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NB3 Bio-SANS preliminary optics design

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Neutron Technologies Division

NB3 BIO-SANS PRELIMINARY OPTICS DESIGN

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ABSTRACT

This report describes the calculations and simulations to determine the optimal guide coatings for the NB3 (Bio-SANS) beam line post beryllium reflector changeout. The reported guide performance meets the Bio-SANS scientific requirements document [1].

1. Instrument description

1.1 POST-HBRR PHYSICAL LAYOUT

The NB3 Beamline utilizes the center part of the right channel (looking downstream, "S1") of the cold guide main shutter as described in [2]. Its initial direction is 0.66° off the center line of the cold source beam tube in horizontal direction, and points 0.5° upwards. Starting directly after the main shutter, the remaining beam line uses a guide. The guide has a square cross section of 4 x 4 cm^2. At 8.93 m after the main shutter, the beam is diverted by 7.35° by means of a double optical filter, followed by another straight guide section with 18.69 m length. At the end of this a velocity selector (VS) is placed. After the velocity selector, the beam line consists of 8 consecutive guide sections ("collimator sections", each 2 m in length), each sitting on a sled with three positions: guide in, aperture in, and empty. The sample can be placed freely in the sample area, which makes the next fixed reference point the entrance window of the detector tank.

Name	Start (along flightpath)	Description	Length
Source		HFIR cold Source	
Main shutter		Channel 2, with guide	0.6
Instrument Start	0.0		
Guide1	0.0	m=1	8.93
Optical filter	8.93	m=6 (outer side), m=1 (top/bottom), m=0 (inner side), 2 consecutive mirrors, each diverting the beam by 3.675°	2.49
Guide2	11.42	m=1, rotated by 7.35° against Guide1	18.69
Velocity Selector Gap	30.11	Exact layout TBD	1.11
Guide2 extension		Within Velocity Selector Gap, m=1	TBD
Velocity Selector		Within Velocity Selector Gap	0.25
8 Collimator Boxes	31.22	m=1, can individually be moved into beam	8 x ~2m
Tank Window	49.15	SANS tank window	

Table 1. Overview of the Bio-SANS beamline components post-HBRR.

1.2 OPERATION

The beamline can move the 8 consecutive guide pieces in and out of the beam to adjust the beam intensity reaching the sample by manipulating the beam divergence. If intensity was not an issue, the instrument would achieve its best performance by measuring at very long wavelengths (~20AA) and at very low divergences (no collimations section in, a setting often referred to as N=0, where N is the number of collimation sections used). In reality, the flux at long wavelengths is often too low. The instrument can increase its flux on sample by two methods: Shifting to lower wavelengths (due to the shape of the cold source's spectrum), and moving more collimator sections in. Usually, the shift to lower wavelengths is done first, and only if this is not enough the divergence is increased.

The most relevant instrument configurations for the guide optimization are therefore:

- N=0, λ=20Å
- N=0, λ as close to the spectral peak flux as possible
- N=8, λ as close to the spectral peak flux as possible

Due to planned detector upgrades, the importance of the 7th and 8th guide sections will be reduced in the future. Losses of short wavelength neutrons at the 6th collimator guide setting and below should be minimized. Due to other limitations, "as close to the spectral peak as possible" means 4Å. Following the last collimation section with a guide piece in the beam, the next collimation section is usually set to insert its circular aperture into the flight path.

1.3 MCSTAS MODEL

See also Appendix A. The instrument was modeled in McStas using the cold source, beam tube and main shutter description developed by Lee Robertson. The precise starting point of the guide system was provided by the engineering group. All guides described hereafter have a square cross section of 4x4 cm^2. The initial straight guide section (Guide1) is described by a single guide piece (8.93m). The "optical filter" which diverts the beam by 7.35° has the shape of a pentagonal prism (Figure 1) and is described using an .off geometry file for guide_anyshape. This is followed by another straight guide section ("Guide2", 18.69m).
The following gap intended for the Velocity Selector measures 1.111 m. To capture only the effects of the guide system changes, the McStas simulations described here all use the currently existing Velocity Selector of 47cm length. Additional benefits by exchanging the Velocity Selector and the layout of the Velocity Selector cave will be discussed in a separate report.
Downstream of this, the beam line consists of 8 "Collimator Sections". Each section starts with an oversized aperture ("InterGuide Shield") which is irrelevant for the actual ray tracing aspect of the simulation, but is in reality one of the few parts accessible by the Survey& Alignment group, and therefore acts as the reference point for comparing placement in McStas and installed components. Precise locations of the InterGuide Shields were provided by Survey& Alignment and reflect the as-built, currently existing instrument. After the InterGuide Shields, the McStas model gives the choice of inserting either an "Entrance Aperture" (a circular slit of 20 mm radius) or two guide sections (1 m each). The exception is the first Collimator Section, where an additional choice is an Entrance Aperture with a radius of only 10 mm. This setting is sometimes referred to as "N = -1" and defines the lowest divergence the instrument can achieve. The 8^{th} collimator section is rarely used.
The instrument has no defined sample position, the sample can be freely moved in the sample area. Therefore, the next fixed point in the instrument is the Vacuum Tank Window at 17.93m from the start of the collimator sections. In all calculations in this report, the sample was placed 20 cm upstream of the Vacuum Tank Window. The standard sample size is 1.4 cm in diameter.

An alternative instrument model foregoes the optical filters in favor of a continuously curved guide from the main shutter exit to the velocity selector position, which is approximated by 81 individual guide pieces, each rotated by 0.09° against the previous one.

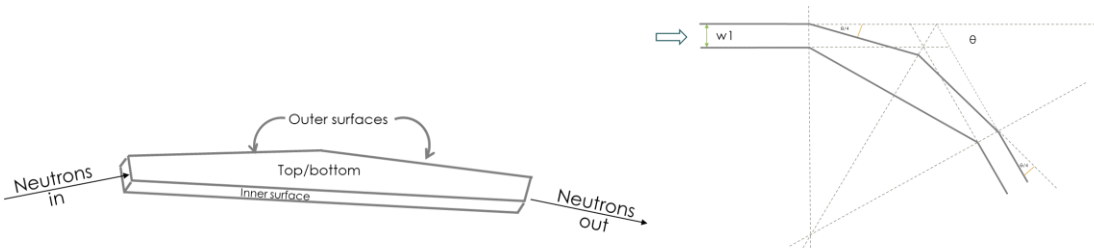

Figure 1. Shape (left) and design (right) of the optical filter. The optical filter will bend the beam by a total of θ=7.35°.

2. MCSTAS CALCULATIONS

2.1 SIMULATIONS

For a detailed description of the source and main shutter used, see [2].
McStas simulations were performed for the following options (“straight sections” includes the collimator sections):

- Current Instrument: m=1 (straight sections) / m=3 (optical filters)

- Curved Guide: m=1 (straight sections) / various m-Values in curved section

- 2 Optical filters: m=1 (straight sections) / m=6 (optical filters)

2.2 RESULTS

Spectra were simulated at the sample position. Table 2 sums up the integrated flux results for the simulations that are discussed in detail in the following sections.

	Wavelength-Integrated Flux [n/s/cm^2]	
Position (Area) / **Guide option**	**Sample, 0 collimator sections, 20 Å (π*0.7^2 cm^2)**	**Sample, 8 collimator sections, 4Å (π*0.7^2 cm^2)**
Current Instrument	6.56x10^4	-
Curved Guide	4.28x10^4	1.25x10^8
2 Optical Filters	6.43x10^4	1.15x10^8
Requirement [1]	1.4x10^4	6x10^7

Table 2. Simulated integrated flux for 3 guide options for various locations and settings in the instrument.

2.2.1 High divergence mode (8 collimator sections)

In high divergence mode, both post-HBRR guide options result in significantly more flux at the sample position at short wavelengths than the currently existing instrument (Figure 2). While the simulation of the currently existing instrument has its peak flux at roughly 6Å, both post-HBRR options reach peak flux at roughly 3Å. At long wavelengths, the post-HBRR guide layouts show an increased flux of roughly 10%. Comparing the flux with the velocity selector set to 4Å shows a slightly higher flux for the curved guide option (Figure 3)

While the curved guide option delivers overall more flux to the sample position than the guide system using 2 optical filters, the divergence distribution (Figure 4) shows that most of this extra intensity comes in the form of very sharp peaks in divergence, and that the optical filter option delivers a smoother beam.

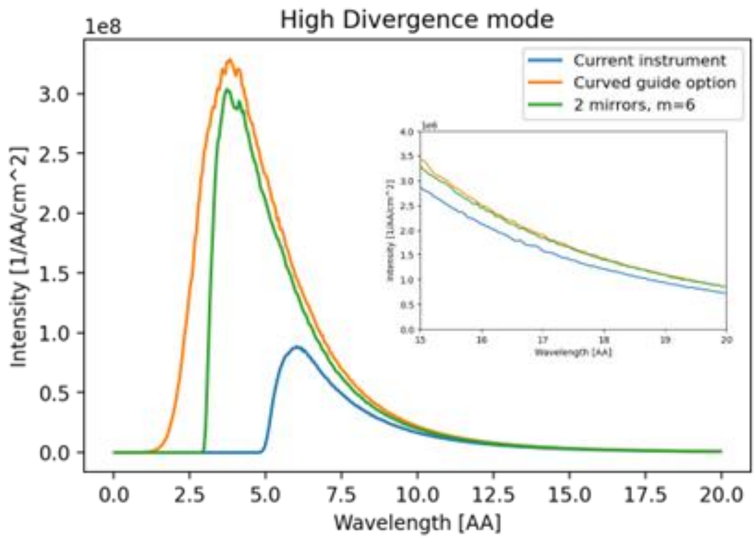

Figure 2. Simulated flux at the sample position for several guide options. Insert: zoomed in long wavelengths.

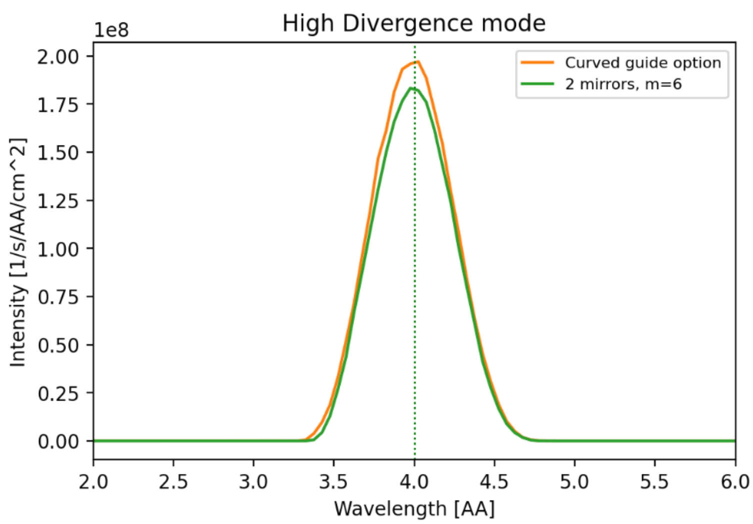

Figure 3. Simulated flux at the sample position for several guide options with the Velocity Selector set to 4Å. All collimator sections are in the beam (N=8). The sample is a circle of 7mm radius.

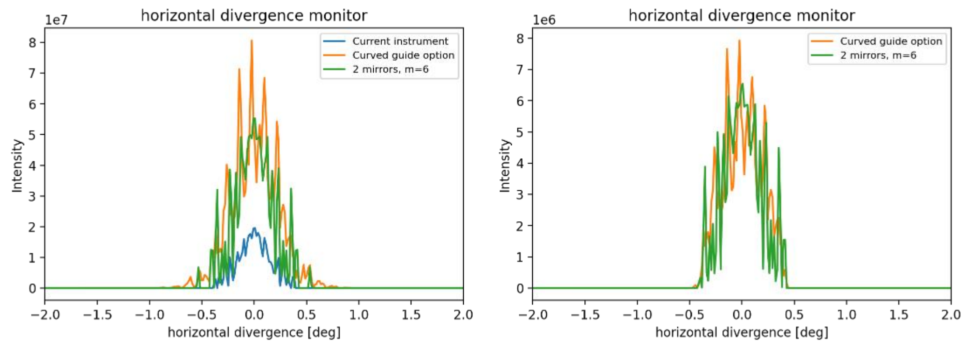

Figure 4. Simulated divergence at the sample position for several guide options. Left: white beam, right: Velocity Selector set to 4Å.

2.2.2 Low divergence mode (0 Collimator sections)

In low divergence mode, both post-HBRR guide options result in significantly more flux at the sample position at short wavelengths than the currently existing instrument (Figure 5). While the simulation of the currently existing instrument has its peak flux at roughly 5.5Å, both post-HBRR options reach peak flux at roughly 3Å.

At long wavelengths however, the curved guide option delivers roughly 20% less neutrons to the sample position than the currently existing instrument and the planned option using 2 optical filters (both the currently existing instrument and the planned version use 2 optical filters, the difference is that the planned version uses a significantly higher m-Value for its mirrors coatings). This can also be seen in the spectrum when the Velocity Selector is set to 4Å (Figure 6).

The reason for that is that a curved guide redistributes the phase space [4] meaning the amount of low divergence neutrons leaving the guide depends on the illumination of the guide entrance across all divergences. Since the Bio-SANS guide is under illuminated, a curved guide cannot deliver as many low divergence neutrons as a flat mirror system, which is optimized around the centerline of the beam, and therefore the lowest divergence neutrons.

The difference in the shape of the divergence profile between the three guide options is marginal (Figure 7).

Since the instrument performance relies heavily on low divergence, long wavelength neutrons, the layout using 2 optical filters is preferred.

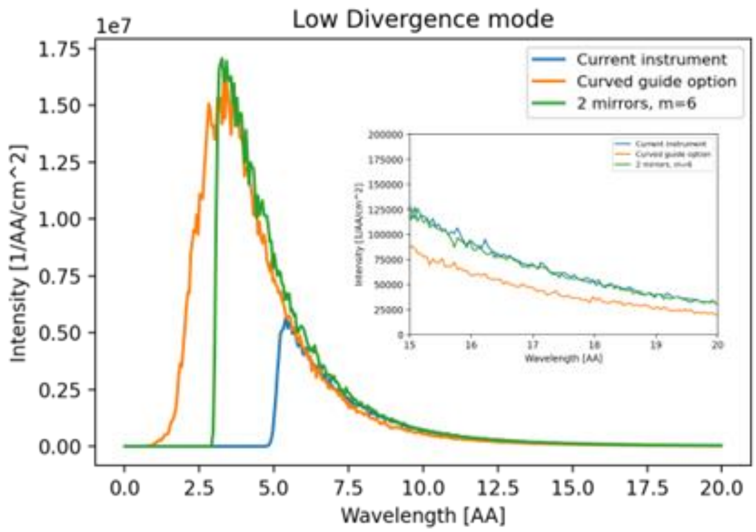

Figure 5. Simulated flux spectrum at the sample position for several guide options. The sample is a circle of 7mm radius. Insert: zoom of higher wavelengths.

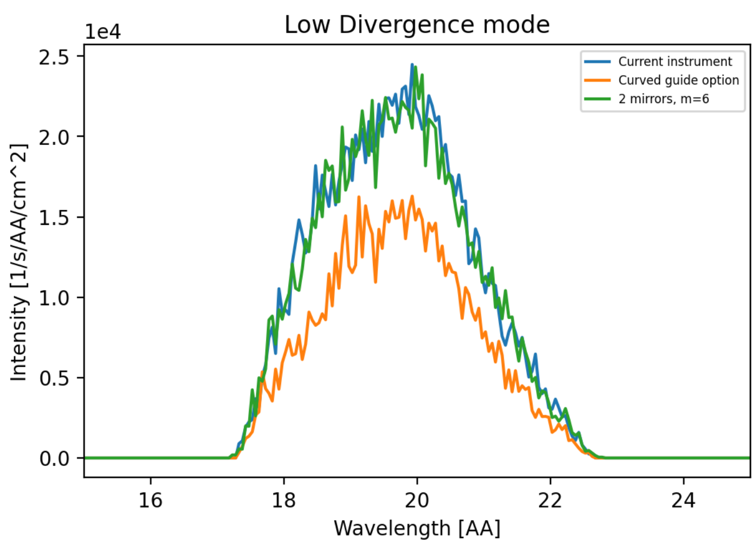

Figure 6. Simulated flux at the sample position for several guide options with the Velocity Selector set to 20Å. No collimator sections are in the beam (N=0), and the source aperture is set to 40mm. The sample is a circle of 7mm radius.

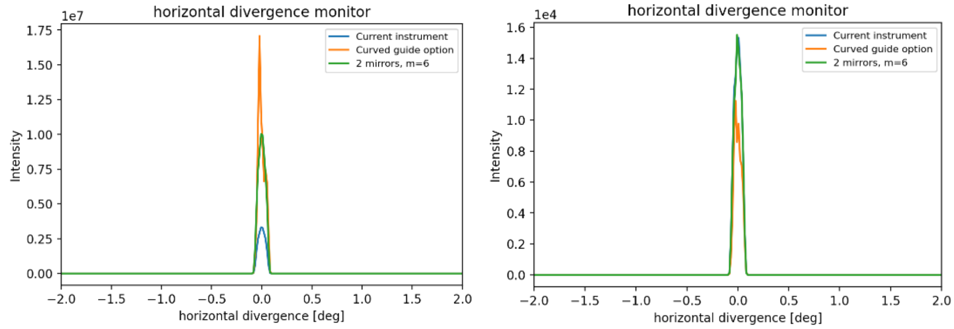

Figure 7. Simulated horizontal divergence at the sample position for several guide options. Left: white beam, right: Velocity Selector at 20Å. No collimator sections are in the beam (N=0), and the source aperture is set to 40mm. The sample is a circle of 7mm radius.

2.2.3 Optimizing the guide coatings

The guide system using two optical filters has 3 different surface types:

- Straight guides (Guide1, Guide2, Collimator Sections, top/bottom of the optical filters)
- Outer surfaces of the optical filter (see Figure 1)
- Inner surface of the optical filter (see Figure 1)

No reflection will occur on the inner surface of the optical filter, and it will be made of either just glass or an absorbing material.
The straight sections will all have the identical m-Value. At the highest divergence setting (8 collimator sections), a small difference exists between all m=1 and m=2 at short wavelengths (Figure 8 (left)). This difference disappears at a slightly lower divergence setting (7 collimator sections, Figure 8 (right)). Since the 8th collimator section is rarely ever used, and exchanging all collimator sections to m=2 would present a significant effort, the instrument will use m=1 in all straight guides.

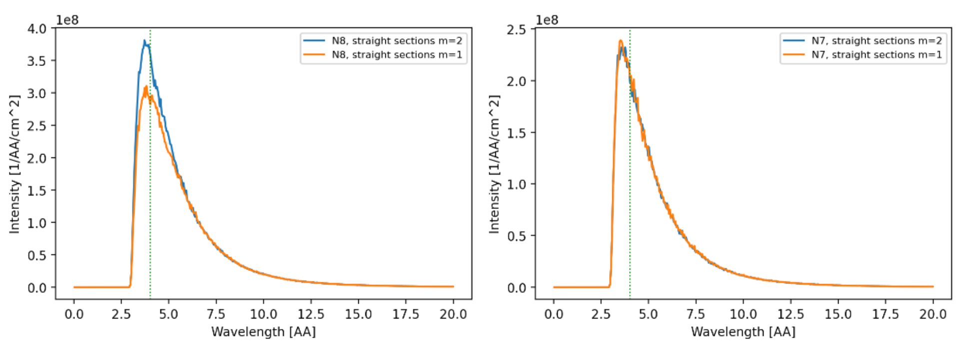

Figure 8. Spectrum of the Instrument option using 2 optical filters in highest divergence mode (N=8, left) and the more commonly used high divergence mode (N=7, right) if all straight guide sections are m=2 (blue) or m=1 (orange).

The most critical surface for the performance of the guide system will be the outer surfaces of the optical filters. Changing the m-Value of these surfaces from m=6 to m=5 changes the peak flux from 4Å to 5Å and will therefore decrease the peak flux available by ~20%. For the instrument to reach is full potential, the outer surface of the optical filters will need to be m=6.

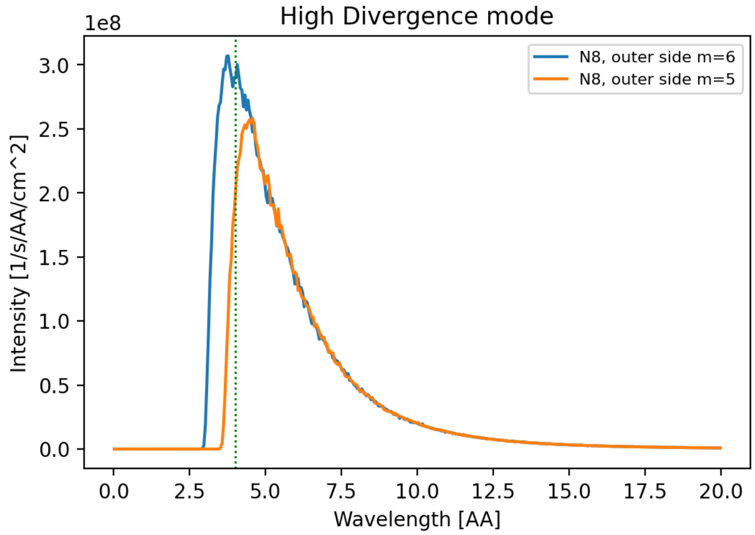

Figure 9. Spectrum of the Instrument option using 2 optical filters in highest divergence mode (N=8) when the outer side of the optical filter is set to m=6 (blue) or m=5 (orange). The straight sections are all set to m=1.

3. SUMMARY

Two different guide options for the post-HBRR Bio-SANS guide system were simulated and compared to the currently existing instrument's performance. The best guide option for the post-HBRR Bio-SANS will be a system using two optical filters, where the optical filters use m=6 mirrors and all other reflecting surfaces are m=1 (Figure 10).
As can be seen in Table 2, the Bio-SANS scientific requirements will be met by the proposed guide design.

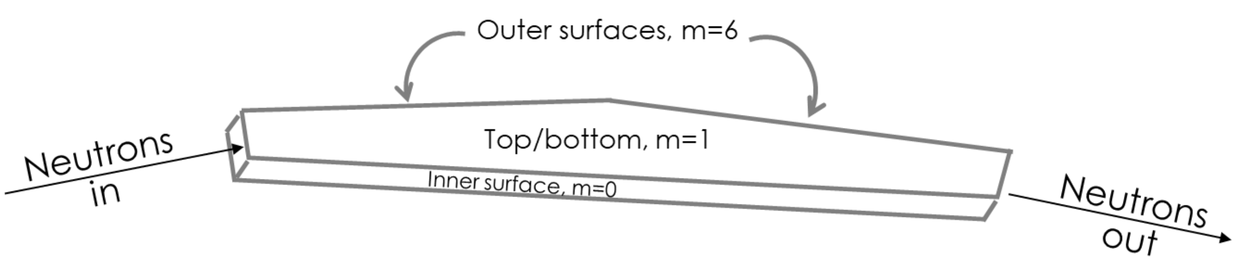

Figure 10. Guide coatings of the optical filter.

4. REFERENCES

[1] Sai Venkatesh Pingali, Cassie Sabens, *HFIR Beryllium Reflector Replacement Project Science Requirements Document for NB3 Bio-SANS*, NB3-SR-00-0001.

[2] Matthew J. Frost et al, *Ray-Tracing Simulations Characterizing the Performance of the Proposed HFIR HB4 Main Shutter*, ORNL-TM-2021/2181, Oak Ridge National Laboratory (August 2021).

[3] R. A. Moon, ORNL internal memo, 2007.

[4] D.F.R. Mildner, *Acceptance diagrams for curved neutron guides*, NIMA, 290, 1990.

APPENDIX A. McStas Instrument file

```
/*******************************************************************
*********
*
* Instrument: NB-3
*
* %Identification
* Written by: Lee Robertson (robertsonjl@ornl.gov)
* Modified by: Thomas Huegle (hueglet@ornl.gov)
* Date: 22may2018
* Modified: 30sept2022
* Origin: ORNL
* McStas Version 2.X
* %INSTRUMENT_SITE: ORNL
*
* %INSTRUMENT_SITE: ORNL
*
* %Description
* NB-3 Beamline.  The New Bio SANS Instrument with curved guide and
inclined by 0.5 degrees
*
*******************************************************************
*********/

DEFINE INSTRUMENT Bio_SANS_tally()
DECLARE
%{
double VS_Central_Wavelength =        20.0;        //Wavelength of the
neutrons transmitted by the velocity selector in Angstroms.  Disk
rotation speed is calculated from this.
double VS_Tilt_Angle =                0.0;        //Rotation of the
whole velocity selector about a vertical axis passing through its
center in degrees.
int N =                          0;        //Number of collimator
guide sections translated into the beam.
double Sample_to_Detector_Distance = 2.5;        //Distance in m from
the sample to the detector.
double Collimator1_Entrance_Aperture =  40;       //Aperture in front
of the guide in collimator section #1 (vaild values = 0, 20, 40)
double Collimator2_Entrance_Aperture =  0;        //Aperture in front
of the guide in collimator section #2 (vaild values = 0, 40)
double Collimator3_Entrance_Aperture =  0;        //Aperture in front
of the guide in collimator section #3 (vaild values = 0, 40)
double Collimator4_Entrance_Aperture =  0;        //Aperture in front
of the guide in collimator section #4 (vaild values = 0, 40)
double Collimator5_Entrance_Aperture =  0;        //Aperture in front
of the guide in collimator section #5 (vaild values = 0, 40)
```

```
double Collimator6_Entrance_Aperture =  0;        //Aperture in front
of the guide in collimator section #6 (vaild values = 0, 40)
double Collimator7_Entrance_Aperture =  0;        //Aperture in front
of the guide in collimator section #7 (vaild values = 0, 40)
double Collimator8_Entrance_Aperture =  0;        //Aperture in front
of the guide in collimator section #8 (vaild values = 0, 40)
char  shutter_filename[255];
double IN2M = 25.4 / 1000.0;   // Unit conversion from inches to
meters

double m_straight = 1;
double m_OF = 6;

//These parameters will only be used by Lee Robertson't tally
components:
  int Tally =                          0;       //Switch to record
neutron tallies (histories)
  int    tally_flag;
  int    tally_neutron_index;
  int    tally_number_of_events;
  int    tally_event_component_index[1000];
  int    tally_event_component_type[1000];
  double tally_event_position[1000][3];
  double tally_event_velocity[1000][3];
  double tally_event_weight[1000];
  double tally_reflection_q[1000];
  int    tally_reflection_mirror_index[1000];
  FILE   *tally_event_list_fp;
  int    tally_number_of_components;
  int    tally_component_index[1000];
  int    tally_component_type[1000];
  char   tally_component_name[1000][255];
  char   tally_module_name[1000][128];
%}

INITIALIZE
%{

Wavelength_Min =               0;        //Minimum neutron wavelength
to be generated.  Should be chosen to with respect to
VS_Central_Wavelength
Wavelength_Max =               20;        //Maximum neutron wavelength
to be generated.  Should be chosen to with respect to
VS_Central_Wavelength
sprintf(shutter_filename,"%s","../hb4-cold-source-
2024/main_shutter_S1.off");

  tally_flag = Tally;
  char tally_output_file_name[255];
  if (tally_flag == 1)
  {  sprintf(tally_output_file_name, "%s",
"BioSANS_neutron_event_list.dat");
```

```
     tally_event_list_fp = fopen(tally_output_file_name, "w");
     if (tally_event_list_fp == NULL)
     {
         printf("Error opening file %s!\n", tally_output_file_name);
         exit(1);
     }
  }
%}

TRACE

//**********************************************************************
**************************************************************
// Define the absolute instrument coordinate system with the origin at
the center line of the reactor pressure vessel.
// Many of the drawings of the HB-4 beamtube use this as the
reference.
// The positive Z-axis is along the beamtube centerline.
// The positive Y-axis is pointing up.
// The positive X-axis is pointing to the left looking down the
beamtube toward the reactor core. (Right handed coordinate system)

COMPONENT Pressure_Vessel_CL_Coordinate_System = Progress_bar()
  AT (0.0, 0.0, 0.0) ABSOLUTE

//**********************************************************************
**************************************************************

%include "../hb4-cold-source-2024/HB4_Beamtube.instr"

//**********************************************************************
**************************************************************

%include "../hb4-cold-source-2024/HB4_Main_Shutter.instr"

//**********************************************************************
****************************************************************

// McSTAS code for the origin of the NB-3 guide system:
COMPONENT NB3_Beam_Coordinate_System = Arm()
  AT (-0.05422055871659287, 0.04101575802119908, 4.70) RELATIVE Source
  ROTATED (-0.5, -0.66101, 0.0) RELATIVE Source

COMPONENT NB3_Guide1_Entrance_Mask = Slit(xwidth=0.040, yheight=0.040)
// Block the neutrons that won't enter the guide before characterizing
the beam at the guide entrance
  AT (0.0, 0.0, 0.0) RELATIVE NB3_Beam_Coordinate_System

COMPONENT NB3_Guide1 = Guide(w1 = 0.04, w2 = 0.04, h1 = 0.04, h2 =
0.04, l = 8.64707449850299, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m =
m_straight, W = 0.0025)
  AT (0.0, 0.0, 0.0) RELATIVE NB3_Beam_Coordinate_System
```

```
COMPONENT End_of_Guide1_Coordinate_System = Arm()
  AT (0, 0, 8.64707449850299) RELATIVE NB3_Guide1

COMPONENT OF =
Guide_anyshape(geometry="2OF_long_sections_tally_o6_i0.off", R0 =
0.99, Qc = 0.0219, alpha = 3.044, m = m_OF, W = 0.0025)
  AT (0,0,0.0005) RELATIVE End_of_Guide1_Coordinate_System

COMPONENT Guide2 = Guide(w1 = 0.04, h1 = 0.04, l = 18.45069491924003,
R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W = 0.0025)
AT (-0.19964322688456265, 0, 3.165464387054288) RELATIVE PREVIOUS
ROTATED (0, -7.21763528893225, 0) RELATIVE PREVIOUS

// Generate a reference position at the end of Guide2
COMPONENT NB3_End_of_Guide2_Coordinate_System = Arm()
  AT (0, 0, 18.45069491924003) RELATIVE PREVIOUS

//*******************************************************************
**************************************************************
// Simulate the helical disk velocity selector bought from Mirrortron

COMPONENT Velocity_Selector_Coordinate_System = Arm()
  AT (0.0, 0.0, 0.10 + (0.475 / 2.0)) RELATIVE
NB3_End_of_Guide2_Coordinate_System  // The z position is the center
of the velocity selector rather than its entrance so the "tilt"
rotation will be about its center, not the entrance
  ROTATED (0.0, VS_Tilt_Angle, 0.0) RELATIVE
NB3_End_of_Guide2_Coordinate_System

COMPONENT Selector = Disk_type_velocity_selector(window_width = 0.100,
window_height = 0.050, slot_width = 2.25, r1 = 0.150, r2 = 0.200,
absorber_width = 0.75, pitch = 17.0, wavelength =
VS_Central_Wavelength, length = 0.420, rotation_direction = 1.0,
housing_length = 0.475)
  AT (0.0, 0.0, 0.0) RELATIVE Velocity_Selector_Coordinate_System
  ROTATED (0.0, VS_Tilt_Angle, 0.0) RELATIVE
Velocity_Selector_Coordinate_System

//*******************************************************************
**************************************************************

// !!!!! The aperture and attenuator and beam monitor assembly should
go in here but I do not know how its configured. !!!!!
//
//*******************************************************************
**************************************************************
//Define a new coordinate system for the collimatopr sections --
millwight data referenced to the end of Guide 2
//  Data from Wayne and Chris (millwrights) for the installation of
the new collimators sections prior to the Be outage
```

```
COMPONENT Collimator_Section_Coordinate_System = Arm()  // Set to be
the end of Guide_2 because that is the reference used for the data
from the millwrights
  AT (0.0, 0.0, 0.0) RELATIVE NB3_End_of_Guide2_Coordinate_System

// Collimator Guide Section #1

COMPONENT NB3_Collimator1_InterGuide_Shield = Slit(xmin = -0.021, xmax
= 0.021, ymin = -0.021, ymax = 0.031)   // See Drawing M11540-0N-332-
E0 Rev0
  AT (0.0, 0.0, 1.110094) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator1_Entrance_Aperture_20mm = Slit(radius =
0.010)   // See Drawings M11540-0N-321-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator1_Entrance_Aperture == 20)
  AT (0.0, 0.0, 1.1100994 + 0.001) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator1_Entrance_Aperture_40mm = Slit(radius =
0.020)   // See Drawings M11540-0N-320-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator1_Entrance_Aperture == 40)
  AT (0.0, 0.0, 1.110094 + 0.002) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator1_Guide_1 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 0)
  AT (0.0, 0.0, 1.1130842) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator1_Guide_2 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 0)
  AT (0.0, 0.0, 1.1130842 + 1.0) RELATIVE
Collimator_Section_Coordinate_System



// Collimator Guide Section #2

COMPONENT NB3_Collimator2_InterGuide_Shield = Slit(xmin = -0.021, xmax
= 0.021, ymin = -0.021, ymax = 0.031)     //See Drawing M11540-ON-332-
E Rev0
  AT (0.0, 0.0, 3.143042) RELATIVE
Collimator_Section_Coordinate_System
```

```
COMPONENT NB3_Collimator2_Entrance_Aperture_40mm = Slit(radius =
0.020)   // See Drawings M11540-0N-321-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator2_Entrance_Aperture == 40)
  AT (0.0, 0.0, 3.143042 + 0.002) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator2_Guide_1 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 1)
  AT (0.0, 0.0, 3.155242) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator2_Guide_2 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha1 = 3.044, alpha2 = 3.044, alpha3 =
3.044, alpha4 = 3.044, m1 = m1, m2 =m2, m3 = m3, m4 = m4, W1 = 0.0025,
W2 = 0.0025, W3 = 0.0025, W4 = 0.0025)
  WHEN (N > 1)
  AT (0.0, 0.0, 3.155242 + 1.0) RELATIVE
Collimator_Section_Coordinate_System



// Collimator Guide Section #3

COMPONENT NB3_Collimator3_InterGuide_Shield = Slit(xmin = -0.021, xmax
= 0.021, ymin = -0.021, ymax = 0.031)     //See Drawing M11540-ON-332-
E Rev0
  AT (0.0, 0.0, 5.167442) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator3_Entrance_Aperture_40mm = Slit(radius =
0.020)   // See Drawings M11540-0N-321-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator3_Entrance_Aperture == 40)
  AT (0.0, 0.0, 5.167442 + 0.002) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator3_Guide_1 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 2)
  AT (0.0, 0.0, 5.179442) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator3_Guide_2 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
```

```
  WHEN (N > 2)
  AT (0.0, 0.0, 5.179442 + 1.0) RELATIVE
Collimator_Section_Coordinate_System



// Collimator Guide Section #4

COMPONENT NB3_Collimator4_InterGuide_Shield = Slit(xmin = -0.021, xmax
= 0.021, ymin = -0.021, ymax = 0.031)   // See Drawing M11540-0N-332-
E0 Rev0
  AT (0.0, 0.0, 7.201423) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator4_Entrance_Aperture_40mm = Slit(radius =
0.020)   // See Drawings M11540-0N-321-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator4_Entrance_Aperture == 40)
  AT (0.0, 0.0, 7.201423 + 0.002) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator4_Guide_1 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 3)
  AT (0.0, 0.0, 7.205383) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator4_Guide_2 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 3)
  AT (0.0, 0.0, 7.205383 + 1.0) RELATIVE
Collimator_Section_Coordinate_System



// Collimator Guide Section #5

COMPONENT NB3_Collimator5_InterGuide_Shield = Slit(xmin = -0.021, xmax
= 0.021, ymin = -0.021, ymax = 0.031)   // See Drawing M11540-0N-332-
E0 Rev0
  AT (0.0, 0.0, 9.233421) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator5_Entrance_Aperture_40mm = Slit(radius =
0.020)   // See Drawings M11540-0N-321-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator5_Entrance_Aperture == 40)
```

```
  AT (0.0, 0.0, 9.233421 + 0.002) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator5_Guide_1 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 4)
  AT (0.0, 0.0, 9.236011) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator5_Guide_2 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 4)
  AT (0.0, 0.0, 9.236011 + 1.0) RELATIVE
Collimator_Section_Coordinate_System  // The 0.5mm gap is for
nstallation clearence



// Collimator Guide Section #6

COMPONENT NB3_Collimator6_InterGuide_Shield = Slit(xmin = -0.021, xmax
= 0.021, ymin = -0.021, ymax = 0.031)   // See Drawing M11540-0N-332-
E0 Rev0
  AT (0.0, 0.0, 11.258565) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator6_Entrance_Aperture_40mm = Slit(radius =
0.020)   // See Drawings M11540-0N-321-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator6_Entrance_Aperture == 40)
  AT (0.0, 0.0, 11.258565 + 0.002) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator6_Guide_1 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 5)
  AT (0.0, 0.0, 11.261524) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator6_Guide_2 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 5)
  AT (0.0, 0.0, 11.261524 + 1.0) RELATIVE
Collimator_Section_Coordinate_System
```

```
// Collimator Guide Section #7

COMPONENT NB3_Collimator7_InterGuide_Shield = Slit(xmin = -0.021, xmax
= 0.021, ymin = -0.021, ymax = 0.031)   // See Drawing M11540-0N-332-
E0 Rev0
  AT (0.0, 0.0, 13.295981) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator7_Entrance_Aperture_40mm = Slit(radius =
0.020)   // See Drawings M11540-0N-321-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator7_Entrance_Aperture == 40)
  AT (0.0, 0.0, 13.295981 + 0.002) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator7_Guide_1 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 6)
  AT (0.0, 0.0, 13.299851) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator7_Guide_2 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 6)
  AT (0.0, 0.0, 13.299851 + 1.0) RELATIVE
Collimator_Section_Coordinate_System  // The 0.5mm gap is for
installation clearence



// Collimator Guide Section #8

COMPONENT NB3_Collimator8_InterGuide_Shield = Slit(xmin = -0.021, xmax
= 0.021, ymin = -0.021, ymax = 0.031)   // See Drawing M11540-0N-332-
E0 Rev0
  AT (0.0, 0.0, 15.321498) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator8_Entrance_Aperture_40mm = Slit(radius =
0.020)   // See Drawings M11540-0N-321-E-Rev0 and See Drawings M11540-
0N-316A-E-Rev1  NOTE: There apertures are reversed on M11540-0N-316A-
E-Rev1
  WHEN (Collimator8_Entrance_Aperture == 40)
  AT (0.0, 0.0, 15.321498 + 0.002) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator8_Guide_1 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
```

```
  WHEN (N > 7)
  AT (0.0, 0.0, 15.324526) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Collimator8_Guide_2 = Guide(w1 = 0.040, h1 = 0.040, l =
1.0, R0 = 0.99, Qc = 0.0219, alpha = 3.044, m = m_straight, W =
0.0025)
  WHEN (N > 7)
  AT (0.0, 0.0, 15.324526 + 1.0) RELATIVE
Collimator_Section_Coordinate_System  // The 0.5mm gap is for
installation clearence



// the final interguide shield

COMPONENT NB3_Collimator8_InterGuide_Shield_Last = Slit(xmin = -0.021,
xmax = 0.021, ymin = -0.021, ymax = 0.031)   // See Drawing M11540-0N-
332-E0 Rev0
  AT (0.0, 0.0, 17.337839) RELATIVE
Collimator_Section_Coordinate_System

//*****************************************************************
***********************************************************
//
// The beam extender and gate valve should go here !!!!!!!!!!
//
//*****************************************************************
***********************************************************
// Model some kind of simple scatterer to check min Q and resolution.

COMPONENT NB3_SANS_Tank_Window_Coordinate_System = Arm()  //
Coordinates from millright data on the collimator sections
  AT (0.0, 0.0, 19.039659) RELATIVE
Collimator_Section_Coordinate_System

COMPONENT NB3_Sample_Position_Coordinate_System = Arm()
  AT (0, 0, -0.200) RELATIVE NB3_SANS_Tank_Window_Coordinate_System
//The 20cm in front of the tank window is aribitray since this
position is adjustable from the end of guide 8 to the sample is just a
guess.

//~ COMPONENT NB3_Tally_Detector = Tally_detector()  // Record neutron
tallies (histories) at the sample position for post processing
  //~ AT (0.0, 0.0, -0.002) RELATIVE
NB3_Sample_Position_Coordinate_System

COMPONENT NB3_Sample_aperture = Slit(radius=0.007)
  AT (0.0, 0.0, -0.001) RELATIVE NB3_Sample_Position_Coordinate_System
```

```
/// NB3_Sample_Position detectors, xwidth=0.02, yheight=0.02,
bins=400, Lbins=500, Lmin=0, Lmax=25, maxDiv=3.0 ///

COMPONENT DetectorPack_NB3_Sample_Position = Arm()
  AT (0.0, 0.0, 0.0) RELATIVE NB3_Sample_aperture

    COMPONENT NB3_Sample_Position_Flux = Monitor(xwidth = 0.02,
yheight = 0.02)
      AT (0.0, 0.0, 0.0) RELATIVE DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Image = PSD_monitor(nx = 400, ny =
400, filename = "NB3_Sample_Position_image", xwidth = 2*0.02, yheight
= 2*0.02)
      AT (0.0, 0.0, 0.0) RELATIVE DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Spectrum = L_monitor(nL = 500,
filename = "NB3_Sample_Position_spectrum", xwidth = 0.02, yheight =
0.02, Lmin = 0, Lmax = 25)
      AT (0.0, 0.0, 0.0) RELATIVE DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Vertical_Divergence =
Hdiv_monitor(nh = 400,
filename="NB3_Sample_Position_vertical_divergence", xwidth = 0.02,
yheight = 0.02, h_maxdiv = 3.0)
      AT (0.0, 0.0, 0.0) RELATIVE DetectorPack_NB3_Sample_Position
      ROTATED (0.0, 0.0, 90.0) RELATIVE
DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Horizontal_Divergence =
Hdiv_monitor(nh = 400,
filename="NB3_Sample_Position_horizontal_divergence", xwidth = 0.02,
yheight = 0.02, h_maxdiv=3.0)
      AT (0.0, 0.0, 0.0) RELATIVE DetectorPack_NB3_Sample_Position
      ROTATED (0.0, 0.0, 0.0) RELATIVE
DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Divergence_Map =
Divergence_monitor(nh = 400, nv = 400,
filename="NB3_Sample_Position_divergence_map", xwidth = 0.02, yheight
= 0.02, maxdiv_h = 3.0, maxdiv_v = 3.0)
      AT (0.0, 0.0, 0.0) RELATIVE DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Horizontal_Phase_Space_Map =
DivPos_monitor(nh = 400, ndiv = 400,
filename="NB3_Sample_Position_horizontal_phase_space_map", xwidth =
0.02, yheight = 0.02, maxdiv_h = 3.0)
      AT (0.0, 0.0, 0.0) RELATIVE DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Vertical_Phase_Space_Map =
DivPos_monitor(nh = 400, ndiv = 400,
filename="NB3_Sample_Position_vertical_phase_space_map", xwidth =
0.02, yheight = 0.02, maxdiv_h = 3.0)
      AT (0.0, 0.0, 0.0) RELATIVE DetectorPack_NB3_Sample_Position
      ROTATED (0.0, 0.0, 90.0) RELATIVE
DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Vertical_divergenceMonitor_xL =
DivLambda_monitor(xwidth = 0.02, yheight = 0.02, nL=500, nh = 400,
filename = "NB3_Sample_Position_vertical_divLambda_map", maxdiv_h =
3.0, Lmin = 0, Lmax = 25)
```

```
      AT (0, 0, 0) RELATIVE DetectorPack_NB3_Sample_Position
      ROTATED (0.0, 0.0, 90.0) RELATIVE
DetectorPack_NB3_Sample_Position
    COMPONENT NB3_Sample_Position_Horizontal_divergenceMonitor_xL =
DivLambda_monitor(xwidth = 0.02, yheight = 0.02, nL=500, nh = 400,
filename = "NB3_Sample_Position_horizontal_divLambda_map", maxdiv_h =
3.0, Lmin = 0, Lmax = 25)
      AT (0, 0, 0) RELATIVE DetectorPack_NB3_Sample_Position
      ROTATED (0.0, 0.0, 0.0) RELATIVE
DetectorPack_NB3_Sample_Position


/// --- ///

FINALLY
%{
    int i;
    char tally_event_list_filename[255];
    char tally_component_list_filename[255];

    if (tally_flag == 1)  fclose(tally_event_list_fp);

    if (tally_flag == 1)
    {  sprintf(tally_component_list_filename,
"BioSANS_component_list.dat");
       FILE *fp = fopen(tally_component_list_filename, "w");
       for (i = 0; i < tally_number_of_components; i++)
       {
           fprintf(fp, "%5d %5d %-64s %s\n", tally_component_index[i],
tally_component_type[i], tally_component_name[i],
tally_module_name[i]);
       }
       fclose(fp);
    }
%}

END
```

APPENDIX B. Optical filter in .off file format

```
OFF
44 40
0.02 -0.02 0.0 #0
0.02 0.02 0.0 #1
0.01 -0.02 0.31742715701462293 #2
0.01 0.02 0.31742715701462293 #3
0.0 -0.02 0.6348543140292459 #4
0.0 0.02 0.6348543140292459 #5
```

```
-0.010000000000000005 -0.02 0.9522814710438687 #6
-0.010000000000000005 0.02 0.9522814710438687 #7
-0.02 -0.02 1.2697086280584917 #8
-0.02 0.02 1.2697086280584917 #9
-0.030000000000000002 -0.02 1.5871357850731147 #10
-0.030000000000000002 0.02 1.5871357850731147 #11
-0.05996034106682942 -0.02 1.9033040598470796 #12
-0.05996034106682942 0.02 1.9033040598470796 #13
-0.08992068213365884 -0.02 2.2194723346210443 #14
-0.08992068213365884 0.02 2.2194723346210443 #15
-0.11988102320048825 -0.02 2.535640609395009 #16
-0.11988102320048825 0.02 2.535640609395009 #17
-0.14984136426731767 -0.02 2.8518088841689737 #18
-0.14984136426731767 0.02 2.8518088841689737 #19
-0.17980170533414708 -0.02 3.167977158942939 #20
-0.17980170533414708 0.02 3.167977158942939 #21
-0.02 -0.02 0.0 #22
-0.02 0.02 0.0 #23
-0.039948474843497825 -0.02 0.31629516151656367 #24
-0.039948474843497825 0.02 0.31629516151656367 #25
-0.059896949686995646 -0.02 0.6325903230331273 #26
-0.059896949686995646 0.02 0.6325903230331273 #27
-0.07984542453049348 -0.02 0.948885484549691 #28
-0.07984542453049348 0.02 0.948885484549691 #29
-0.0997938993739913 -0.02 1.2651806460662547 #30
-0.0997938993739913 0.02 1.2651806460662547 #31
-0.11974237421748912 -0.02 1.5814758075828184 #32
-0.11974237421748912 0.02 1.5814758075828184 #33
-0.13969084906098694 -0.02 1.897770969099382 #34
-0.13969084906098694 0.02 1.897770969099382 #35
-0.15963932390448476 -0.02 2.214066130615946 #36
-0.15963932390448476 0.02 2.214066130615946 #37
-0.17958779874798259 -0.02 2.5303612921325094 #38
-0.17958779874798259 0.02 2.5303612921325094 #39
-0.1995362735914804 -0.02 2.846656453649073 #40
-0.1995362735914804 0.02 2.846656453649073 #41
-0.21948474843497823 -0.02 3.1629516151656367 #42
-0.21948474843497823 0.02 3.1629516151656367 #43
4 0 1 3 2
4 2 3 5 4
4 4 5 7 6
4 6 7 9 8
4 8 9 11 10
4 10 11 13 12
4 12 13 15 14
4 14 15 17 16
4 16 17 19 18
4 18 19 21 20
4 22 23 25 24
4 24 25 27 26
4 26 27 29 28
4 28 29 31 30
```

4 30 31 33 32
4 32 33 35 34
4 34 35 37 36
4 36 37 39 38
4 38 39 41 40
4 40 41 43 42
4 0 2 24 22
4 2 4 26 24
4 4 6 28 26
4 6 8 30 28
4 8 10 32 30
4 10 12 34 32
4 12 14 36 34
4 14 16 38 36
4 16 18 40 38
4 18 20 42 40
4 1 3 25 23
4 3 5 27 25
4 5 7 29 27
4 7 9 31 29
4 9 11 33 31
4 11 13 35 33
4 13 15 37 35
4 15 17 39 37
4 17 19 41 39
4 19 21 43 41