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Theory documentation for software to control the pgII phiro2 automated sample mount and analyzing data obtained

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Abstract

The phiro2 sample holder is a device used for controlling the angle of incidence for anisotropic samples with the pgII photogoniometer.

The first topic covered is how to control the instrument using the `allmess` command line tool which allows the measurement sequence to be more flexible than the `pgc` GUI tool usually used for control. A method to monitor drift over long measurement sessions is also covered. Tangential to this is several syntax examples of how bash shell script is used to call `allmess`. Code to generate bash scripts for samples with different degree of symmetry is discussed as well as how to modify a script to continue from a certain point if a measurement was aborted.

The second half of the document describes how to access the data and compile the data into the Klems XML format. A path for future combination with the Radiance interpolation format is also given.

Finally verification and visualization of BSDF data is discussed.

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1 Introduction

When the pgII goniophotometer was purchased by LBNL in 2009 it was believed that it would be used to measure material properties and that those measured properties would be fed with a geometry into a raytracing tool to obtain the bi-directional scattering distribution function (BSDF) of any window or façade element. That approach assumed that the materials studied would have a full rotational symmetry, e.g. single color Venetian blind slats, diffuse laminates, and fritted glass. For such samples only 9 out of the 145 angles of incidence in the Klems coordinate system has to be measured and all the others can be calculated through rotation of those nine. This could be accomplished by rotating the sample around a single axis.

The assumption that materials would be studied and geometries raytraced has failed on two fronts since the instrument was obtained. Raytracing tools are limited to ray optics, and phenomena like diffraction, that require wave optics to describe them, cannot be accurately modeled using that method. The pgII goniophotometer was used to characterize shape-shifting diffraction gratings as part of an LBNL LDRD (laboratory directed research and development) project in 2012. The sample could only be characterized at a limited number of angles of incidence, but in this case it was enough since the goal was to see if the shape-shifting occurred rather than to use the result for running building and daylighting simulations. In addition to studying wave optics there has also been a need to verify that a manufactured material behaves in the way that it was designed to to. So even for a material that can be modeled using ray optics it is still important to be able to confirm behavior of produced materials.

With the procurement of a novel sample holder that enables measurement of the BSDF at an arbitrary angle of incidence, thanks to allowing sample rotation around two axis, it became possible to automate measurements of complete BSDFs without rotational symmetry at LBNL. The sample holder is unique in the world, neither PAB who makes it or any other pgII owner has one so the amount of shared user knowledge is non-existent. One of the first choices that was made was to move away from the graphical user interface and instead use the command-line tool. Scripting calls to the command line tool allows for varying theta steps and theta dependent phi steps which is crucial to describe the Klems coordinate system. It also allows for easy continuation of an interrupted measurement series, more a convenience than a necessity but it does save a lot of time to not have to start over from scratch when a week long measurement failed half-way through.

This document details the different steps with which the controls were tailored to the needs of LBNL and also describe post processing of the data. Finally visualization and verification of BSDF data is discussed.

2 pgII command-line tool – `allmess`

All the options available are given in table 1. The most important options will be discussed in this section. In addition to calling `allmess` with the correct options and flags it is

important to set the GUI tool `pgc` in the correct state. Sect 2.8 in the *pgII* manual states that `pgc` is started and used to set the instrument in the run state. After that is important to select the `pgc` measurement tab to avoid the interaction between the manual control and the instrument interfering with the measurement.

Option	Function
<code>-acp index</code>	number of sample place in auto changer (default 0)
<code>-beam id</code>	beam-shape id (as in database)
<code>-com string</code>	comment
<code>-filterlamp id</code>	id of filter at lamp (as in database)
<code>-filterdet id</code>	id of filter at detector (as in database)
<code>-intheta</code>	incident angle theta
<code>-inphi</code>	incident angle phi
<code>-slabel strng</code>	sample label, (overridden by <code>-sid</code>)
<code>-lamp</code>	number of lamp (as specified in db, default 1)
<code>-mcc mcname</code>	measurement channel control (name in db, default "std-chan0")
<code>-msid id</code>	measurement session id (default -1, start new session)
<code>-pfile file</code>	(default "std-full")
<code>-sid id</code>	sample number
Flags:	
<code>-lampoff</code>	switch off lamp after measurement
<code>-lamppre</code>	get and check for pre-run time of lamp from db
<code>-moff</code>	switch off machine after measurement (does not imply <code>-loff</code>)
<code>-nodb</code>	don't write anything to db, (demo mode)

Table 1: Options of the `allmess` command-line tool

The basic idea is that a sequence of calls to this program is made so that all angles of incidence that are being measured can be measured in sequence without human interaction. This is accomplished by using the bash scripting language.

The two parameters that control the angle of incidence are `--intheta` and `--inphi`, the angles are given in degrees. See section 3 for conversion between *pgII* and Klems coordinates.

The measurement channel control option `--mcc mcname` selects which detector is used. The main choices are `std-chan0` and `std-chan3` for visible and NIR, respectively. This can be expanded with different `mcnames` to improve scan speed at the cost of dynamic range.

The measurement path is defined by the `--pfile file`. This controls the density of the mesh that `fullmeas` covers. The `pfile` is also where the inplane path would have been defined. These files are predefined rather than defined at runtime.

The sample number is important since that controls where in the database that the sample is stored. The definition of samples is done using the web interface to the database.

The `--lamppre` can be set without noticeable penalty and by doing it for all calls reduces the risk that an aborted measurement will be continued with this flag forgotten.

2.1 Preserving the measurement session ID

The `--msid id` is the most intricate part is not the most interesting or important, but it significantly increases the accessibility of the database if it is handled correctly. The in a sequence of `allmess` calls the first one is called with `--msid -1` to pick the next available number in the database. This has to be done in a way so that the id given is stored in a variable that can be accessed for future calls in the bash script.

The `msid` given during the first call is reported in the `stderr` output stream. It is assumed that this is done on a line containing the string 'got msid' and that the new id is the last portion of that line.

The getting access to the `stderr` stream is done by redirecting it to `stdout` which in bash is written as `2> &1`. The result is piped to `grep` to select the line containing `got msid` and finally that line is piped to `sed` (overkill, but it works) to replace the unwanted parts with nothing. The result creates a first call that looks something like

```
mysid="/usr/local/pab_pg/bin/allmess --msid -1
--sid 1 --pfile std-beam-square-5.0 --intheta 0
--mcc std-chan0 --beam 3 --filterlamp 2
--filterdet 2 --lamppre 2>&1 | grep "got msid"
| sed 's/\got msid: //g' "
```

Subsequent calls are simply called with `--msid $mysid`.

3 Converting between Klems and pgII coordinate systems

There is a difference in representation of spherical coordinates between pgII `pgc` and the Klems coordinate system used for BSDF matrices used in WINDOW and Radiance. The range of angles of incidence for the `pgc` are go from 0 to 180 for theta and 0 to 360 for any phi and all these angles are unique with regard to the positioning of the sample.

Four example cases are demonstrated in figure 1. Each case have different points to note:

- a Normal angle of incidence requires no special care. However, `pgc` allows for altering the phi-angle which in reality is undefined for normal angles. This just changes what is up for the sample for this specific measurement and should not be done.
- b Propagating in positive x and z direction in the Klems coordinate system means phi=0.

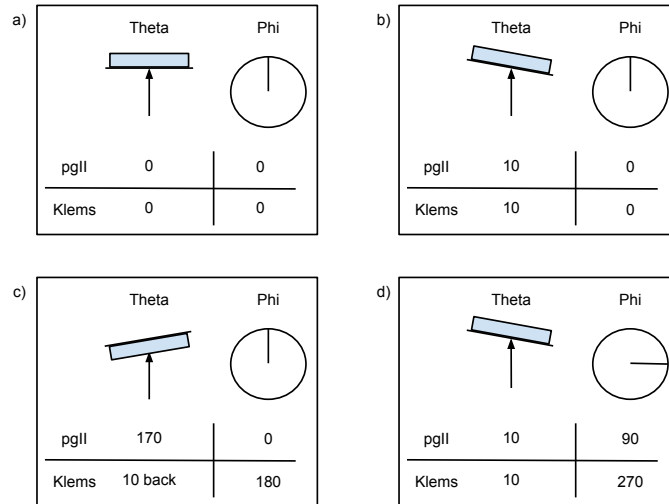


Figure 1: Example of sample configurations in the pgII with its respective theta and phi values for the two different coordinate systems. The for configurations are a) normal angle of incidence, b) 10 degrees from the right, c) 10 degrees from the left incident on the backside of the sample, and d) 10 degrees from above. is no confusion,

- c As theta increases above 90 the beam is instead incident on the back of the sample. The beam is now going to the right which corresponds to phi = 180 in the Klems system. The theta value for Klems is calculated as 180 - theta for pgc . The pgII setup still defines transmittance and reflectance based on the front of the sample requiring a switch of R to T and T to R for the back side measurements.
- d The incident beam is traveling from above towards the sample resulting in a Klems phi-value of 270. As theta increases and the back side is getting measured this angle stays the same.

There is another format on the near horizon for use with angle of incidence interpolation for Radiance's variable resolution coordinate system. This intermediate format could be used to produce a BSDF according to any basis, including the Klems, so being open to work with that system is important.

4 Repeating first measurement to track instrument drift

Without a way to remove the sample from the beam path there is no way to directly track the instrument response in a single beam instrument such as the pgII. The suggested solution is to track drift by repeating the first measurement of the measurement series at some interval.

4.1 Magnitude of drift over multi-day measurements

The reference beam was measured over more than two days with three detector channels, first under regular operating conditions and then a second time with the local air chiller set at 68°F to try to minimize the influence of temperature fluctuations.

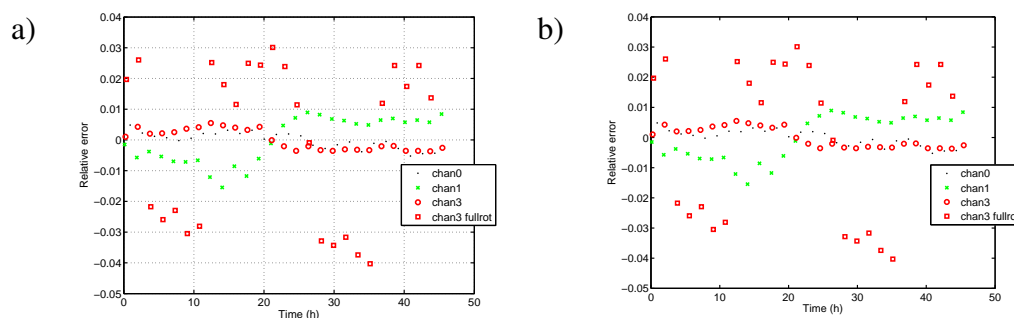


Figure 2: Long time monitoring of the chan0 (vLambda filter), chan1 (Si with hot mirror) and chan3 (InGaAs) reference measurements. The beam was characterized using the square-5 measurement strategy. The NIR channel was characterized using the fullrot measurement strategy as well. The absolute integrated values are shown in a) and relative values calculate in b). This only measurement that has more than $\pm 1\%$ relative variation is the over the whole time.

There are some interesting points shown in figure 2. There is fairly good correlation between chan0 and chan3 indicating that the system drift is mostly due to lamp drift rather than detector. However, chan1 is not following that trend so it is hard to draw any certain conclusions.

The fullrot measurement which is highly influenced by the zero signal fluctuates between two fairly narrow bands. The third measurement point with this channel is the first one of the first low band, it was started at 8.23 pm. Data point number 8 is the first one in the higher band, it was started at 5.05 am.

Further digging into building temperature control indicated that airflow schedule changes at 4 am and 7 pm. Figure 3 shows how the temperature in the room varies over time. A text bar is also shown marking the 4 am to 7 pm time span. The temperature sensor is in the half of the room with the lamp so it separated from the detectors with a heavy curtain. However, air vents are present on both sides of the curtain so the temperature is expected to be following a similar pattern over time.

4.1. Magnitude of drift over multi-day measurements

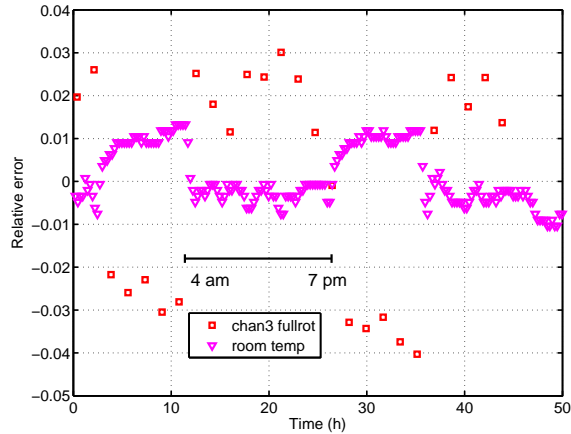


Figure 3: Long time monitoring of the chan3 fullrot and temperature in the room. The absolute temperature variation in the room spanned from 71.3°F to 72.8°F during the period of the measurement.

The local chiller controlling the temperature in rooms 14, 16, and 16A was set to override the temperature in an attempt to keep the temperature stable. However, figure 4 shows how the temperature varies over a period with both building control (up to about hour 80) and with the local chiller operating. The local chiller does not keep the temperature stable, nor does it operate during the night period (7 pm to 4 am).

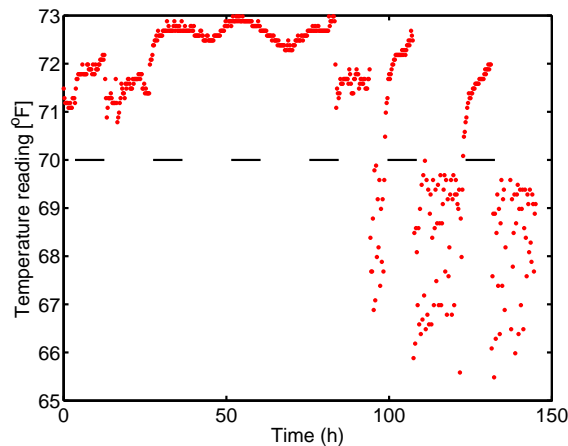


Figure 4: Temperature of room 90-0016A during a six day period. The time the building air fan and heater is shut down (7 pm to 4 am) is marked with black lines at the 70 degree level. At approximately hour 90 the local chiller was set to 68 degrees to keep the temperature stable, instead a larger variation occurred and control was lost during the night time.

4.2 Conclusion and requirements for drift control

The NIR detector seems to have a strong temperature dependence when measuring zero signal, resulting in an integrated value variation of $\pm 2\%$. This is an issue when measuring samples where the BSDF is close to zero in large areas of the angle space. For samples with a reasonable diffuse component this effect is not expected to be present.

There seems like there is only one way to tackle this problem. By adapting to the cycling schedule and avoid measurements between 4 am and 5 am as well as 7 pm and 8 pm. And measuring an already measured angle of incidence at these times before continuing with the required measurements.

5 Data processing

After the measurement has been carried out there are several stages to get the data into an XML file that can be used in WINDOW and Radiance.

5.1 One measurement

The pgII SQL database stores the measurement of each angle of incidence with a single measurement ID (MID). Each MID contains outgoing measured intensity (detector response, not BSDF), for a single angle of incidence, for a single detector, however, it contains both reflected and transmitted data for those conditions. The code to obtain this digitally is hidden in `pabsqlloaddatapr2.m`, that function takes a MID and returns a struct with two matrices containing intensity values for R and T. Each of these matrices contain both theta, phi, and intensity value. The struct furthermore contains information about the channel (detector) used for the measurement. This function is not intended to be used directly, more a low level function.

There are some subtleties with the access of the database. The first would be that some “bad” data is collected and stored, e.g. when the detector arms and head block the incident light. These are marked in the database and have to be omitted from the data set. Furthermore it is recommended to avoid data points that are close to theta equals 90. For the phirot2 sample holder the values within 5 degrees from grazing should not be used due to the shading and high reflectance of the sample holder rim. One of the issues with measured data points at high angles is that the BSDF is proportional to $1/\cos(\theta)$ which goes to infinity at 90 so the detector response must go to $1/\infty$. Few detectors have that dynamic range and some have thermal noise that makes it hard to measure zero. In addition to ignoring some sample the negative values that comes from noisy zero measurements are made physical, but since that adds intensity to the total integrated value some intensity is removed from positive values near zero.

To convert the result into BSDF values the all intensity values have to be divided with the integrated value of the reference beam and divided with the cosine of the outgoing theta-angle. The code to do this is also a low-level function `pabsqlloadmidpr2` which

takes both a sampleMID and the MID for the reference beam. This calls the function mentioned above and in addition to changing the R and T matrices to contain BSDF values instead of intensity, it also adds information about the angle of incidence (in the pgII coordinate system), maximum R, and maximum T.

The process to convert the measured data into the Klems format is the most time consuming part. Perhaps the most important consideration in this transformation is to preserve the direct-hemispherical transmittance and reflectance of the data-set. The Klems basis system is much coarser than the individual points. A typical measurement contains anywhere from 200000 to 600000 data points depending on the measurement strategy. However, due to the scanning behavior of the pgII the density is greater than needed along the scan paths so the first step is to delete points that are not adding a lot of data. This is possible without losing accuracy in the end, think of it as how two points describe a line with close to zero derivative as well as a hundred.

The outline of the process is as follows

1. Project data from the spherical source coordinates θ, φ onto the the Cartesian xy -plane.
2. Create a Voronoi-diagram in the xy -plane.
3. For each patch in the Klems basis, find polygons in the Voronoi-diagram that is fully or partially inside the patch. Polygons partially inside are intersected with the patch and the result is then treated as fully inside.
4. Project the polygon areas back to spherical coordinates and calculate the BSDF of the patch.
5. translate isotropic data obtained at a given θ for a single incident φ -angle to other φ -angles

5.1.1 Creation of a Voronoi diagram

The creation of the Voronoi diagram is the least intuitive part of the process so that is described in more detail here. Voronoi formulated a method using nearest-neighbors to create areas around data points in space. Difficult to put in a compact mathematical form, this method is perhaps best described as a geometrical construction. A two-dimensional Voronoi diagram creates polygons associated to points or sites in a plane. The polygons are defined so that all points in the polygon associated with a certain site are closer to that site than any other site. This also means that the boundaries of the polygons will be equidistant to one or more sites.

Data measured with a goniophotometer are typically described by the the detector position relative the sample normal given in spherical coordinates. These data points are

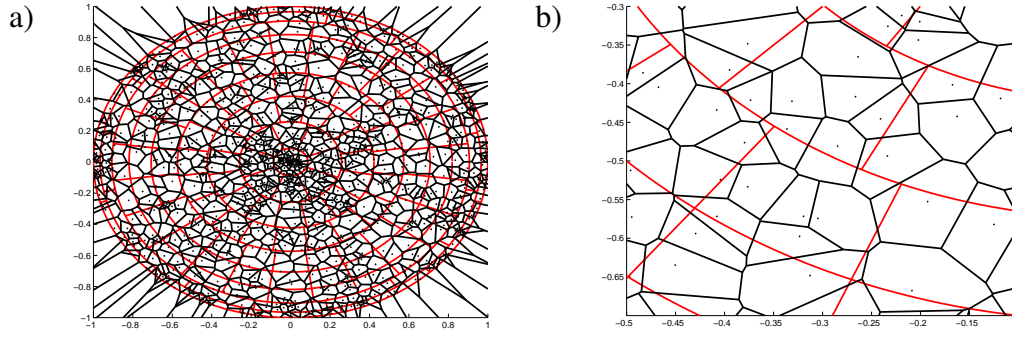


Figure 5: A picture of a 1000 random data points, the black dots, distributed over the hemisphere. The red lines are the Klems patches projected to a 2D surface. The black lines make up the Voronoi diagram for the black dots.

A close-up is shown in b) demonstrating how data points, especially those close to patch borders, have polygons that span over several target patches.

projected onto a plane with a Cartesian coordinate system according to

$$x = \sin \theta \cos \varphi \quad (1)$$

$$y = \sin \theta \sin \varphi. \quad (2)$$

All data points are now inside the unit circle. To avoid getting infinite polygons for the points close to the edge it is easy to mirror the points at the edge in the unit circle so that a boundary will follow the edge of physical values.

An interesting aside is that the Klems coordinate system is not a Voronoi diagram of the data points used to describe the center of the patches in it.

The code for converting a data set to the Klems basis system is hidden in `points2Klems.m` which is called by the functions described in the following section. Since this is a very time-consuming process it is good practice to always save the result from a `points2Klems` call in a data file.

5.2 A group of measurements

If the measurement was carried out correctly all the measurements are stored in the SQL database under the same *measurement session ID*, *MSID*, which can be used to iterate the single measurement process over all the measurements for the sample.

The function `pabsqlmsid2Klems` takes a *MSID* and converts all of the measurements into files with the data in the Klems format. The input arguments are the *MSID* that we want and the *MID* beam reference measurement. At this point it worth to recall that the real reference is a measurement of the beam with out a sample mounted, this is not the same as the drift correction measurements that occur during a scan. If there was a way to automatically remove the sample from the beam line this would be the methodology

of choice but since that is not an option, reflectance of the sample at 10 degrees angle of incidence is remeasured through to quantify the drift, from this the drift in beam intensity can be calculated.

Once all the data has been loaded and trimmed of bad and uninteresting data points the conversion to the Klems coordinate system begins. This is written so that each incident direction is processed on a single core, hence multiple angles of incidence can simultaneously be processed on a multi-core machine.

After each measured dataset has been converted to the Klems basis all these results are used to fill the whole matrix. When there is rotational symmetry in the sample it is now time to mirror and rotate the data for the corresponding incidence angles.

6 Verification and visualization

The BSDFs generated from the pgII measurements can be looked at as a function of multiple variables: angle of incidence ($\theta_{in}, \varphi_{in}$) outgoing angle ($\theta_{out}, \varphi_{out}$), wavelength band, and sample side. Even when fixing the wavelength and sample side it is a 4D function which makes it hard to visualize in a simple graph.

Rather than relying on visual inspection of the data it is important to maximize the amount of numerical verification that can be done before it is inspected by eye.

6.1 Data verification

There are multiple basic checks that can be done to verify that the BSDF is within physical limits. There are two levels to verify the data: first is on the individual level of single BSDF-values for unique combinations of incident and outgoing angle and the second is on complete function level.

On the individual value level it should be noted no single value can be lower than zero. However, in contrast to the classical transmittance and reflectance values for specular samples, the individual BSDF values can be larger than 1. This rises from the definition of the BSDF as a function with unit per steradian.

The energy conservation verification has to happen at a whole function level. For each angle of incidence the direct-hemispherical reflectance and transmittance is calculated. From this the absorption can be calculated just like for classical transmittance and reflectance with the simple relationship of $A = 1 - R_{dh} - T_{dh}$. If the absorption is negative it means that there is not conservation of energy and the reflectance and/or transmittance is to large.

Qualitative verification is harder to define. For most samples the specular reflectance and transmittance will have a significant component but that is not a rule. The goal of many systems is to change that, either by blocking the direct transmittance or redirecting it to go somewhere else. For the reflectance only a smooth surface would require a specular reflection component, something like an array of mirrored Venetian blind slats angled at 45

degrees will not have a strong component in the specular direction. Due to the complexity of the materials studied it is hard to make general rules for quantities like which direction the maximum or minimum value should be. that is part of the usefulness of the BSDF concept, it can describe any scattering profile.

6.2 BSDF Visualization

With knowledge of the sample studied it is possible to look at partial visualizations of the data to see if it makes sense with regards to the scatter direction with the maximum intensity or shape of the scattered light.

Assuming you know approximately what the data should look like the most power is found in an interactive tool such as `BSDF viewer`¹ written by Andrew McNeil at LBNL. However, since you have to interact with it is hard to use for auto-generated reports similar to the ones used in the IGDB peer-reviews.

There are two common way to reduce the 4D nature of the angles used for the BSDF. The first is to integrate the outgoing values over the whole hemisphere to get a direct-hemispherical value for each angle of incidence. One such graph is shown in figure 6. The Klems incident directions on the x-axis go from 1 to 145. The first one is normal angle of incidence, after that each theta-band follows with phi-values going from 0 to 360, and then the next theta band and so forth. This makes it hard to just pick out a profile angle of the sample and learn the transmittance for all theta values along that profile.

¹Available for download at
<https://www.radiance-online.org/download-install/bsdf-viewer>

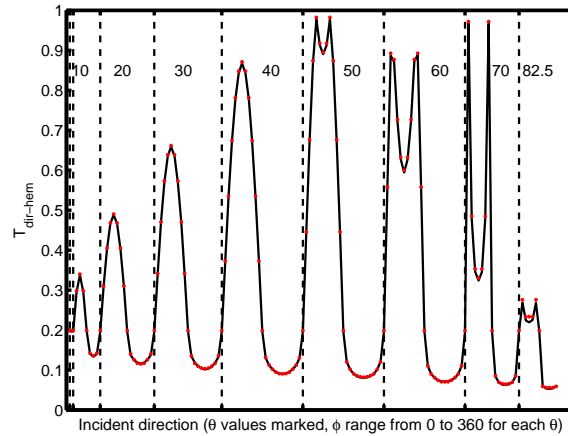


Figure 6: Direct-hemispherical transmittance for each of the 145 angles of incidence in the Klems coordinate system. Each theta-band is labeled in the graph from 10 to 82.5. Within each theta band phi varies from 0 to 360. This means that the first value is incident going left coming from the right, the following rotates clockwise so it is going up coming from below. A quarter through each band means going straight up coming from below, and three quarters through corresponds to going down coming from above. Knowing that, can you guess what kind of sample is being shown in the graph? Correct answers emailed to jcjonsson@lbl.gov are rewarded with a picture of my dog.

As with all overviews there is a loss of detail; a compact way of showing all 145 angles of incidence is convenient from a data point and spotting discrepancies but it is not intuitive to read. The direct-hemispherical value completely deletes all information about the outgoing scattering distribution which makes it hard tell if the sample is Lambertian, specular, or anything in between.

To learn about the two-dimensional outgoing scattering distribution it is common to fix the function to a single incident angle. All the outgoing BSDF values can then be projected on a virtual hemisphere using a false color scale to show the magnitude of each individual outgoing direction. An example of such a plot is shown in figure 7.

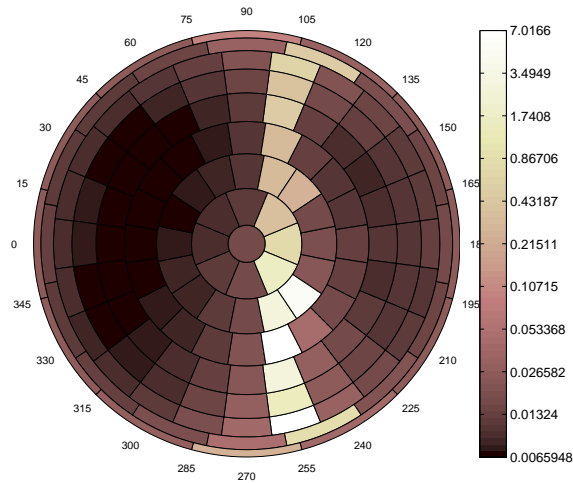


Figure 7: All outgoing BTDF values for a single angle of incidence projected on a virtual hemisphere. The false color values show the BSDF value (in unit sr^{-1}) on a logarithmic scale. Without a logarithmic scale it is hard to see the scattering due to the dynamic range of the BSDF.

This shows the scattering pattern generated for light incident at this specific angle of incidence. It gives the detailed information about how light is distributed over the outgoing hemisphere. One variant to plotting the BSDF values on the false color scale is to integrate the BSDF over the patch to generate a ratio of how much of the incident light that was transmitted through that patch.

Other specialized visualization methods can be tailored to specific materials. An example could be visualization of light-redirecting materials whose purpose is to redirect light above the horizon. In such a scenario it is relevant to take a cross section of a single outgoing plane, such as the vertical axis, it is demonstrated in figure 8.

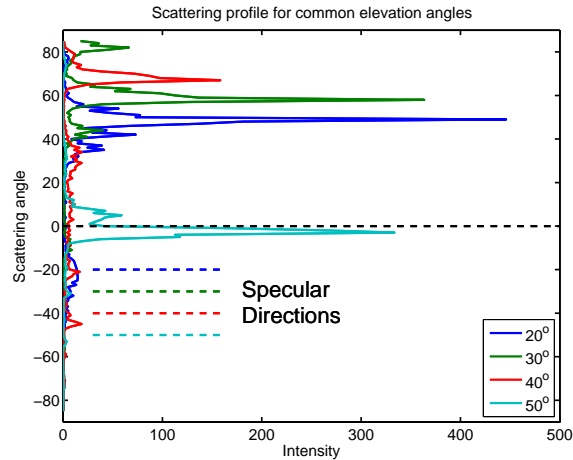


Figure 8: Scattering intensity for a vertical cross section of the the outgoing hemisphere for four different angles of incidence. The specular directions are all marked as dashed lines for the four incident angles. The horizon is marked as a black dashed line. Positive scattering angles signify light scattered over the horizon and negative below the horizon. For all incident angles but the 50 degree one, the light is redirected well above the horizon. The specular component is very small compared to the redirected peaks.

One obvious advantage of this graph is that we can compare multiple angles of incidence in the same graph, something that is not possible with the projection on the virtual hemisphere. However, this visualization would make little sense to use to look at data of e.g. a piece of fritted glass.

As a conclusion to the visualization part of this document it is relevant to remember that the BSDF is a function that is hard to describe in fewer than four dimensions. The correct way to slice those dimensions depends on the sample being studied and what behavior is of interest. Even though the methods described here are considered useful it is important that you do not limit yourself to only these methods if they do not tell the story you are after.

7 Conclusions and future work

The current state of the code is that the chain works but it is not automatic. However, having manual steps allows for dealing with issues such as if the instrument crashed and the format of the data set is not the expected.

Greg Ward's work with interpolation of BSDFs shows a promising general purpose format to store BSDF data in. Being able to automate generation of the Gaussian basis sets that it uses is a goal for the near future. Greg's code is written to handle symmetry so those steps can be removed, however, they expect text-file input so rather than making Klems basis data files there would be a need to generate data files with all measured points in them.

Right now there is no correction built in for the drift in the system. Data is collected but the effort to interpret the time stamp data of the drift measurements and modify the data set according to this has not been automated. This is partially because few data sets have been without interruption and interpreting the reference measurements under those conditions is not easy to automate. A two step process is to start with a manual correlation between sample measurements and reference measurements and then if that works try to write logic for doing the correlation. This process would have to be inserted before the passing of data to the generation of the Gaussian basis functions.