_{zij} - k_{zij} R_{yij} = kU^1_{xij}(0)$$
$$\delta_{ij00}[k_z u_x - k_x u_z] + k_{xij} R_{zij} - k_{zij} R_{xij} = kU^1_{yij}(0)$$

where *R*, *u*, *S*, and *U* are defined in Sections 16.2.1 and 16.2.2. For s total orders (2*orders+1), each field component (x, y, z) has s entries. At the internal interface, between the n^{th} and $n+1^{th}$ layers, the tangential fields require

$$S^n_{xij}(d) = S^{n+1}_{xij}(0)$$
$$S^n_{yij}(d) = S^{n+1}_{yij}(0)$$
$$U^n_{xij}(d) = U^{n+1}_{xij}(0)$$
$$U^n_{yij}(d) = U^{n+1}_{yij}(0)$$

where *d* is the thickness of the n^{th} layer. At the last interface, with the substrate, the boundary conditions dictate that

$$T_{xij} = S^N_{xij}(d)$$
$$T_{yij} = S^N_{yij}(d)$$
$$k_{yij} T_{zij} - k_{zij} T_{yij} = kU^N_{xij}(d)$$
$$k_{xij} T_{zij} + k_{zij} T_{xij} = kU^N_{yij}(d)$$

where *d* is now the thickness of the n^{th} layer. This set of equations, together with the divergence free conditions (no charge is accumulating within the grating) lead to two more equations

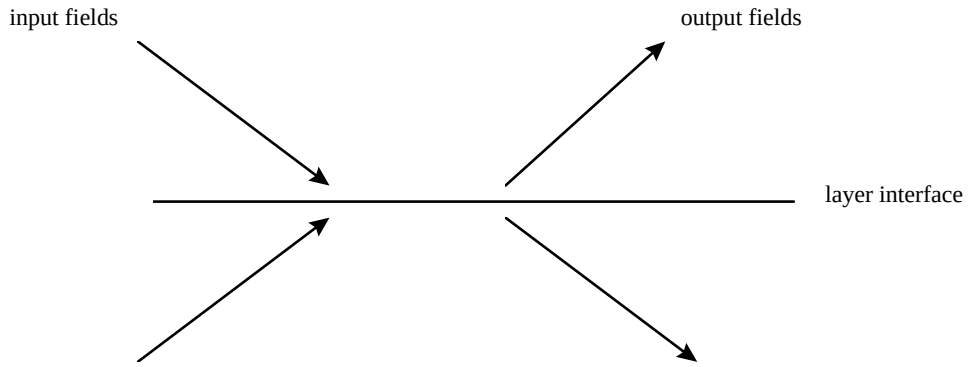
$$k_{1xij} R_{xij} + k_{1yij} R_{yij} + k_{1zij} R_{zij} = 0$$
$$k_{3xij} T_{xij} + k_{3yij} T_{yij} + k_{3zij} T_{zij} = 0$$

which represent a solvable system. The trick is to solve the internal fields iteratively, eliminating dependence on the internal fields top down (or bottom up), ending up with the sets of equations in R and T. This final system (in R and T) are then solved. The internal fields are iteratively solved, reusing the same matrix work storage area for each layer in turn.

Thus the fields are first calculated in the first layer, and numerical values are found for all field components at the top and bottom of the layer. These fields are solutions to Maxwell's equations within the layer. They can be multiplied by any arbitrary constant, which allows scaling such that numerical overflow is avoided. The fields are then solved for in the next layer, at the top and bottom. The internal interface boundary condition is then solved using Gaussian elimination to remove the internal interface, leaving field solutions at the top of the first layer and the bottom of the second layer. This proceeds through the grating stack, ending with field solutions at the superstrate interface (top), and substrate interface (bottom). These fields are then matched, using the remaining boundary conditions, and divergence-free conditions to solve for the *R*'s and *T*'s in terms of the *u*'s and *k*'s.

19.2.2.2 Stack Matrix Methods

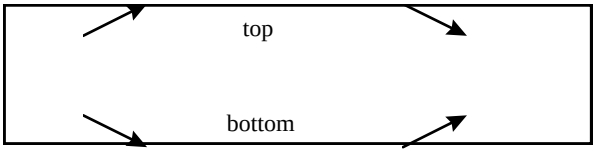
Boundary condition solving based on the stack matrix method is illustrated in the following figure.



Each interface has fields approaching it and leaving it (the substrate has only outgoing fields). The input and output fields are all multiplied by an

appropriate exponential function. By reordering the way the fields are solved in the Gaussian case (16.2.3.1), which is solved top to bottom, the stack matrix method solves the fields input to output. This reordering of the equations has the added effect of guaranteeing that there are no exponentially growing fields.

To make this idea explicit, consider the fields in one layer



They are written in terms of the eigenvectors and eigenvalues as

$$\begin{bmatrix} \mathbf{E}_{11} & \mathbf{E}_{12}\exp(-\Lambda d) \\ \mathbf{E}_{21} & \mathbf{E}_{22}\exp(-\Lambda d) \end{bmatrix}\begin{bmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{S}^t \\ \mathbf{U}^t \end{bmatrix} \quad \begin{bmatrix} \mathbf{E}_{11}\exp(-\Lambda d) & \mathbf{E}_{12} \\ \mathbf{E}_{21}\exp(-\Lambda d) & \mathbf{E}_{22} \end{bmatrix}\begin{bmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{S}^b \\ \mathbf{U}^b \end{bmatrix}$$

where the **C**'s are to be solved (eliminated) by application of the boundary conditions, the **E**'s are the eigenvector components, and Λ is the diagonal eigenvalue matrix. For the stack matrix method these equations become

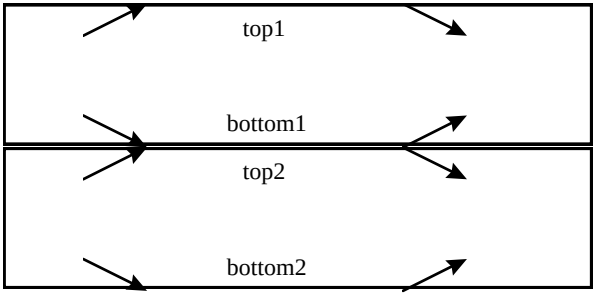
$$\begin{bmatrix} \mathbf{E}_{11} & \mathbf{E}_{12}\exp(-\Lambda d) \\ \mathbf{E}_{21}\exp(-\Lambda d) & \mathbf{E}_{22} \end{bmatrix}\begin{bmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{S}^t \\ \mathbf{U}^b \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{E}_{11}\exp(-\Lambda d) & \mathbf{E}_{12} \\ \mathbf{E}_{21} & \mathbf{E}_{22}\exp(-\Lambda d) \end{bmatrix}\begin{bmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{S}^b \\ \mathbf{U}^t \end{bmatrix}$$

and the matrix multiply results in the stack matrix for this layer.

$$\begin{bmatrix} \mathbf{E}_{11} & \mathbf{E}_{12}\exp(-\Lambda d) \\ \mathbf{E}_{21}\exp(-\Lambda d) & \mathbf{E}_{22} \end{bmatrix}\begin{bmatrix} \mathbf{E}_{11}\exp(-\Lambda d) & \mathbf{E}_{12} \\ \mathbf{E}_{21} & \mathbf{E}_{22}\exp(-\Lambda d) \end{bmatrix}\begin{bmatrix} \mathbf{S}^b \\ \mathbf{U}^t \end{bmatrix} = \begin{bmatrix} \mathbf{S}^t \\ \mathbf{U}^b \end{bmatrix}$$

The next step is to find the algorithm which combines two stack matrices, or equivalently combines the fields of two layers. This is illustrated below.



The two stack matrices defined by layers 1 and 2 are combined to form a new stack that connects top1 and bottom2, and so forth down through the layers. If S^1 is the stack for layer 1, and S^2 is the stack for layer 2, the combined stack is found to be

$$\begin{bmatrix} \mathbf{S}_{11}^2\left(1-\mathbf{S}_{12}^1\mathbf{S}_{21}^2\right)^{-1}\mathbf{S}_{11}^1 & \mathbf{S}_{11}^2\left(1-\mathbf{S}_{12}^1\mathbf{S}_{21}^2\right)^{-1}\mathbf{S}_{12}^1\mathbf{S}_{22}^2+\mathbf{S}_{12}^2 \\ \mathbf{S}_{22}^1\left(1-\mathbf{S}_{21}^2\mathbf{S}_{12}^1\right)^{-1}\mathbf{S}_{21}^2\mathbf{S}_{11}^1+\mathbf{S}_{21}^1 & \mathbf{S}_{22}^1\left(1-\mathbf{S}_{21}^2\mathbf{S}_{12}^1\right)^{-1}\mathbf{S}_{22}^2 \end{bmatrix}\begin{bmatrix} \mathbf{S}^{b1} \\ \mathbf{U}^{t2} \end{bmatrix}=\begin{bmatrix} \mathbf{S}^{t2} \\ \mathbf{U}^{b1} \end{bmatrix}$$

Note that one 4s x 4s matrix inversion is replaced by two 2s x 2s inverses. Thus the stack method is not only faster, it is more stable than the Gaussian method. The stack methods are used in all solvers other than the 3D grating case.

The final stack matrix is complicated by the fact that the external fields require all vector components, and are, therefore, of a different dimension. When the grating layers have been solved there is found a single stack matrix, **S**. This is placed in the following 6s x 6s final boundary condition solver as follows

$$\begin{bmatrix} 1-\mathbf{S}_{12}(\mathbf{k}_1\times) & 0 \\ -\mathbf{S}_{22}(\mathbf{k}_1\times) & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} u_x\delta_{i0} \\ u_y\delta_{i0} \\ u_z\delta_{i0} \\ 0 \\ 0 \\ 0 \end{bmatrix}=\begin{bmatrix} -1+\mathbf{S}_{12}(\mathbf{k}_1\times) & \mathbf{S}_{11} \\ \mathbf{S}_{22}(\mathbf{k}_1\times) & \mathbf{S}_{21}-(\mathbf{k}_3\times) \\ \mathbf{k}_1 & 0 \\ 0 & \mathbf{k}_3 \end{bmatrix}\begin{bmatrix} \mathbf{R}_x \\ \mathbf{R}_y \\ \mathbf{R}_z \\ \mathbf{T}_x \\ \mathbf{T}_y \\ \mathbf{T}_z \end{bmatrix}$$

where the sub-blocks are appropriately dimensioned. GSolver calls the matrix that pre-multiplies the RT vector the **F** matrix. This matrix is

formed in Fnlmat(TE,TM) and a final partial inverse is performed. Since the bottom rows of the terms on the left are all 0, only those rows that are needed in the inverse are computed. The notation **k**x indicates a matrix that, when multiplied by a vector, results in a vector cross product. If there is no grating, then **S** is initialized to the identity and the final calculation simply turns out to be a solution of the interface Fresnel equations.

The implementation of the stack method is somewhat altered if the problem is purely a TE or a TM mode. In that case certain vector components are identically zero.

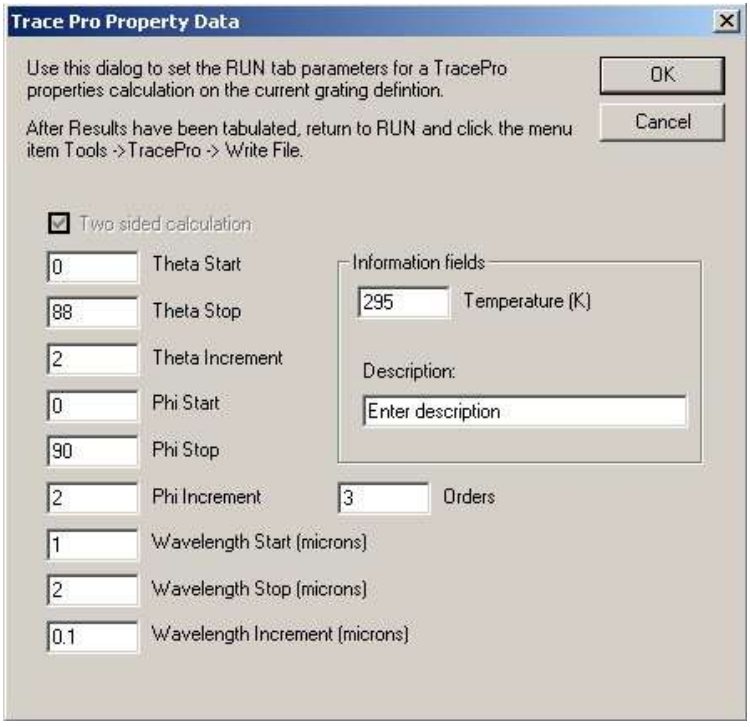
20 Trace-Pro Material Runs

GSolver has an integrated tool for generating a material property file (essentially a BRDF for a grating) suitable for reading into TracePro®. The idea is to set up a grating and loop through all the angles, and wavelengths for radiation incident from the superstrate to the substrate (normal mode) as well as from the substrate to the superstrate (reverse normal). For normal parameter selections, a large number of GSolver runs may be generated. On completion of the normal mode the results of the calculation are stored to temporary arrays and the grating structure is then temporarily inverted (the superstrate and substrate materials are swapped, and the order of the grating layer structure is inverted) and the series of loops are run through again. Finally, the run data from both sets of runs (normal and inverted) are written to a text file in a format suitable for import into TracePro®, and the grating structure is returned to its normal orientation.

GSolver expects the superstrate to have only real-valued indices of refraction. If the TracePro® tool is run on grating structures that have complex substrate indices of refraction, the imaginary part is ignored on the second run through the parameter set.

20.1 TracePro® Run Example

1. Start a new GSolver top-level window by opening GSolver, or by clicking on File→New)
2. Define a grating structure using the Editor tools and click on the Approximation button in the usual manner.
3. Click on the RUN tab.
4. Click on the menu item Tools→TracePro→Setup/Run
5. The following Dialog should now be showing



This dialog lists the parameter settings that will be executed in the TracePro® run.

1. Set the various parameters to the desired values
2. Click OK to continue
3. GSolver estimates the number of calls needed to complete the loop and reports the result in a dialog. Click OK.
4. When the first set of loop conditions are completed, a second dialog pops up asking if the user wishes to invert the grating and complete the second set of loop conditions. Click OK.
5. On completion, a file dialog pops up. Enter the name of the text file in which to record the results. If that file already exists, the contents are over written.

21 References

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