

Introduction to VITESS

- VITESS team
 - Phillip Bentley (HMI, Germany)
 - Heloisa Bordallo (HMI, Germany)
 - Dickon Champion (ISIS, UK)
 - Michael Fromme (HMI; Germany)
 - Klaus Lieutenant (IFE, Norway)
 - Sergey Manoshin (JINR; Russia)
 - Judith Peters (ILL, France)
 - Geza Zsigmond (PSI, Switzerland)

Virtual
Instrumentation
Tool for the
E
S
S

History of VITESS

- Origin
 - Idea of Ferenc Mezei to realize a package well suited to simulate instruments on neutron spallation sources, as European spallation source (ESS) is planned
- Important dates
 - 1998: Some existing programs put together, GUI added
 - 1999: Release of VITESS 1.0
First complete instruments simulated
 - 2000: SCANS collaboration started (McStas, VITESS, ...)
 - 2001: Release of VITESS 2.0 containing polarisation, absolute flux values, improved GUI
several ESS instruments simulated
 - 2003: Decision: ESS will not be built in the near future
VITESS will be used for (TOF) instruments on other sources
 - 2004: VITESS supported by SCANS successor MCNSI

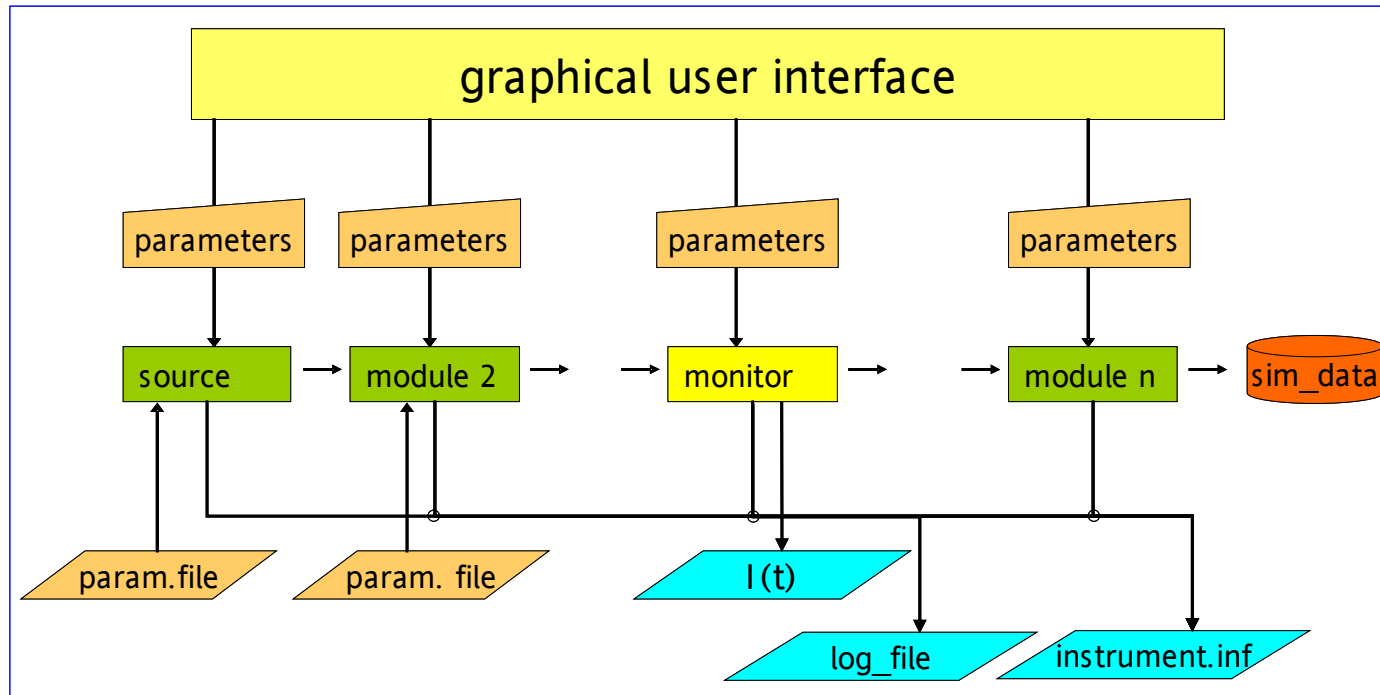
Some general features

- Published under GNU licence
 - Free of charge
 - Can be downloaded from internet.
Address: <http://www.hmi.de/projects/ess/vitess/>
 - Code developed by a limited number of persons
- Staff
 - 8 persons from 6 different facilities in the development team
 - Open to new members
- Platforms
 - Executables for Windows/DOS, Linux 32 bit and 64 bit
 - Macintosh support on demand
- Version 2.7 currently under test
- A few hundred downloads
- Collaborations
 - Supported by European Commission in MCNSI
 - Collaboration with McStas in VnCS

Why using VITESS ?

- VITESS is easy to install
- VITESS is easy to use
 - Practically everything can be done from a graphical user interface
 - Simulation can be run without writing any code or using any meta-language
 - Advanced users can write own modules or change existing ones
- VITESS is nearly complete
 - TOF option (even on constant wave sources)
 - Many modules treating polarisation
 - Gravity is included
- VITESS is ideal for small projects (and powder diffraction)

Concept of Vitess



- Advantages of the piping concept:
 - No need of large memories
 - Shorter calculations times
 - Instrument can easily be split
- Disadvantages
 - Little information about the whole instrument
 - No calculation of dependent parameters (from some independent parameters)

Parameter set transferred

- criterion 'ray tracing'
- ID
- Time of flight t [ms]
- wavelength λ [Å]
- probability/current p [n/s]
- location of neutron x [cm]
- location of neutron y [cm]
- location of neutron y [cm]
- flight direction $v_x/|\underline{v}| = \cos \alpha$
- flight direction $v_y/|\underline{v}| = \cos \beta$
- flight direction $v_z/|\underline{v}| = \cos \gamma$
- Spin S_x
- Spin S_y
- Spin S_z

GUI after Starting the Program

Instrument 1 Click parameter names for help!

VITESS 2.7

input file Browse BrowseN

output file Browse BrowseN

parameter directory Browse NewDir

random seed random number generator min. neutron weight gravity

Check Start Kill Stop Fresh Exit

Getting Help

You can get help about every

- parameter by clicking on its name (see also help for module)
- module by clicking on the module number or choosing the menu Help

Help

Alternatively, you can use the help system in the internet:
<http://www.hmi.de/projects/ess/vitess/DOC/index.html>

For further questions, please send an email to vitess@hmi.de

Getting Started Tutorial
Inserting/Deleting a Module Visualising Results
Troubleshooting

output file

The data of all trajectories will be written to the 'output file' at the end (of the first part) of the simulation. These data can be used to start a second part the simulation by giving the name of this file as 'input file'.
command option --F

Big Clear Save

Help

VITESS Module Source

The module **source** initialises neutrons originated at a short pulsed (SPSS), long pulsed (LPSS), or a continuous source (CWS). Their starting positions are randomly distributed over a rectangular moderator surface. Further parameters like wavelength, divergence and time at the moderator are determined at random, too.

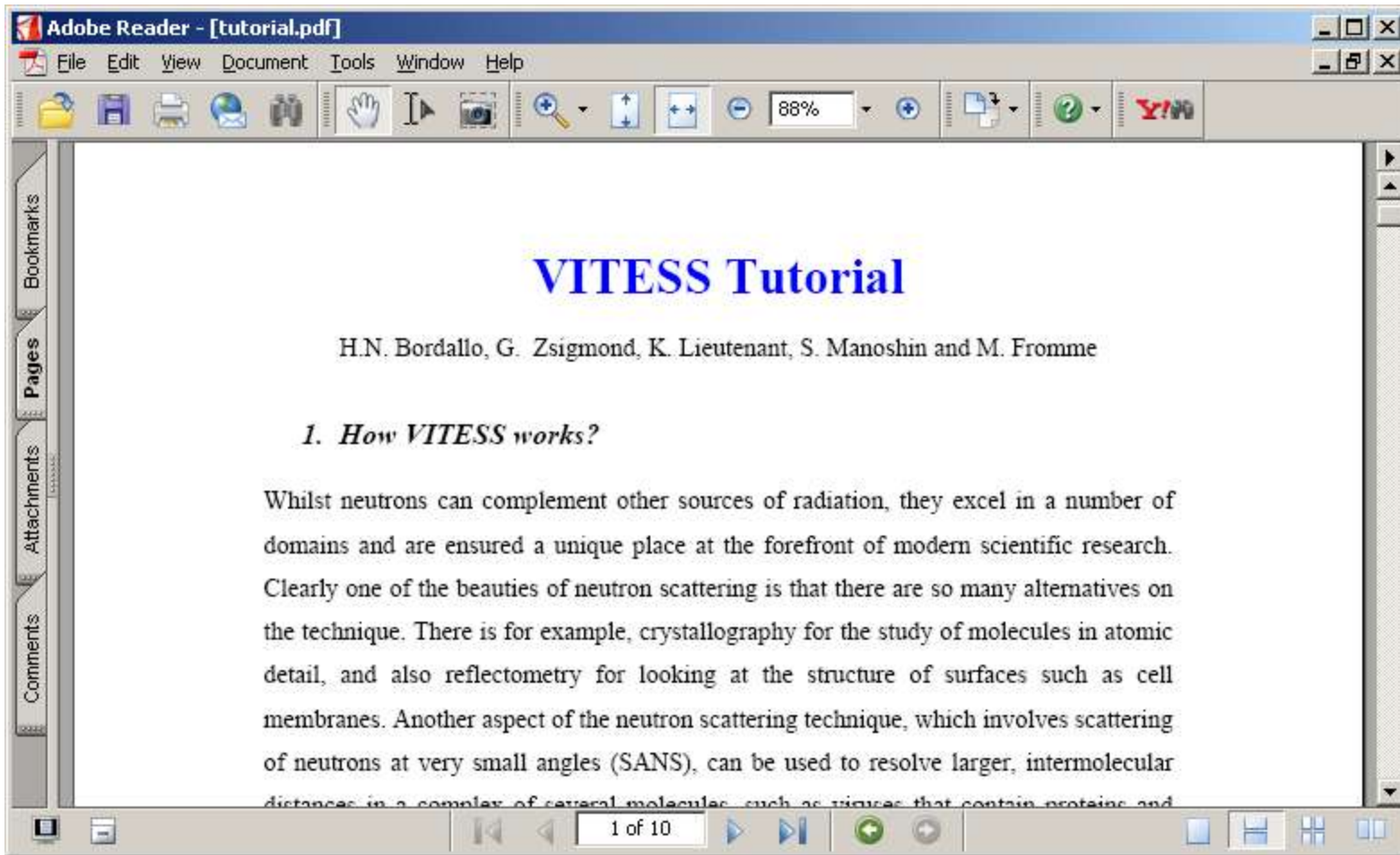
This module simulates also subsequent free propagation which can be limited in such a way, that only neutrons reaching a certain region of space are considered further on. The coordinate system is oriented as illustrated in the figure, it is centered in the middle of the moderator surface and shifted parallel to the x-axis to the position of the propagation window (i.e. the x-coordinate of each neutron which hit the propagation window is zero).

SPSS
LPSS
CWS

Moderator
at $x=0$

propagation window

Tutorial



The screenshot shows the Adobe Reader interface. The title bar reads 'Adobe Reader - [tutorial.pdf]'. The menu bar includes 'File', 'Edit', 'View', 'Document', 'Tools', 'Window', and 'Help'. The toolbar contains various icons for file operations and viewing. The main content area displays the following text:

VITESS Tutorial

H.N. Bordallo, G. Zsigmond, K. Lieutenant, S. Manoshin and M. Fromme

1. *How VITESS works?*

Whilst neutrons can complement other sources of radiation, they excel in a number of domains and are ensured a unique place at the forefront of modern scientific research. Clearly one of the beauties of neutron scattering is that there are so many alternatives on the technique. There is for example, crystallography for the study of molecules in atomic detail, and also reflectometry for looking at the structure of surfaces such as cell membranes. Another aspect of the neutron scattering technique, which involves scattering of neutrons at very small angles (SANS), can be used to resolve larger, intermolecular distances in a complex of several molecules, such as viruses that contain proteins and

The status bar at the bottom indicates '1 of 10' pages.

Modules representing Hardware

Sources	Reactor	SPSS	LPSS		
Space + Windows	Space	window or beamstop	multiple Windows	grid	
Choppers	Disk	Fermi str.	Fermi cur	Vel.select	
Monochr/ Analys.	Flat	Focus	Foc.user		
Modules f. Polaris.	³ He-Pol.	Coil Flip.	Prec.field	Resonat. Drabkin	
	SMir-Pol.	Grad.Flip.	Rot. field		
Samples	Elastic + isotropic	Inelastic	Powder	SANS	
		Sngl.crys.	S(Q)	Reflecto.	
	Guide	Bender	SM-Ensemble	elliptic mirror	Collimat.

GUI after loading of an instrument

The screenshot shows the Xcontrol K:/ VITESS 2.7 GUI. The main window has a menu bar (File, Edit, Configure, Tools, Options, Help) and a title bar (Xcontrol K:/). The main area is titled "Instrument SANS" and "VITESS 2.7". On the right, it says "Click parameter names for help!".

On the left side, there are four buttons: Check, Start, Kill, and Stop. Below these is a list of modules (1-11) with up/down arrows and a checkbox. The selected module is "mon2_pos".

The main configuration area for "Module 13 mon2_pos" includes:

- input file: [] Browse BrowseN
- output file: no_file Browse BrowseN
- parameter directory: Y:/Tutorials/SANS_PSI Browse NewDir
- random seed: 1 random number generator: ran3 min. neutron weight: 1.0e-25 gravity: on
- monitor file: pos_detector.dat Browse BrowseN Edit Plot AutoPlot
- number of y-bins: 100 number of z-bins: 100
- minimal y-value [cm]: -50 maximal y-value [cm]: 50
- minimal z-value [cm]: -50 maximal z-value [cm]: 50
- probability weight: yes exclusive counts: no

At the bottom, there are three buttons: Big, Clear, and Save. Below them is a text area showing the simulation command line and a status message "description O.K.". The command line is:

```
Parameter directory is Y:/Tutorials/SANS_PSI
Starting simulation
K:/MODULES/source.exe -S1 --Z1 --U1.0e-25 --B10000 --PY:/Tutorials/SANS_PSI --LY:/Tutorials/SANS_PSI/vpipelog1 -aY:/Tutorials/SANS_PSI/src_sans.mod -n1000000 -m3 -y0.5 -M7 -z0.5 -d1 -f
|K:/MODULES/monitor1.exe -k1 --Z1 --U1.0e-25 --B10000 --PY:/Tutorials/SANS_PSI --LY:/Tutorials/SANS_PSI/vpipelog2 -OY:/Tutorials/SANS_PSI/mambda_src.dat -n50 -C0 -f0 -m3 -M7 -p1 -e0
|K:/MODULES/guide.exe --Z1 --U1.0e-25 --B10000 --PY:/Tutorials/SANS_PSI --LY:/Tutorials/SANS_PSI/vpipelog3 -Y2 -Z0 -w3 -h4 -W3 -H4 -p50 -N20 -R1000 -iY:/Tutorials/SANS_PSI/mirr1a.dat -iY
|K:/MODULES/mon2_pos.exe --Z1 --U1.0e-25 --B10000 --PY:/Tutorials/SANS_PSI --LY:/Tutorials/SANS_PSI/vpipelog4 -OY:/Tutorials/SANS_PSI/pos_guide.dat -y60 -z60 -w3 -W3 -h3 -H3 -p1 -e0
|K:/MODULES/space.exe --Z1 --U1.0e-25 --B10000 --PY:/Tutorials/SANS_PSI --LY:/Tutorials/SANS_PSI/vpipelog5 -d20
|K:/MODULES/vselect.exe --Z1 --U1.0e-25 --B10000 --PY:/Tutorials/SANS_PSI --LY:/Tutorials/SANS_PSI/vpipelog6 -i25 -s395.6 -w70 -c45 -r15 -o12.5 -d0.02
|K:/MODULES/monitor1.exe -k1 --Z1 --U1.0e-25 --B10000 --PY:/Tutorials/SANS_PSI --LY:/Tutorials/SANS_PSI/vpipelog7 -OY:/Tutorials/SANS_PSI/mambda_select.dat -n50 -C0 -f0 -m3 -M7 -p1 -e0
```

Output

- Every module writes to log file and instrument file
- This output comes for free

VITESS Output

Horizontal: Vertical : constant height

19 kink(s) with an angle of 0.0286 deg each
 Inside guide abutment loss is disabled
 The walls have no waviness

3 number of trajectories read : 999999
 number of trajectories written : 38198
 (time averaged) neutron count rate : 2.5239e+009 +/- 1.442e+007 n/s

VITESS version 2.6 module mon2_pos 1.2
 4 number of trajectories read : 38198
 number of trajectories written : 38198
 (time averaged) neutron count rate : 2.5239e+009 +/- 1.442e+007 n/s

VITESS version 2.6 module Space 1.0a
 Distance between entrance and exit plane: 20.000 cm
 Center of beam at exit: (20.000, -0.253, -0.002) cm, TOF = 15.8940 ms

5 number of trajectories read : 38198
 number of trajectories written : 38198
 (time averaged) neutron count rate : 2.5239e+009 +/- 1.442e+007 n/s

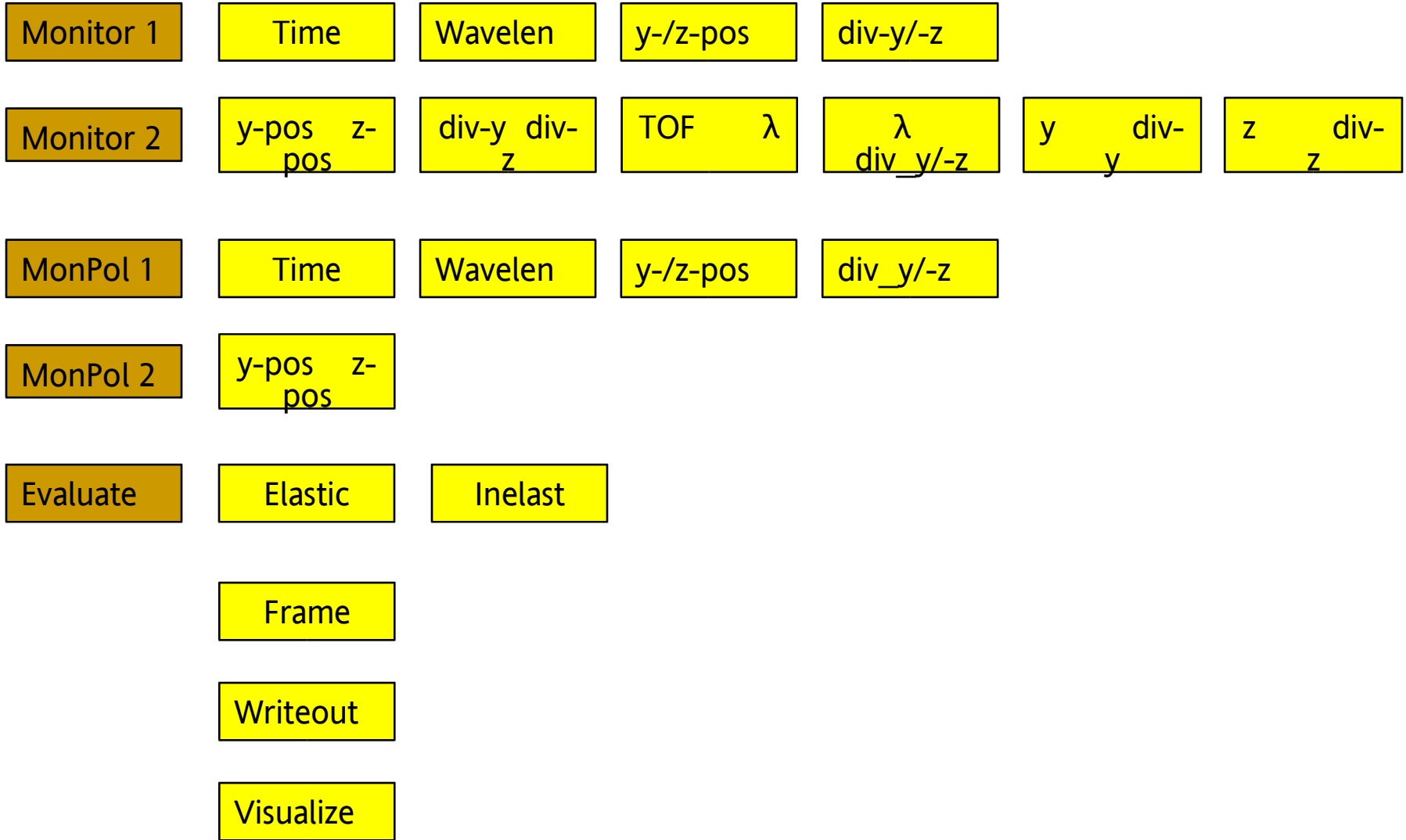
VITESS version 2.6 module velselect 1.2a
 6 number of trajectories read : 38198
 number of trajectories written : 4892
 (time averaged) neutron count rate : 4.1554e+008 +/- 5.983e+006 n/s

VITESS version 2.6 module monitor1_wavelength 1.6
 Binning : 50 bins from 3.00000 to 7.00000 Ang
 File : Y:\Tutorials\SANS_PSI\lambda_select.dat
 total neutron count rate within binning and eval. time: 4.1554e+008 n/s

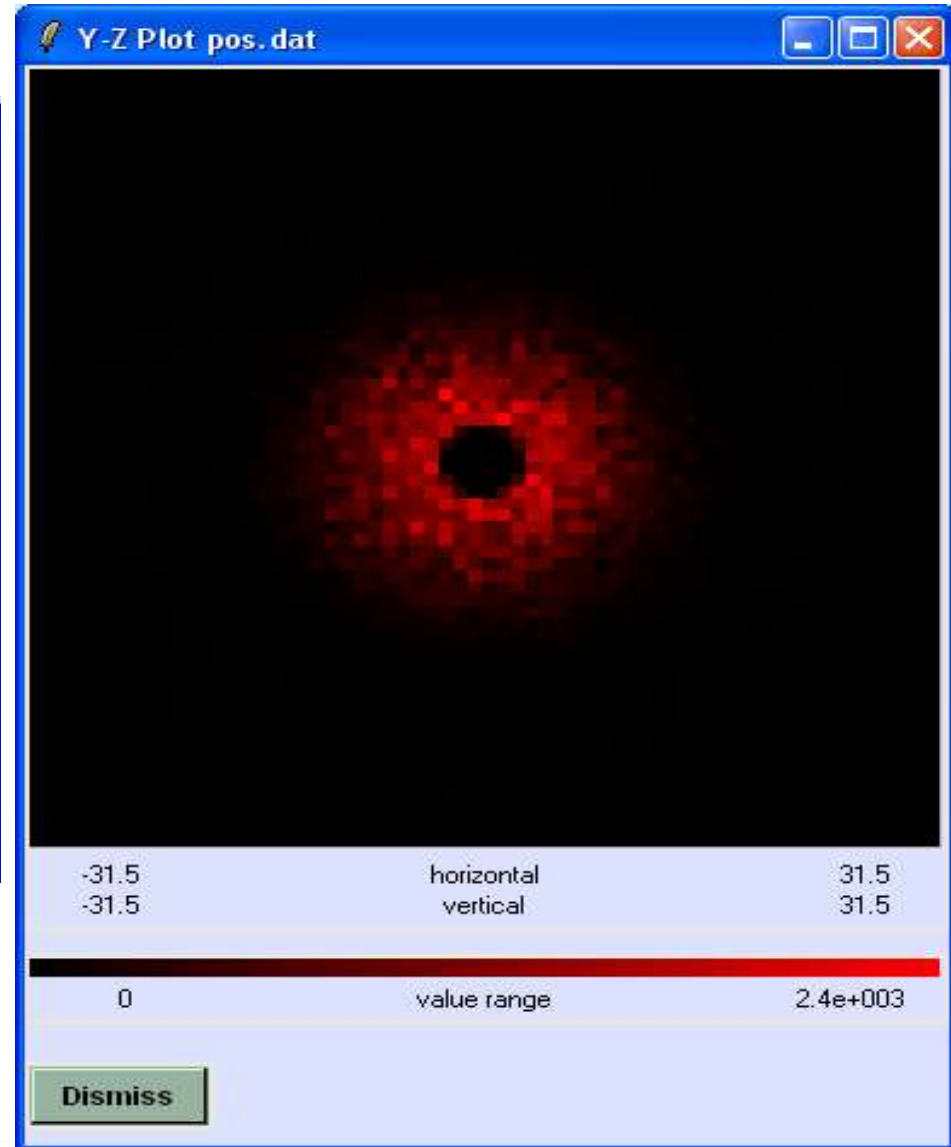
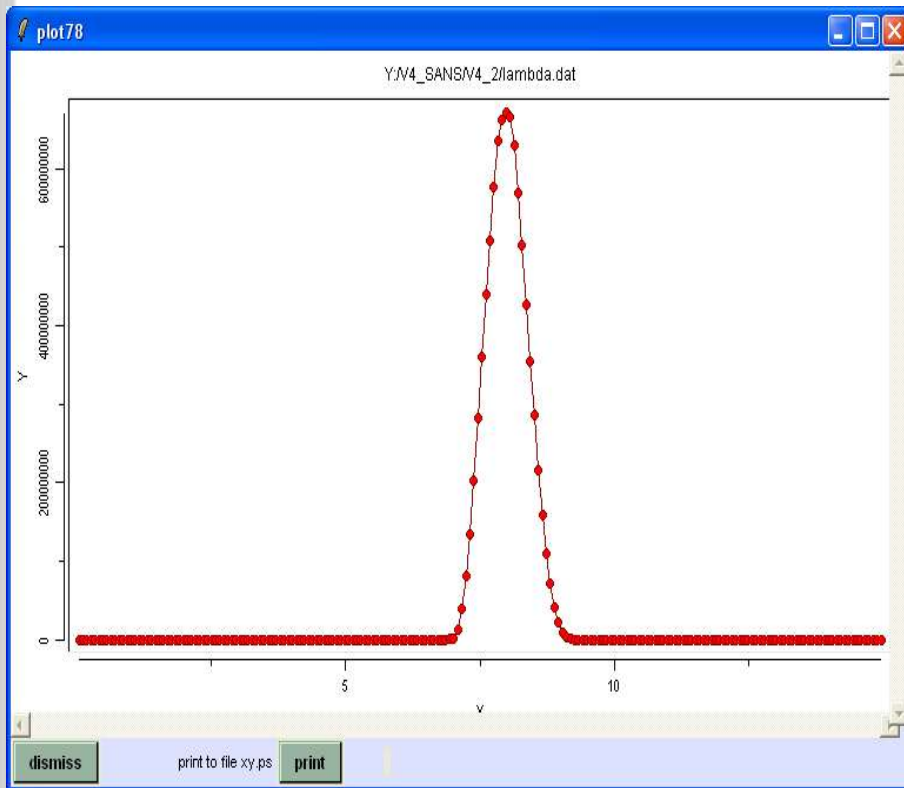
7 number of trajectories read : 4892
 number of trajectories written : 4892
 (time averaged) neutron count rate : 4.1554e+008 +/- 5.983e+006 n/s

#	No	ID	module	len [m]	x [m]	y [m]	z [m]	hor. [deg]	ver.	W-Par.	H-Par.	R-Par.	number	type	Descr
0	1		Source and Window	0.000	0.000	0.000	0.000	0.000	0.000	1.8000e+001	0.0000e+000	0.0000e+000	1	1	30.0 K
1	1		Source and Window	2.000	2.000	0.000	0.000	0.000	0.000	3.0000e+000	0.0000e+000	0.0000e+000	0	0	
2	101		monitor1_wavelength	2.000	2.000	0.000	0.000	0.000	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	1	
3	11		guide	12.000	12.000	0.047	0.000	0.544	0.000	3.0000e+000	3.0000e+000	1.0000e+003	20	20	
4	102		mon2_pos	12.000	12.000	0.047	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0	
5	20		Space	12.200	12.200	0.049	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0	
6	41		velselect	12.450	12.450	0.051	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0	
7	101		monitor1_wavelength	12.450	12.450	0.051	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	1	
8	21		Window	12.450	12.450	0.051	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0	
9	21		Window	20.450	20.450	0.127	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0	
10	87		sample_sans	20.500	20.500	0.127	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	1	
11	21		Window	28.400	28.400	0.202	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0	F
12	71		detector	28.500	28.500	0.203	0.000	0.544	0.000	1.0000e+002	1.0000e+000	8.0000e+002	1	2	
13	102		mon2_pos	28.500	28.500	0.203	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0	
14	111		eval_elast	28.500	28.500	0.203	0.000	0.544	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	2	

Modules for Monitoring



Graphical output



Tools

AsciiToBinary

GenerMirrorFile

ChopPhases

DefineDirection

GenerSurfFile

ChopSystem

Direct View

StdDeviation

DistTimePlot

GenerateBatch

LatticeDist.

VisualOutput

CrysAnalySpec

- Tool can be used
 - to generate input files
 - to visualize output data
 - to help designing the instrument

Series of Simulations

L_eff [cm]	take-off [deg]	h	k	l	coll 1 [min]	num traj.	impile window 2				coll. 1				mono.			lambda		
137.0	60.0	1	1	3	30.0	15000000	-3.50	3.50	-6.00	6.00	9.6	9.6	15	0.0125	137.0	547.8	Ge113_060.par	1.686	1.726	1.7060
137.0	90.0	1	1	5	30.0	15000000	-2.25	2.25	-5.00	5.00	9.6	9.6	15	0.0125	193.7	387.4	Ge115_090.par	1.520	1.560	1.5399
137.0	90.0	1	1	5	10.0	15000000	-2.25	2.25	-5.00	5.00	9.7	9.7	44	0.0113	193.7	387.4	Ge115_090.par	1.520	1.560	1.5399
137.0	135.0	3	3	5	10.0	15000000	-1.75	1.75	-3.50	3.50	9.7	9.7	44	0.0113	253.1	0.0	Ge335_135.par	1.574	1.614	1.5943

Generate Series

Name	number_o	min_y	max_y	min_z	max_z	enter_wid	exit_width	num_chan	spacer_w	cradius	chradius	parfile	min_wave	max_wave	refwave	refwave
Option	1:n	4:w	4:W	4:h	4:H	6:w	8:W	6:b	8:s	12:r	12:s	12:P	1:m	1:M	25:r	26:r
delta	0									0	0	0	0	0		0
1.	15000000	-3.50	3.50	-6.00	6.00	9.6	9.6	15	0.0125	137.0	547.8	Ge113_06	1.686	1.726	1.7060	1.7060
2.	15000000	-2.25	2.25	-5.00	5.00	9.6	9.6	15	0.0125	193.7	387.4	Ge115_09	1.520	1.560	1.5399	1.5399
3.	15000000	-2.25	2.25	-5.00	5.00	9.7	9.7	44	0.0113	193.7	387.4	Ge115_09	1.520	1.560	1.5399	1.5399
4.	15000000	-1.75	1.75	-3.50	3.50	9.7	9.7	44	0.0113	253.1	0.0	Ge335_13	1.574	1.614	1.5943	1.5943

Step Selection

Files to be copied

Copy Target Directory

<< Cancel

4 Iterations

space separated Module:Option:Name list
name may be omitted
e.g. 1:n 3:P

1:n:number_of_neutrons 4:w:min_y 4:W:max_y 4:h:min_z 4:H:max_z 6:w:enter

Cancel >>

all

instrument.inf impile_exit.mtl impile_exit.pos collim1

Y:/C3PO/C3PO_6_Detector/SeriesA

Import Table File Series Start Series

'Instrument Digest'

Define Instrument Digest

space separated list of Name:Module and free variable items e.g.
 wavelength min_width:1 max_width:1
 where wavelength is a free variable, and the next two belong to module 1

deswl:1 rounds:7 min_wavelength:1 max_wavelength:1 offset:7

Cancel >>

Instrument NEAT_test_digest

VITESS 2.6

Click parameter names for help!

Check Start Kill Stop

input file Browse BrowseN

output file chop.int Browse BrowseN

parameter directory Y:/NEAT/NEAT_Test Browse NewDir

random seed 1 min. neutron weight 1.e-25 gravity on

Fresh Exit

Instrument Digest

1 source_const_wave

2 mon1 lambda

Instrument Digest

desired wavelength [A] 3 rounds / min. 5000

min. wave-length [A] 1 max. wave-length [A] 5 offset [deg] 843.64762

Propagate Values Change Digest

Define Instrument Digest

deswl:1 edit store formula

rounds:7 edit store formula

min_wavelength:1 edit store formula

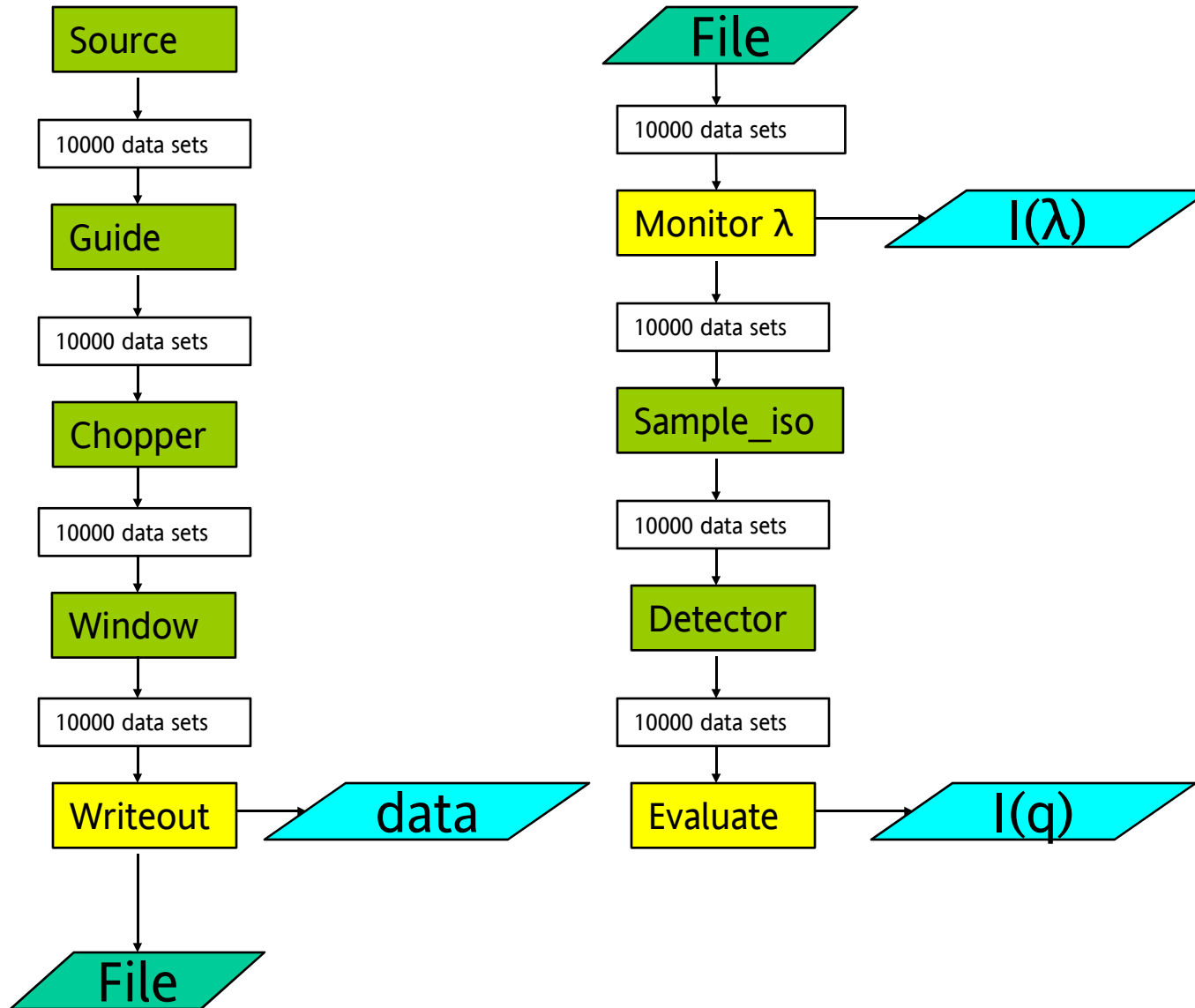
max_wavelength:1 edit store formula

offset:7 edit store formula

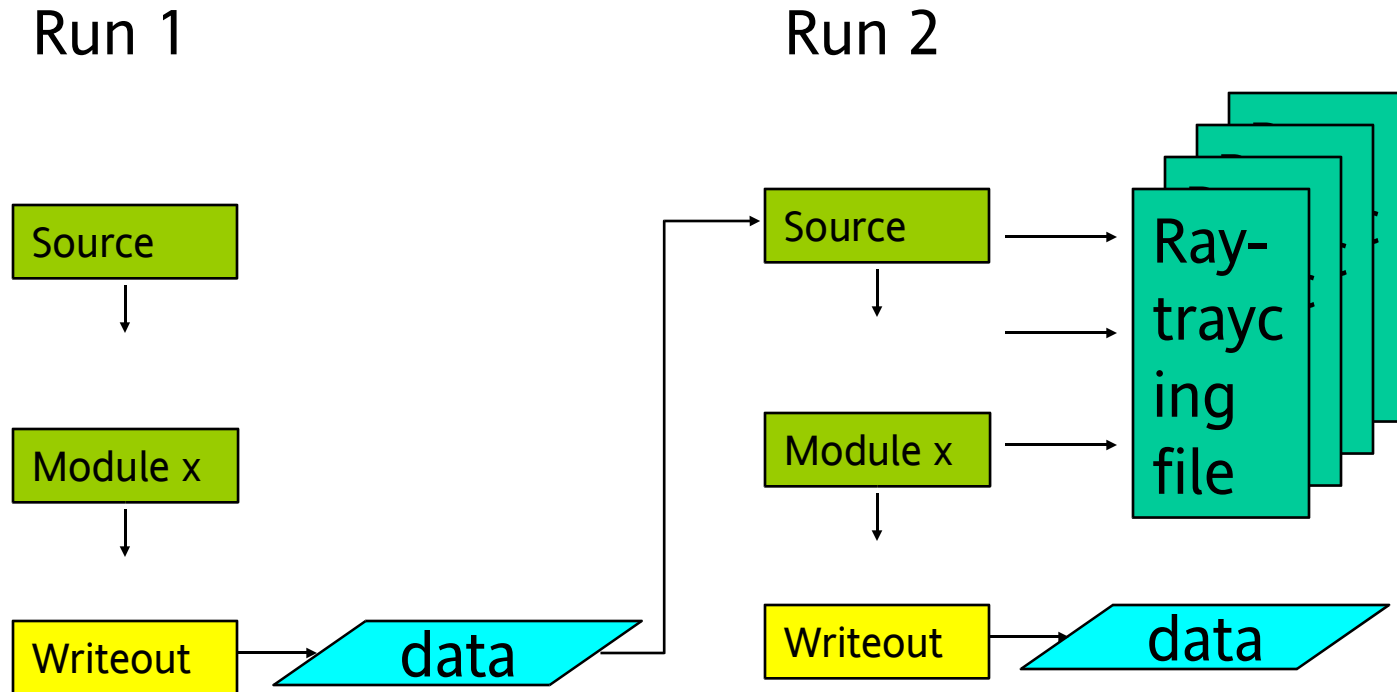
<< Cancel >>

Programme/ViteSS2_6
 lgui successfully loaded ---
 test.gui successfully loaded ---

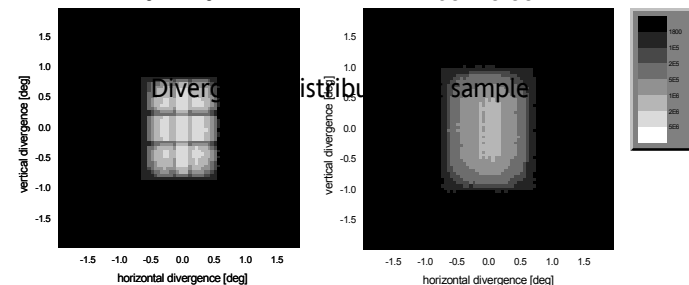
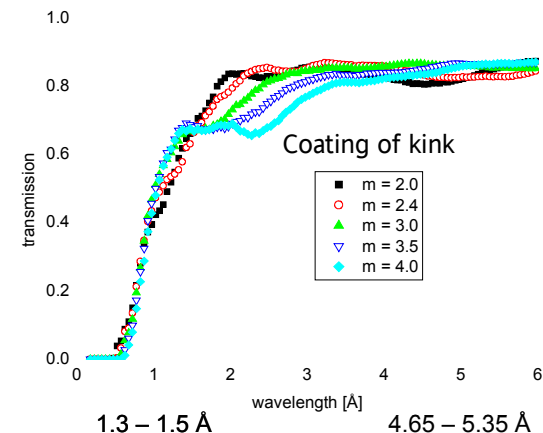
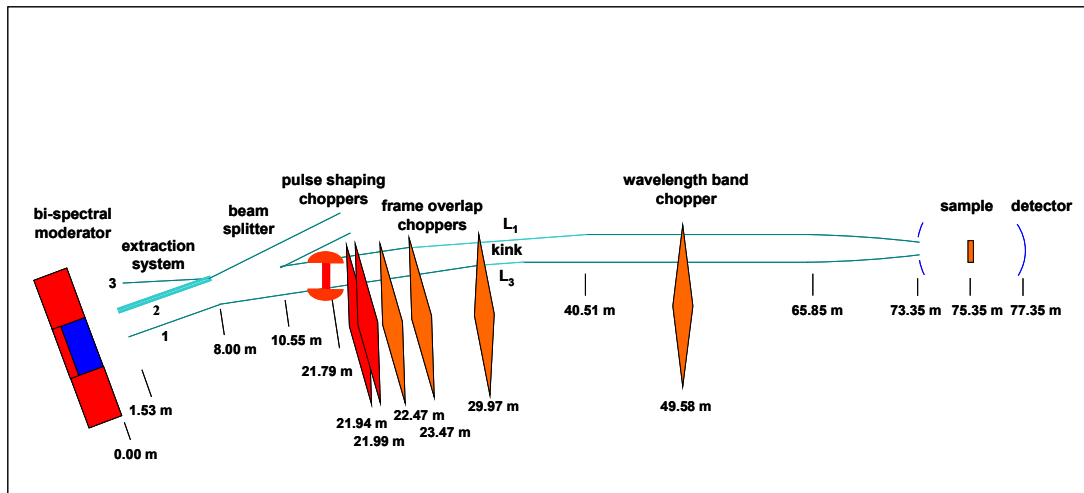
Splitting of the Simulation



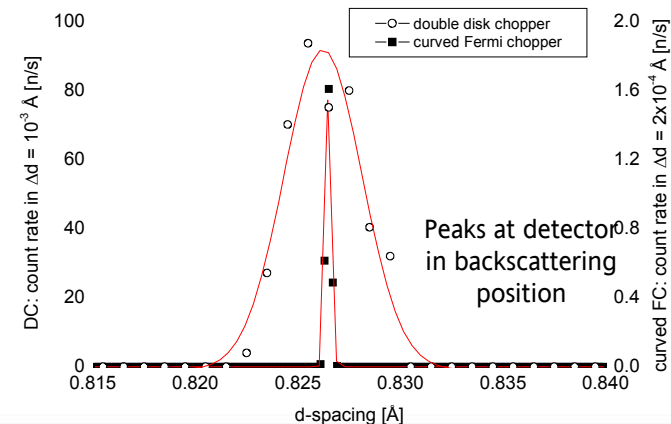
Ray tracing



TOF powder diffractometer EXED at HMI

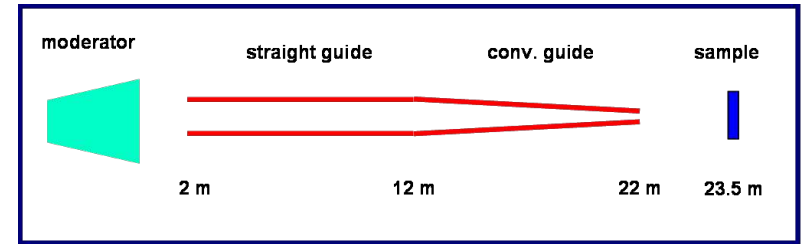
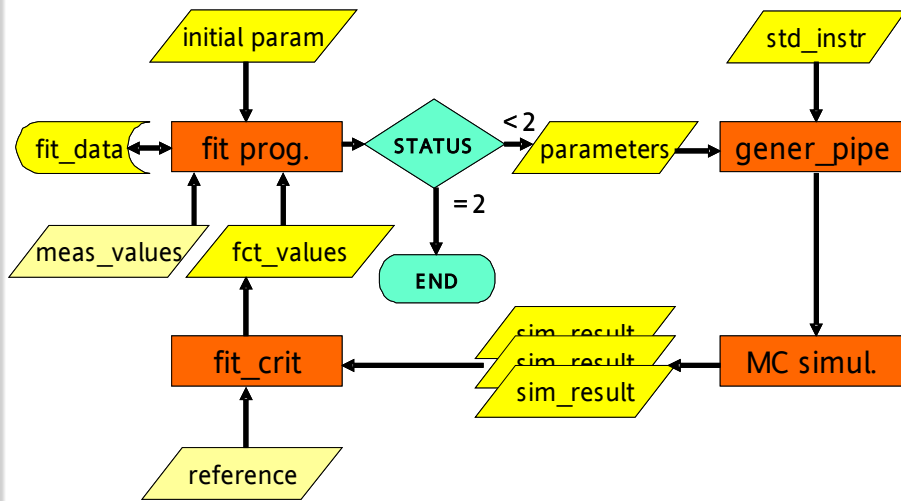


- Concept of EXED
 - TOF diffractometer
 - beam extraction system to use neutrons of cold and thermal moderator
 - kink to suppress hot neutrons
 - pulse generation by double chopper system or Fermi chopper
 - elliptic tapered guide
- Whole instrument simulated and optimized
- Results
 - resolution of 2×10^{-4} possible

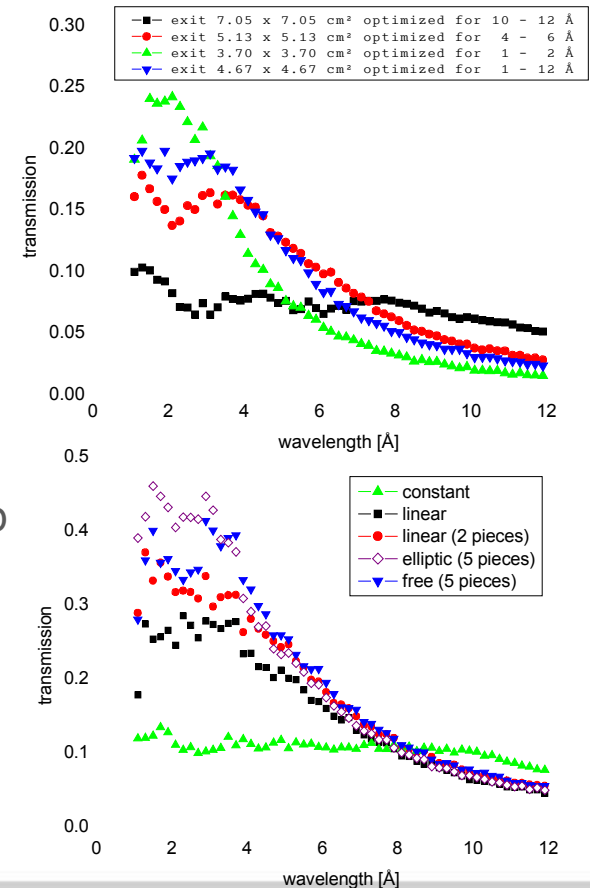


J. Peters, K. Lieutenant, D. Clemens, F. Mezei, Z. Kristall. (accepted for publication)
 K. Lieutenant, J. Peters, F. Mezei, J. Neutron Res. (submitted for publication)

Optimization (of guide exits)



- MC simulation and numerical optimisation combined
 - Instrument split into 2 parts
 - About 500000 trajectories treated in the 2nd part of the simulation
 - Exit varied and MC simulation performed for each set-up
- Calculations performed on model instrument and real instruments



K. Lieutenant, G. Zsigmond, Physica B 350, Suppl. 1 (2004) E687-689.
 K. Lieutenant et al., SPIE Proc. 5536 (2004) 134-145.
 K. Lieutenant, J. Phys.: Cond. Matter 17 (2005) S167-S174.

Task in Tutorial: Simulation of a SANS Instrument

VITESS tutorial – MC workshop at PSI

02. oct 2006

2

Task: designing a SANS instrument on a reactor source

1. Source

The instrument is placed on the thermal source of a reactor. The effective surface has a size of 18 cm diameter. The flux at the surface is 1×10^{13} n/(cm²s). It is described by a Maxwellian distribution of 30 K.

- Monitor the wavelength distribution in a window of 3 x 4 cm² (W x H) in 2 m distance between 3 and 7 Å

- What is total intensity in [n/s] ?
- What is the (spatially) averaged flux ?
- Which wavelength delivers the highest intensity ?

Alternative task: Describe the source by 2 Maxwellians of 30 K (75% of the total intensity) and 300 K

2. Guide

Transport the neutrons to the instrument by means of a 10 m long nickel-coated (mirr1a.dat) curved guide of 1000 m radius consisting of 50 cm pieces and a cross-section of 3 x 4 cm² (W x H) starting 2 m from the moderator

- Check the positions of the components using the 'instrument.inf' file
- Monitor the spatial distribution of the intensity

3. Velocity selector

Add a velocity selector of 25 cm length and 30 cm diameter and 45° twist angle 20 cm behind the end of the guide to select neutrons of 5 Å. 70 blades of 0.2 mm thickness shall be used.

- What is the maximal usable distance between the axle and the centre of the guide ?
- Which rotational speed has to be used ?
- Check the average wavelength and its FWHM by a monitor

4. Windows

Put apertures of 2 x 2 cm² directly behind the guide and in a distance of 8 m.

- What is the intensity behind the 2nd aperture

5. Sample

Put a rectangular sample of 1 x 1 cm diameter and 1 mm thickness 5 cm behind aperture 2. It has to simulate the scattering of spherical sample of 100 nm diameter taking 10 % volume fraction. Density of the sample is 4×10^{19} cm⁻², for the surrounding it is 1×10^{19} cm⁻². Scattering into a 1 x 1 m detector in 8 m distance shall be regarded.

- Which fraction of the neutrons is scattered

Alternative task: use a cylindrical sample of 1 cm diameter and 1 mm thickness

6. Beamstop (module 'spacewindow')

Put a beam-stop of 5 x 6 cm² in a distance of 7.9 m from the sample

- Is that size sufficient to catch all neutrons that are not scattered ?

7. Detector

Put a detector of 1 x 1 m² size, 2 cm thickness, 1 x 1 cm² resolution and 90 % efficiency 8 m after the sample.

- Check the positions of the components using the 'instrument.inf' file
- Monitor the distribution of neutrons over the detector
- Evaluate the detector count rate as a function momentum transfer (module 'eval_elast') from $Q = 0.001 \text{ \AA}^{-1}$ to 0.1 \AA^{-1} logarithmically.
Hint: don't forget to give the wavelength used

Thank you for your attention !