

A Guide for Designing with Spherical Gradient-Index Materials Constrained to Real Material Properties in Code V

Written by Peter McCarthy
University of Rochester

I. Material Model

The gradient-index material model assumes a smooth change in composition from one homogeneous material to another. Any two-component GRIN system can be modeled with these tools. The refractive index is represented as

$$n = n_1 + C_2(n_2 - n_1),$$

where n_1 is the refractive index of material one and C_2 is the fractional concentration of material two (ranging from zero to one). This linear relationship is not strictly true for all materials, but it is a useful approximation for modeling the material properties.

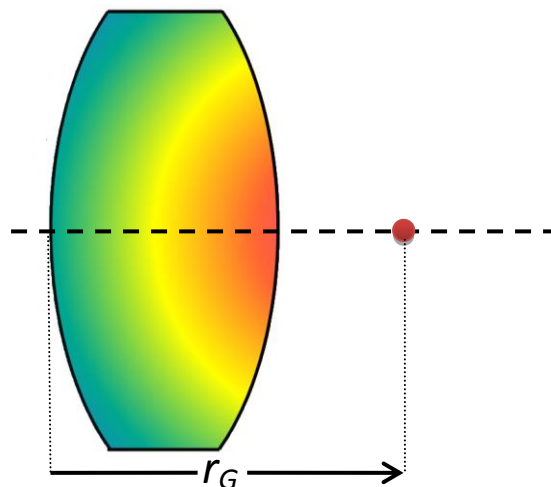
The refractive index distribution is given the usual polynomial expansion representation. For spherical gradients, this is

$$n(\rho) = N_0 + N_1\rho + N_2\rho^2 + N_3\rho^3 + N_4\rho^4,$$

where

$$\rho = \sqrt{x^2 + y^2 + (z - r_G)^2}.$$

The center of curvature of the spherical GRIN is located a distance r_G from the origin along the z-axis as shown in the figure below.



One can also consider the composition profile of the material

$$C(\rho) = C_0 + C_1\rho + C_2\rho^2 + C_3\rho^3 + C_4\rho^4.$$

For a given composition profile, the refractive index profile is fixed for all wavelengths based on the linear model of index vs. composition. However, the standard implementation of gradient-index materials in Code V uses the index function representation. As such, it is essential for the designer to ensure the index profile at different wavelengths agrees with the real material properties. The following sections of this document describe a set of tools to accomplish this task.

II. Entering a GRIN Profile in Code V

Currently the built-in spherical GRIN type in Code V does not allow for the coefficients of the GRIN profile to be fully constrained due to a known bug. As such, the University of Rochester has written a user-defined GRIN for the spherical geometry. The functional form and implementation are similar to the built-in spherical GRIN except that it now requires a dynamic link library (.dll) file to properly trace rays.

The bulk of the design tools are contained within one Excel spreadsheet. This file contains material properties for several possible GRIN materials as well as the constraints for optimization in Code V. The first worksheet of the Excel file, “Material Properties”, contains the material properties for several candidate GRIN materials, including ALON, ZnS/ZnSe, PMMA-Polystyrene, and a Titania-Silicate GRIN glass. For a given material the spreadsheet looks like this:

PMMA-Polystyrene	Wavelength (um)	0.656273	0.587562	0.486133	0	0	0	0	0	0	0
Index measurements in literature from 435.8 nm to 1064 nm	n2-n1	0.097317	0.100302	0.108296	1	1	1	1	1	1	1
	n1	1.487957	1.491402	1.497298	1	1	1	1	1	1	1

The cells that are highlighted in yellow indicate fields that require user input. The user can enter up to ten wavelengths (in microns, ordered from longest to shortest). The first three wavelengths are required and the remaining seven are optional. Use a value of zero for any wavelength you do not wish to use. The values for n_1 and n_2 are calculated based on the material and the wavelengths chosen. New materials combinations can be added if the dispersion formulae for the two homogeneous materials are known. Keep in mind that manufacturing limitations should also be considered.

The second worksheet, “Create New Materials”, includes the framework for adding new GRIN materials, as well as a way to easily select the materials for n_1 and n_2 from a drop-down menu. New homogeneous materials can be added to the available choices by simply inserting a Sellmeier equation (or equivalent dispersion fit) in the same manner that the existing materials are defined.

		Wavelength (um)	5	4	3	2	1	0	0	0	0	0
Material 1	ZnS	n2-n1	0.183140797	0.181188	0.180271	0.181528	0.195987	0	0	0	0	0
Material 2	ZnSe	n1	2.246386391	2.251971	2.257308	2.264671	2.292837	1	1	1	1	1

Second Material
 Select GRIN material
 endpoint from the
 list.

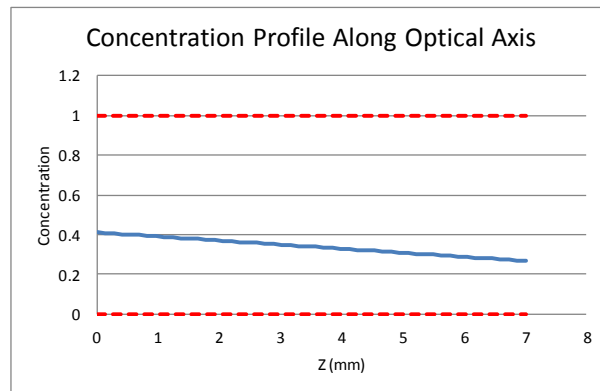
Once the desired material and wavelengths have been selected, the user should copy the wavelength, n_2-n_1 , and n_1 data and paste it in the fourth worksheet of the file (“Spherical GRIN Controls”) as seen below.

Material Data:	Wavelength (um)	0.6562725	0.5875618	0.4861327	0	0	0	0	0	0
$n = (n_2-n_1) * (\text{Concentration}) + n_1$	n2-n1	0.0973169	0.100302084	0.108296359	1	1	1	1	1	1
	n1	1.4879565	1.491402003	1.497297857	1	1	1	1	1	1

From here, the next step is to input the GRIN profile that you wish to start with. Again, cells that are highlighted and outlined in bold require user input. The controls for the starting profile include the concentration at $\rho = 0$ and the index polynomial coefficients (N_1, N_2, N_3, N_4) at the longest wavelength. The location of the GRIN center of curvature is represented as a curvature value, or $1/r_G$. This curvature is represented with the C5 coefficient in Code V.

Input initial GRIN profile		Refractive Index									
		Concentration	0.6562725 um	0.5875618 um	0.4861327 um	0 um	0 um	0 um	0 um	0 um	0 um
At $\rho = 0$	0	1.487956538	1.491402003	1.497297857	1	1	1	1	1	1	
Maximum	4.1103E-01	1.527956538	1.532629007	1.541810735	1.411028389	1.411028389	1.411028389	1.411028389	1.4110E+00	1.411028389	
Minimum	0.2672	1.513956538	1.518199556	1.526231228	1.267168453	1.267168453	1.267168453	1.267168453	1.2671685	1.267168453	
	$ \Delta n $	1.400E-02	1.443E-02	1.558E-02	1.439E-01	1.439E-01	1.439E-01	1.439E-01	1.439E-01	1.439E-01	
	Vary Coefficient? (yes or no)										
n_0	yes	1.487956538	1.491402003	1.497297857	1	1	1	1	1	1	
n_1	yes	2.0000E-03	2.0614E-03	2.2256E-03	2.0551E-02	2.0551E-02	2.0551E-02	2.0551E-02	2.0551E-02	2.0551E-02	
n_2	yes	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
n_3	yes	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
n_4	yes	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	
c (GRIN CoC)	yes	5.00E-02									
r_G (1/c)			20								

A plot of the concentration profile along the optical axis is provided so the user can make sure the profile is within the material bounds (usually zero to one). There is a thickness input which controls the z-axis limits for the plot.



The user can also control whether the coefficients are varied during optimization in Code V by inputting “yes” or “no” in the appropriate boxes.

Below the profile controls, the Abbe numbers of the N_0 term and of the GRIN are calculated.

Based on 0.486, 0.587, 0.656 um	
V0 =	52.62892977
VGRIN =	9.133838404

Next, the user has control over the concentration bounds of the material (C_2 from section I above). For example, with a PMMA-Polystyrene gradient the physical material bounds are between zero and one. If a manufacturing process is not able to achieve that full composition change, then the designer would change those appropriately (for example, make them 0.1 to 0.9). When using the gradient ALON, there is some flexibility here. The composition range of zero to one represents the range of composition that has been fabricated in a set of homogeneous ALON samples. However, GRIN samples have been made with an effective composition range of -1.64 to 1.57. These values are reasonable for the designer to use. This tool allows the designer to change these limits and explore the design space, in turn motivating further development of the ALON GRIN material.

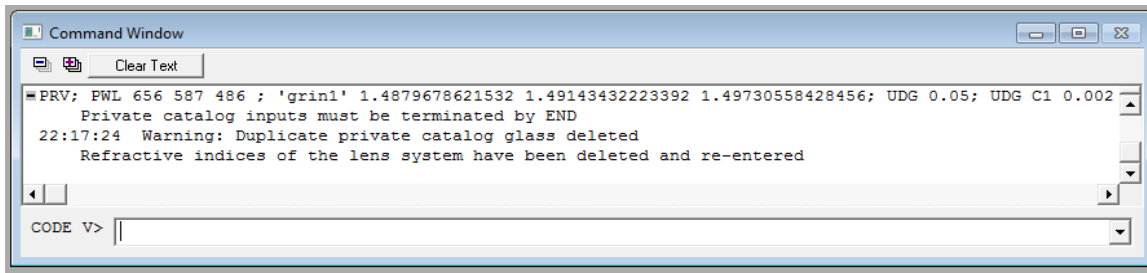
Minimum concentration	0	Constrain concentration to be within these manufacturable limits
Maximum concentration	1	Should be (0,1) for all real materials, and ALON can safely be pushed to (-1.64,1.57)

The last user-entered values relate to inserting this gradient profile into Code V. The “Element ID” field is used to name the private catalog glass. The ID can be a number or it can be up to four characters that describe the GRIN material (for example “pmma” or “ALON”). This same name also must be given to the surface that contains the GRIN material. For example, if the user enters “3” for the element ID then the private catalog glass is titled ‘grin3’ and the surface that contains this material must also be labeled grin3. If the element ID is “pmma” then the private catalog glass is titled ‘grinpmma’ and the surface must be labeled grinpmma. The last user input is the step size (in mm) for the ray tracing calculation. A smaller value will be more accurate but require longer processing time. The designer should ensure that the step size is small enough so it is not introducing ray trace errors. This can be checked by tracing a real ray through the lens system and monitoring how its output height changes with step size. The step size can be changed in the “Surface Properties” section of the Code V GUI.

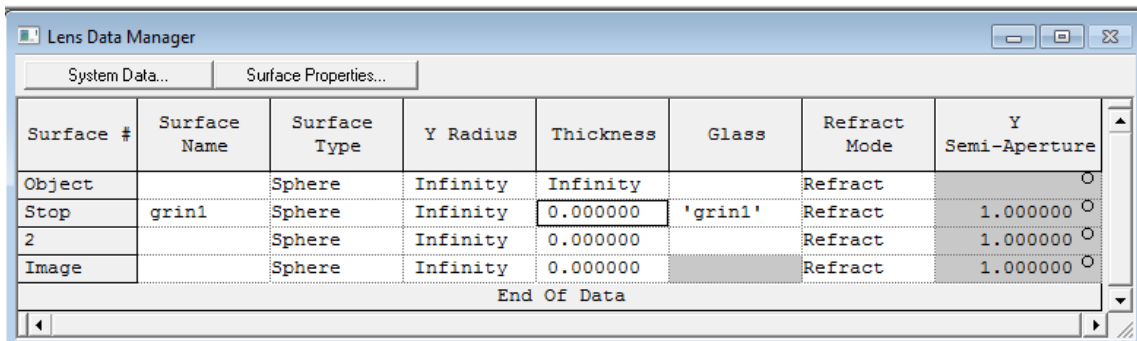
Create private catalog GRIN	Element ID	1	step size	0.05
	Note: Can't be more than 4 characters			

After all user input fields have been entered, there is a cell that contains a list of commands that create the private catalog glass with the given profile and material properties. This list of commands should be copied and pasted into the Code V command window.

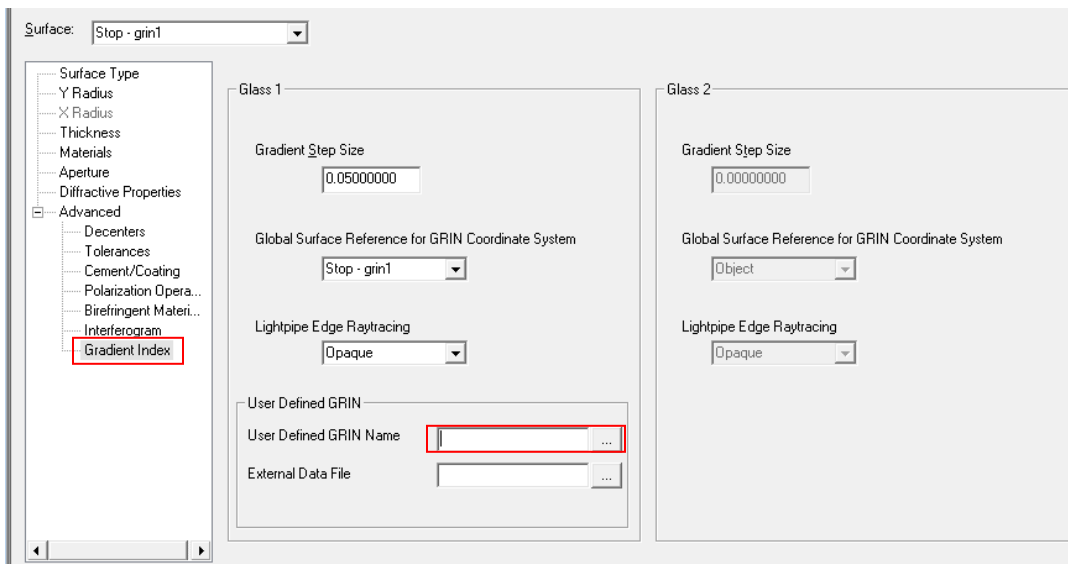
Use the following commands for user defined gradient (UDG) in CodeV (requires .dll)
PRV; PWL 656 587 486 ; 'grin1' 1.4879678621532 1.49143432223392 1.49730558428456; UDG 0.05; UDG C1 0.002 0.00206175472975232 0.00222572708631239;



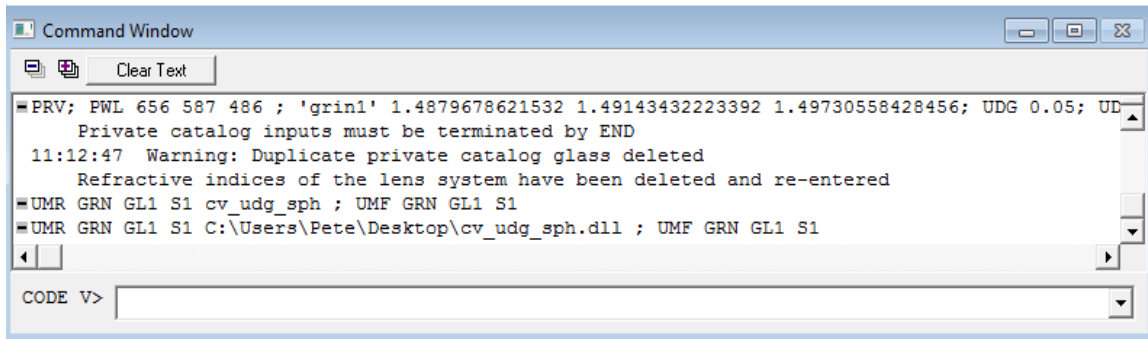
To assign the new GRIN material to one of the surfaces, simply enter the private catalog glass name in the lens data manager. Remember, again, to also label the surface with the same name.



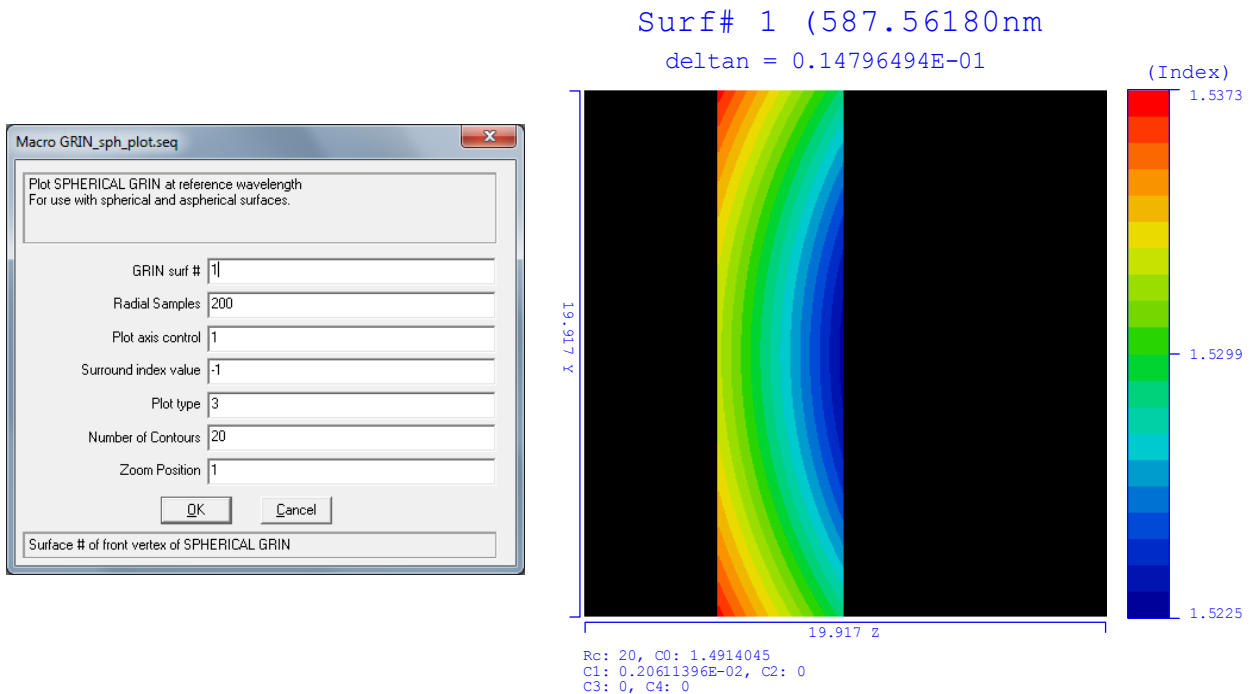
Since the GRIN material that has been defined is a UDG, or user-defined GRIN, the user needs to tell Code V how to trace rays through this material by pointing to the .dll file. The spherical GRIN .dll file is called “cv_udg_sph.dll”. Once the GRIN material has been applied to a surface there are several ways to link to the .dll file. The most straightforward is by using the GUI. Go to the surface properties of the GRIN surface and find the “Gradient Index” field under “Advanced”. If the .dll file is located in the current working directory (check with “eva(cd)”), you can simply type “cv_udg_sph” into the User Defined GRIN Name dialog box.



The .dll can also be loaded by pressing the button with the three dots and browsing for the location of the .dll file. The last method of applying the .dll is to use the command prompt. Issue the command “UMR GRN GL1 S# cv_udg_sph ; UMF GRN GL1 S#” if the .dll file is in the current working directory. Or issue the command “UMR GRN GL1 S# C:\File Location\cv_udg_sph.dll; UMF GRN GL1 S#”. Both of these commands are demonstrated in the figure below for applying the .dll to surface 1. Rays will not trace if the .dll is not loaded properly.



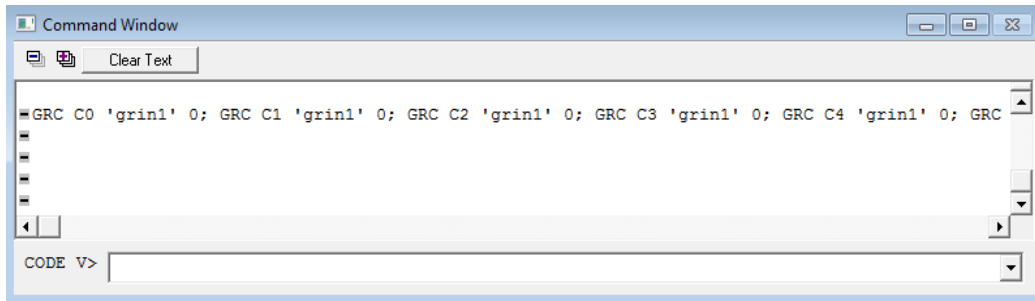
The designer can view the index profile by running the accompanying macro file “GRIN_sph_plot.seq”. The user must indicate the surface, number of samples in the radial dimension, plot axis aspect ratio control, the value to plot in the background, plot type, number of contours, and zoom position.



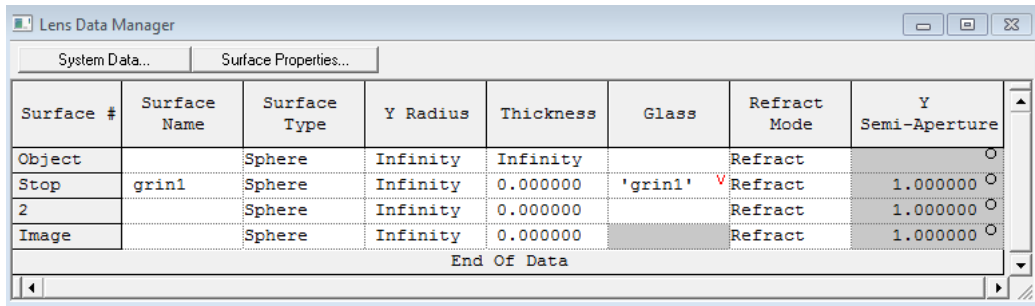
This material with the entered profile can be used in a design just as any other private catalog glass. This is useful for doing polychromatic evaluation of a profile that has been manufactured and measured. The next section covers the basics of optimizing the coefficients of the index polynomial.

III. Optimizing the GRIN Coefficients in Code V

The Excel spreadsheet contains an additional command to vary the GRIN profile coefficients. This should be copied and pasted into the Code V command window. Alternatively, the command can be placed before the AUT command in the optimization sequence file so that it is clear which coefficients are varying for every use of the optimization file.



Now the index profile coefficients at all wavelengths can vary. This can be seen by the small “v” in the lens data manager.



The Excel file creates a list of constraints (over 100 lines) that must be copied and pasted into a .seq file for optimization in Code V.

Creat Optimization Constraints							
! CONSTRAINTS FOR OPTIMIZING SPHERICAL GRADIENT WITH RHO^1, RHO^2, RHO^3, and RHO^4 TERMS ON ELEMENT grin1							
! ADAPTED FROM CODE WRITTEN BY PETER MCCARTHY BY JAMES CORSETTI ON JULY 18 2012							
! Define gradient coefficients at all wavelengths							
@N0_10_1 ==	(GRN C0 S'grin1' W1)						
@N0_9_1 ==	(GRN C0 S'grin1' W2)						
@N0_8_1 ==	(GRN C0 S'grin1' W3)						

This optimization file should also contain any other constraints needed for the designer’s system, including focal length, thickness, etc.

```

GRC C0 'grin1' 0;
GRC C1 'grin1' 0;
GRC C2 'grin1' 0;
GRC C3 'grin1' 0;
GRC C4 'grin1' 0;
GRC C5 'grin1' 0

AUT
INT Y
DRA S1..I

EFL = 100
CT S'grin1' > 2 < 10
ET S'grin1' > 1 < 5

! CONSTRAINTS FOR OPTIMIZING SPHERICAL GRADIENT WITH RHO^1, RHO^2, RHO^3, and RHO^4 TERMS ON ELEM
! ADAPTED FROM CODE WRITTEN BY PETER MCCARTHY BY JAMES CORSETTI ON JULY 18 2012
! Define gradient coefficients at all wavelengths
@N0_10_1 == (GRN C0 S'grin1' W1)
@N0_9_1 == (GRN C0 S'grin1' W2)
@N0_8_1 == (GRN C0 S'grin1' W3)
@N10_10_1 == (GRN C1 S'grin1' W1)
@N10_9_1 == (GRN C1 S'grin1' W2)
@N10_8_1 == (GRN C1 S'grin1' W3)
@N20_10_1 == (GRN C2 S'grin1' W1)
@N20_9_1 == (GRN C2 S'grin1' W2)
@N20_8_1 == (GRN C2 S'grin1' W3)
@N30_10_1 == (GRN C3 S'grin1' W1)
@N30_9_1 == (GRN C3 S'grin1' W2)
@N30_8_1 == (GRN C3 S'grin1' W3)
@N40_10_1 == (GRN C4 S'grin1' W1)

```

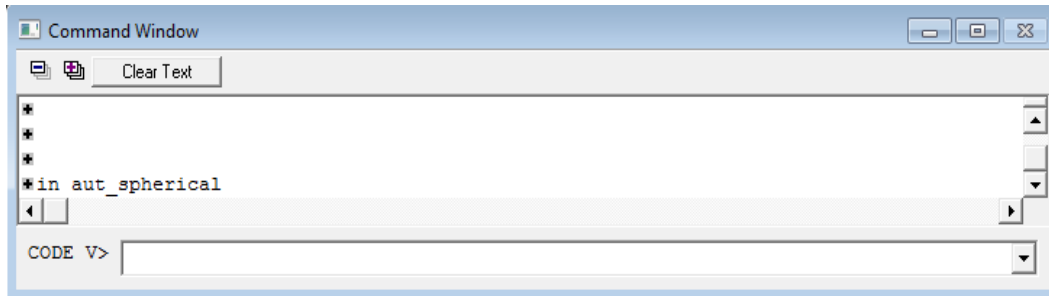
There is a constraint on the location of the GRIN center of curvature that the user may wish to modify. The variable “@grnCoCtol_1” is a number that defines how close the center of curvature can get to either surface of the lens for “grin1”. In the example below, this constraint will keep the center of curvature greater than 10mm away from the lens surfaces. This constraint is imposed for the typical manufacturing processes for spherical GRIN materials, but it can be modified or removed if desired.

```

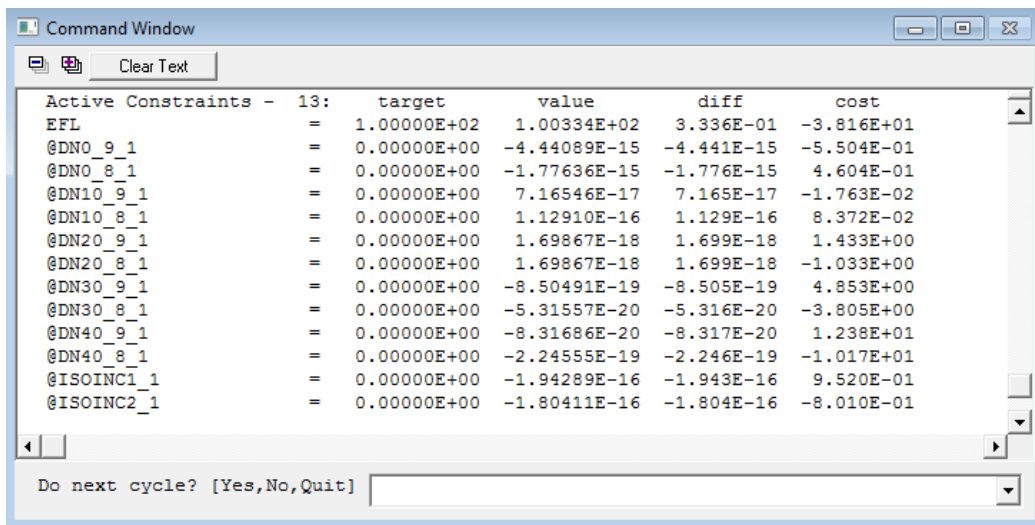
! Constrain center of isoindicial surfaces to be outside of lens. (
! These constraints can be removed if the GRIN center of curvature
@grnCoCtol_1 == 10
@grnCoC_1 == ((CT S'grin1'))/((@grnCoCtol_1) + 0.5*(CT S'grin1'))-
@grnCoC_1 > 0

```

The lens can now be optimized while maintaining the correct dispersion properties. It is essential that the wavelengths used in the lens file are the same as those used when creating the optimization constraints because each user-defined constraint is tied to the material properties at a specific wavelength.



During the optimization process, it is important to monitor the constraints on the GRIN coefficients. Each coefficient is scaled by the appropriate power of the radius so that the value of the user-defined constraint is in Δn space.



In the example above, the GRIN coefficient constraints are all of order 10^{-15} or smaller, which is very well constrained. The designer should be concerned when the magnitudes of these constraints are larger than 10^{-8} . In cases where the constraints are not being obeyed, there are two options the designer can use to gain more control over the optimization. The first is changing the derivative type from default to finite differences, and the second is changing the update interval for the GRIN variable derivative increments. First, it is necessary to attain a list of all variables in the system so the designer can identify which ones correspond to gradient coefficients. This is done with the “DER LIS” command.

```

Command Window
Clear Text
=der lis

VARIABLE LIST
NO  DER INCREMENTS  INCREMENT TYPE  REFRESH  UPDATE  FREEZE  PARAMETERS *
1   0.20349E-04     def      -      -      yes     no      CUY S1      CU
2   0.20867E-04     def      -      -      yes     no      CUY S2
3   0.47362E-01     def      -      -      yes     no      THI S1
4   0.47362E-01     def      -      -      yes     no      THI S2
5   0.20261E-04     def      -      -      yes     no      GRN W1 'grin1'
6   0.20261E-04     def      -      -      yes     no      GRN W2 'grin1'
7   0.20261E-04     def      -      -      yes     no      GRN W3 'grin1'
8   0.20261E-04     def      -      -      yes     no      UDG C1 W1 'grin1'
9   0.20261E-04     def      -      -      yes     no      UDG C1 W2 'grin1'
10  0.20261E-04     def      -      -      yes     no      UDG C1 W3 'grin1'
11  0.20261E-04     def      -      -      yes     no      UDG C2 W1 'grin1'
12  0.20261E-04     def      -      -      yes     no      UDG C2 W2 'grin1'
13  0.20261E-04     def      -      -      yes     no      UDG C2 W3 'grin1'
14  0.20261E-04     def      -      -      yes     no      UDG C3 W1 'grin1'
15  0.20261E-04     def      -      -      yes     no      UDG C3 W2 'grin1'
16  0.20261E-04     def      -      -      yes     no      UDG C3 W3 'grin1'
17  0.20261E-04     def      -      -      yes     no      UDG C4 W1 'grin1'
18  0.20261E-04     def      -      -      yes     no      UDG C4 W2 'grin1'
19  0.20261E-04     def      -      -      yes     no      UDG C4 W3 'grin1'
20  0.20261E-04     def      -      -      yes     no      UDG C5 W1 'grin1'
21  0.20261E-04     def      -      -      yes     no      UDG C5 W2 'grin1'
22  0.20261E-04     def      -      -      yes     no      UDG C5 W3 'grin1'

CODE V>

```

In this example, the variables starting at number 5 and going all the way down to number 22 are associated with the gradient. Now, to change the derivative update interval, use the command “DER i5..22 DRC #”, where # is how often you want the derivatives recomputed. For example, use “DER i5..22 DRC 1” to update the derivatives after every optimization iteration. Note that the optimization will be noticeably slower when using DRC 1. To change the derivative type to finite differences issue the command “DER i5..22 FDF”. Now you can see that the GRIN variables have been changed.

```

Command Window
Clear Text
=der lis

VARIABLE LIST
NO  DER INCREMENTS  INCREMENT TYPE  REFRESH  UPDATE  FREEZE  PARAMETERS *
1   0.20349E-04     def      -      -      yes     no      CUY S1      CU
2   0.20867E-04     def      -      -      yes     no      CUY S2
3   0.47362E-01     def      -      -      yes     no      THI S1
4   0.47362E-01     def      -      -      yes     no      THI S2
5   -              FDF      -      -      yes     no      GRN W1 'grin1'
6   -              FDF      -      -      yes     no      GRN W2 'grin1'
7   -              FDF      -      -      yes     no      GRN W3 'grin1'
8   -              FDF      -      -      yes     no      UDG C1 W1 'grin1'
9   -              FDF      -      -      yes     no      UDG C1 W2 'grin1'
10  -              FDF      -      -      yes     no      UDG C1 W3 'grin1'
11  -              FDF      -      -      yes     no      UDG C2 W1 'grin1'
12  -              FDF      -      -      yes     no      UDG C2 W2 'grin1'
13  -              FDF      -      -      yes     no      UDG C2 W3 'grin1'
14  -              FDF      -      -      yes     no      UDG C3 W1 'grin1'
15  -              FDF      -      -      yes     no      UDG C3 W2 'grin1'
16  -              FDF      -      -      yes     no      UDG C3 W3 'grin1'

CODE V>

```

It can also be instructive to monitor the location of the GRIN center of curvature during optimization. This can be done with the following commands in the optimization sequence file:

```
@GRINradius == 1/(GRN C5 s'grin1' w1)
dsp @GRINradius
```

Now the variable, @GRINradius, will be displayed at every cycle of optimization.

```
Display-only Constraints:  value
@GRINRADIUS              =  2.06093E+01
```

A GRIN element can be optimized inside a more complicated multi-element system by following this same procedure. Additionally, multiple GRIN elements can be optimized in the same lens system, provided they are given different element ID's when creating the constraints. When using multiple gradient materials, it is good practice to use a descriptive ID or comment in the optimization file what the materials are for each GRIN element. These tools will also allow the designer to constrain a GRIN element when using the new Glass Expert feature in Code V. Note that Glass Expert cannot insert a GRIN element into the system, but it will constrain an existing GRIN while it searches for better homogeneous materials in other elements. Early versions of Glass Expert had some issues with changing the user-set derivative properties of the GRIN variables. The designer should make sure that the GRIN constraints are being obeyed.

IV. Quick Start Guide

1. In the “Material Properties” or “Create New Materials” worksheets of the Excel file, choose which material and wavelengths you wish to use.
 - a. Use at least 3 wavelengths and as many as 10. Enter a value of zero for any wavelengths you don't wish to use.
 - b. List wavelengths from longest to shortest.
2. Copy and paste wavelength, n_2 - n_1 , and n_1 values into the top of the “Spherical GRIN Controls” worksheet.
3. Input initial GRIN profile.
 - a. Select concentration at $\rho = 0$ and the polynomial coefficients at the longest wavelength.
 - b. Use the thickness of the lens and the plot of the concentration profile to ensure your starting position is within the material bounds.
 - c. First-order properties can be monitored.
4. Input optimization controls.
 - a. Determine which coefficients you wish to vary during optimization.
 - b. Enter upper and lower concentration bounds based on real material properties.
 - c. Enter element ID (limited to 4 characters).
 - d. Enter ray trace step size.
5. Insert initial GRIN profile into Code V.
 - a. Copy the command that starts with “PRV; PWL” and paste it into the Code V command window.

- b. If you wish to optimize the GRIN profile, also copy and paste the command that starts with “GRC”.
 - c. In the lens data manager, change the material to the correct private catalog glass ‘grinID’, where *ID* is the (less than 4 character) ID you entered in Excel.
 - d. Label the surface with the same name, grinID.
 - e. Load the .dll file either through the surface properties GUI or the command line. For best results place .dll file in current working directory.
6. Copy and paste optimization constraints into a sequence file with any other constraints needed for the lens system.
7. Optimize the system as you normally would by loading in the .seq file.
 - a. Use the same wavelengths in Code V as you did when you created the optimization constraints.
 - b. Monitor the user-defined constraints for the GRIN profile and adjust the derivatives appropriately.
 - c. View the index profile plot periodically.
 - d. Change the derivative type to FDF or change the derivative increment to improve optimization behavior.

V. Caveats and Warnings

1. Ray trace errors may occur when the center of curvature of the GRIN is inside the element or very close to one of the element’s surfaces. This is caused by the linear term of the index profile which introduces a discontinuity in the index derivative at the center of curvature.
 - a. This can result in incorrect first-order calculations and other analyses.
 - b. This can be mitigated by setting the linear coefficient, N_1 , to zero, or by placing the center of curvature safely outside the lens (larger than the raytrace step size).
2. The C5 variable, or r_G , can be difficult to control during optimization. It can often be very slow to converge to a good solution.
 - a. Manually moving the center of curvature can be helpful in the initial optimization stages.
 - b. The constraint that prevents the center of curvature from moving inside the lens element does allow for the center of curvature to move from one side of the element to the other. However, the optimizer may not always be able to push it from one side to another. It is recommended to check for solutions with the center of curvature to the left and to the right of the GRIN element.
3. Code V 10.6 made a change to the predefined INDEX function. Code V version 10.5 and earlier are unaffected. From the 10.6 release notes:

"The behavior of the INDEX macro function has been changed. The input (X, Y, Z) coordinates now refer to the global reference surface coordinate system defined with the GGS command rather than the local surface coordinates."

- a. The INDEX function is used in the constraints to make sure the index values within the lens element are constrained within the material bounds. It is also used in the plotting macros.
 - b. This is only an issue if you change the reference coordinate system for the GRIN to be a surface other than the GRIN surface.
 - c. For small shifts of the GGS surface relative to the GRIN surface, the existing constraints might be tolerable.
 - d. For a workaround in version 10.6 please contact the UR GRIN group.
4. The refractive index data in the Excel file is either from literature sources or it has been measured at University of Rochester. Verify that the index data is appropriate for the materials you are using.
 5. These constraints are based on a linear material model, which may not be the most accurate model for all GRIN materials. Users need to verify that this model adequately describes their materials of interest.