



- VITeSS team
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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, especially for the ESS
- 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
 - 2005: Collaboration with McStas in VnCS
 - 2006: published under GNU public license

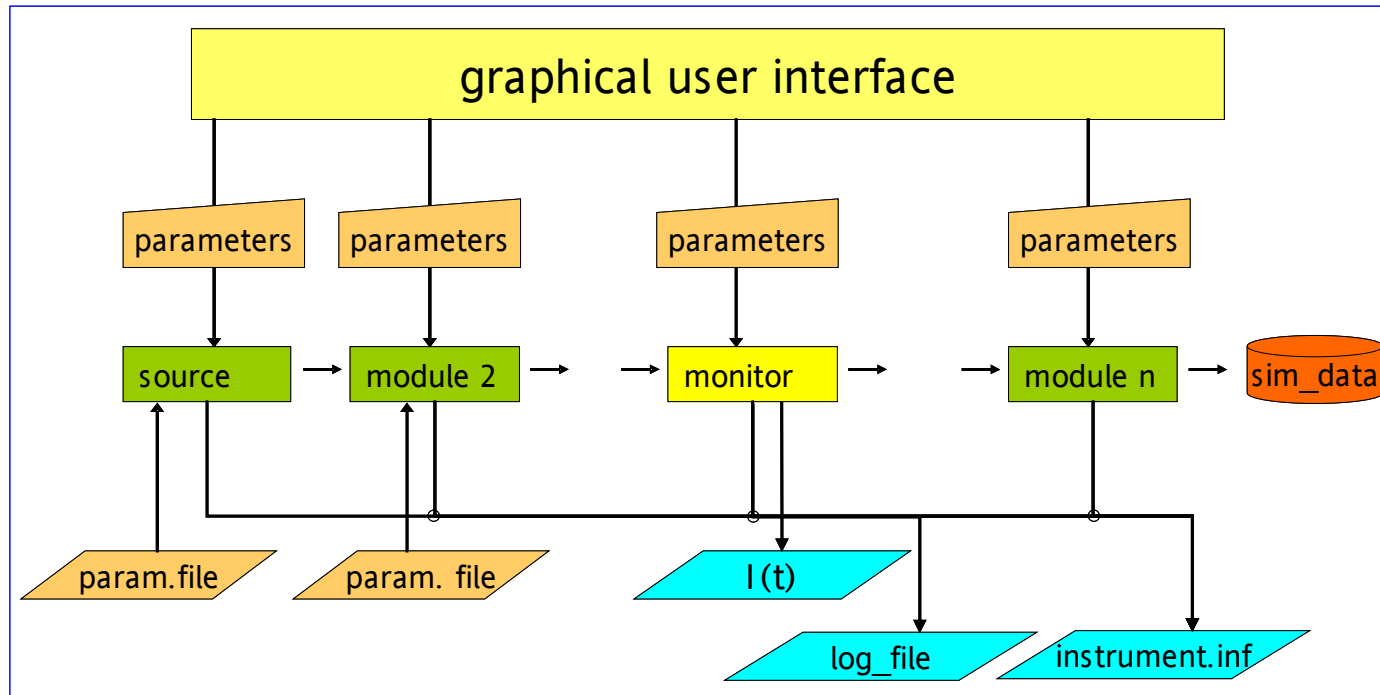
Some general features

- Staff
 - 9 persons from 6 different facilities in the development team
 - Open to new members
- Published under GNU public licence
 - Free of charge
 - Can be downloaded from internet
 - Code developed by a limited number of persons
- Program and platforms
 - Written in C
 - 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
 - Download includes everything needed for simulations and basic visualisation
- 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
 - Components automatically positioned
 - Advanced users can write own modules or change existing ones
- VITESS has all essential features
 - 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
- Challenges
 - Information about the whole instrument
 - Calculation of dependent 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

File **Edit** **Configure** **Tools** **Options** **Help**

Instrument 1 **VITESS 2.7** Click parameter names for help!

Check **Start** **Kill** **Stop** **Fresh** **Exit**

input file Browse BrowseN

output file Browse BrowseN

parameter directory Browse NewDir

random seed random number generator min. neutron weight gravity

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**

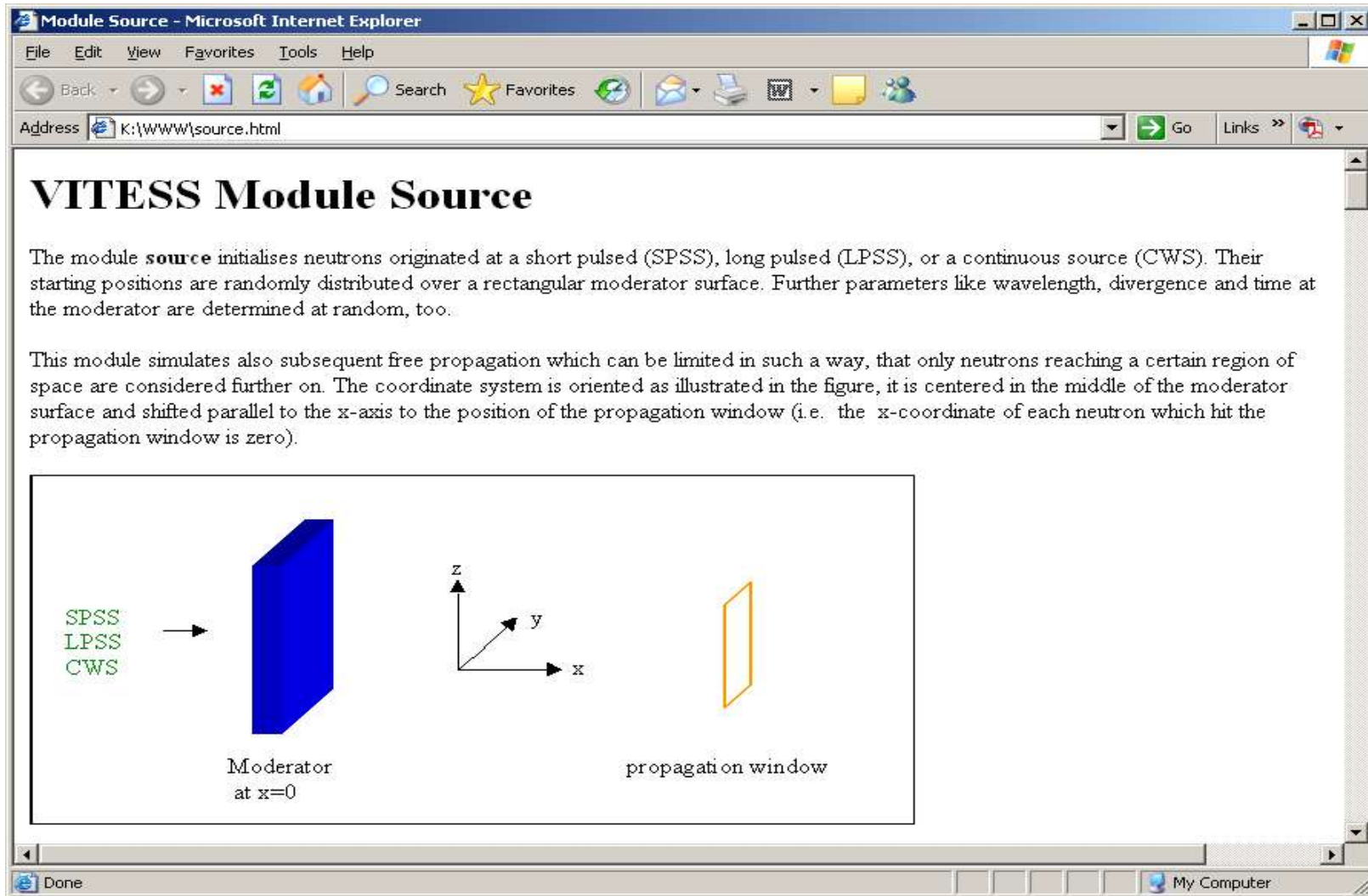
Troubleshooting

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**

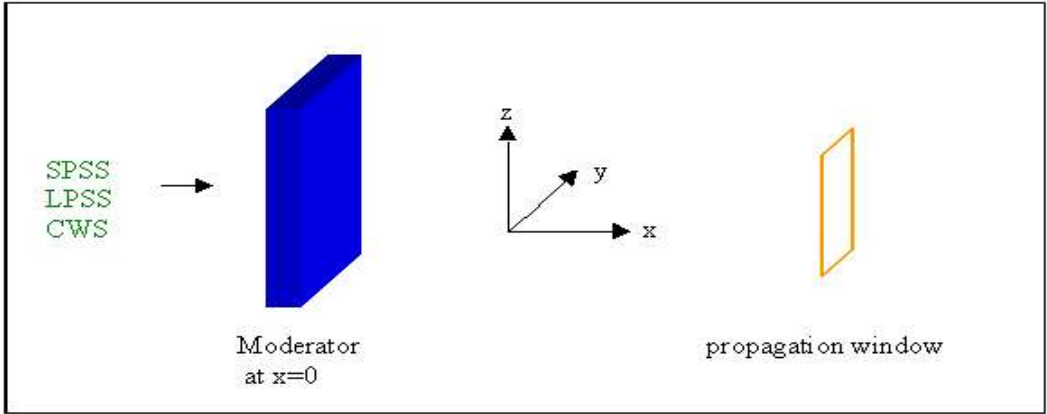
Help



VITESS Module Source

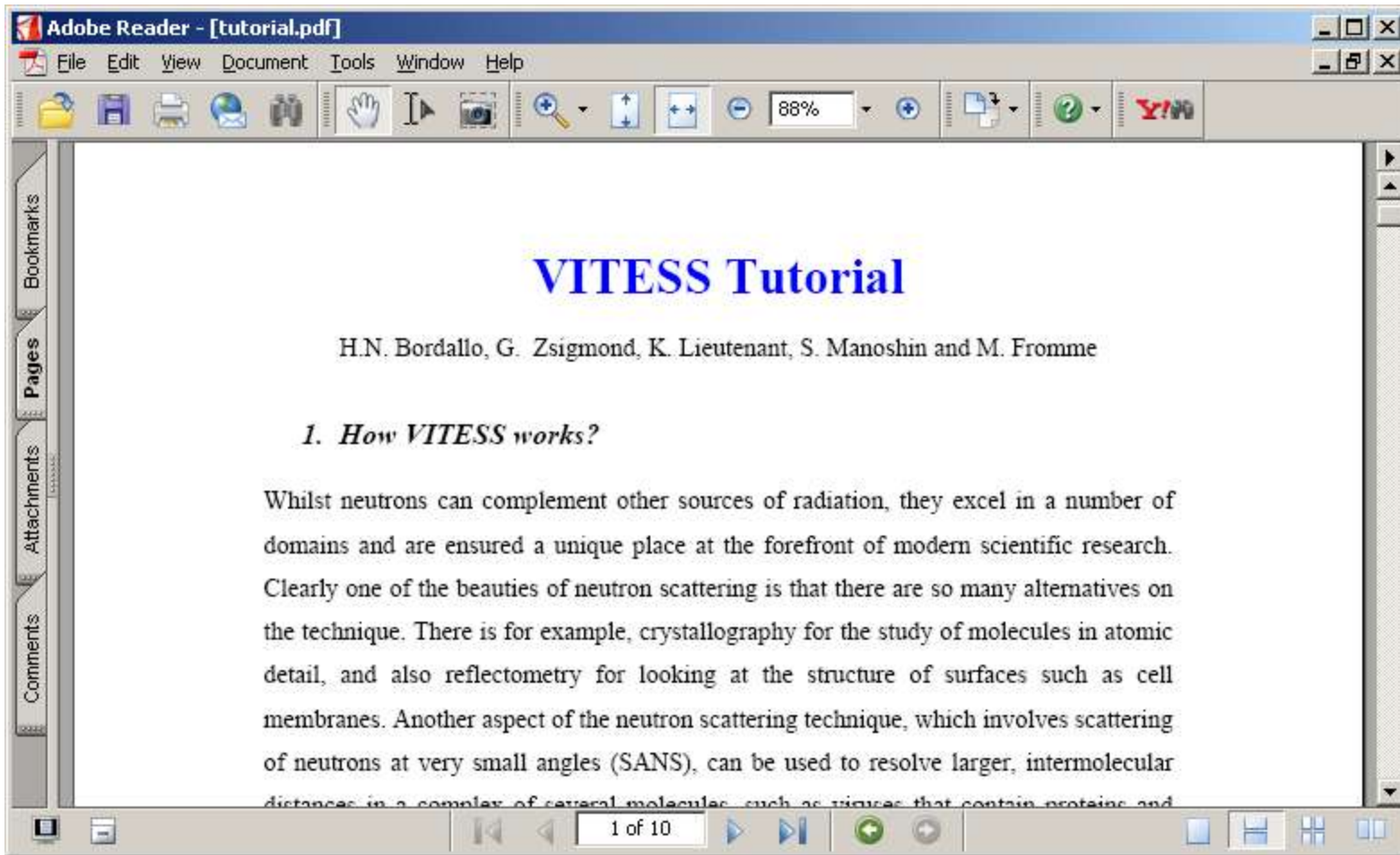
The module **source** initialises neutrons originated at a short pulsed (SPSS), long pulsed (LPSS), or a continuous source (CWS). Their starting positions are randomly distributed over a rectangular moderator surface. Further parameters like wavelength, divergence and time at the moderator are determined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



Done My Computer

Tutorial



The screenshot shows the Adobe Reader interface with the following elements:

- Title Bar:** Adobe Reader - [tutorial.pdf]
- Menu Bar:** File, Edit, View, Document, Tools, Window, Help
- Toolbar:** Includes icons for file operations (Open, Save, Print, Copy, Paste), navigation (Home, Previous, Next, Last), zoom (88%), and search.
- Left Panel:** Bookmarks, Pages, Attachments, Comments
- Main Content Area:**
 - ## 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
- Bottom Panel:** Navigation controls and page indicator showing "1 of 10".

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

Xcontrol K: File Edit Configure Tools Options Help

Instrument SANS VITESS 2.7 Click parameter names for help!

Check Start Kill Stop

input file Browse BrowseN

output file Browse BrowseN

parameter directory Browse NewDir

random seed random number generator min. neutron weight gravity

Exit

Module 13 mon2_pos

monitor file Browse BrowseN Edit Plot AutoPlot

number of y-bins number of z-bins

minimal y-value [cm] maximal y-value [cm]

minimal z-value [cm] maximal z-value [cm]

probability weight exclusive counts

1 source_const_wave 2 mon1_lambda 3 guide 4 mon2_pos 5 space 6 velselect 7 mon1_lambda 8 spacewindow 9 spacewindow 10 sample_sans 11 spacewindow

Big Clear Save

description O.K.

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/velselect.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

VITESS version 2.6 module Source and Window 1.13

> Simulation of constant wave source <

moderator temperature : 30.000 K
 total neutron flux (in 2*pi) : 1.0000e+013 n/(cm*s)
 moderator position : (0.000 0.000 0.000) cm
 moderator diameter : 18.000 cm
 divergence defined by propagation window
 time averaged neutron current: 1.2137e+011 n/s in 0.000300 str
 wavelength band used : 3.000 Ang - 7.000 Ang

real window (WxH) : 3.000 cm x 4.000 cm
 in a distance of : 2.000 m
 with a declination of : 0.000°
 polarization : 0.000 % X: 1.000 Y: 0.000 Z: 0.000
 Center of beam at window : (200.000 0.000 -0.001) cm
 Average TOF : 2.285 ms

Gravity is enabled
 Cutoff probability per traj. : 1.000e-025

number of trajectories started : 1000000
 1 number of trajectories read : 0
 number of trajectories written : 999999
 (time averaged) neutron count rate : 8.8402e+010 +/- 9.613e+007 n/s

VITESS version 2.6 module monitor1_wavelength 1.6
 Binning : 50 bins from 3.00000 to 7.00000 Ang
 File : Y:/Tests/SANS_PSI/lambda_src.dat
 total neutron count rate within binning and eval. time: 8.8402e+010 n/s

2 number of trajectories read : 999999
 number of trajectories written : 999999
 (time averaged) neutron count rate : 8.8402e+010 +/- 9.613e+007 n/s

VITESS version 2.6 module guide 2.12c

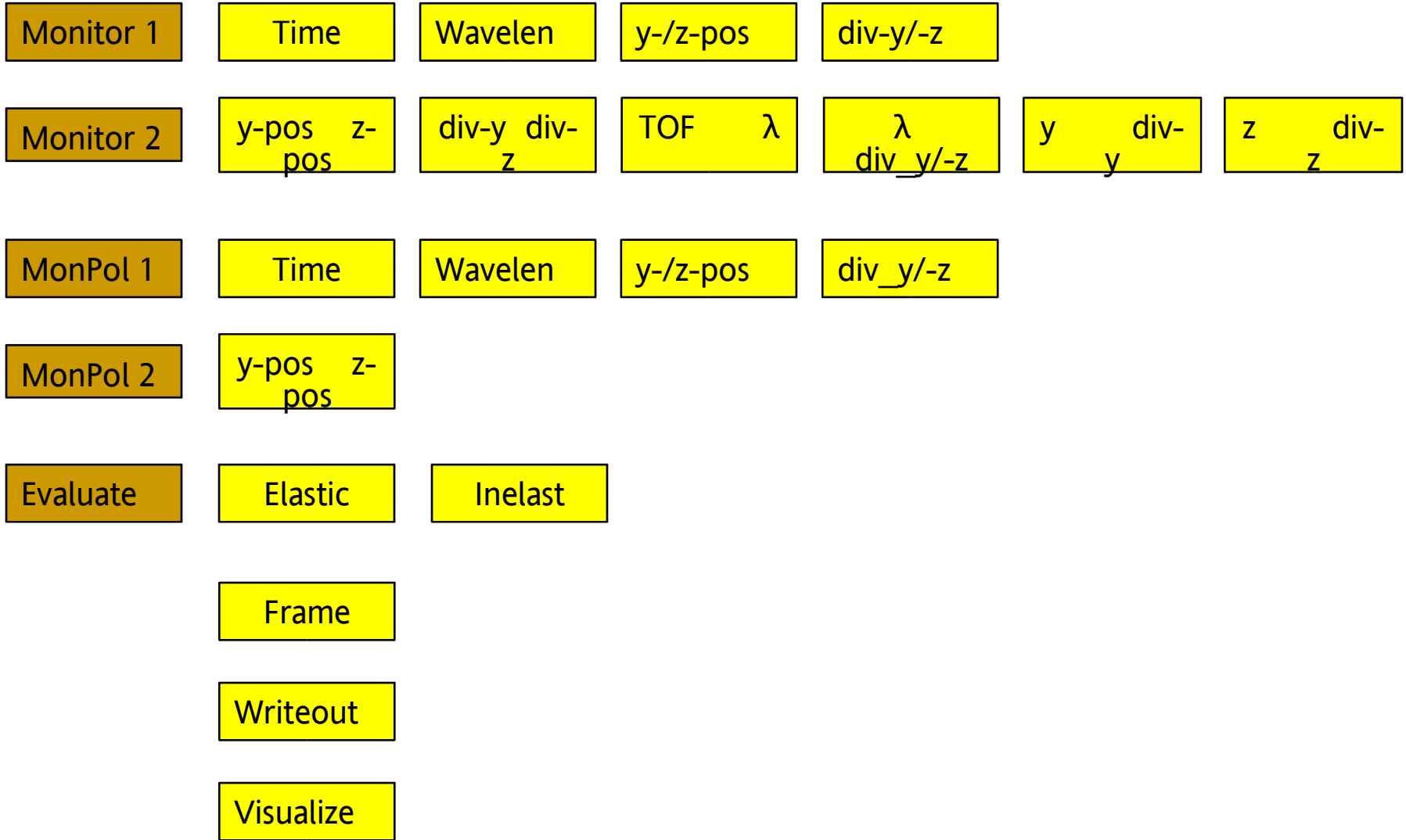
NOTE: coating of top wall also used for bottom wall

Total length of guide : 10.000 m
 Width x Height : 3.000 x 4.000 cm²

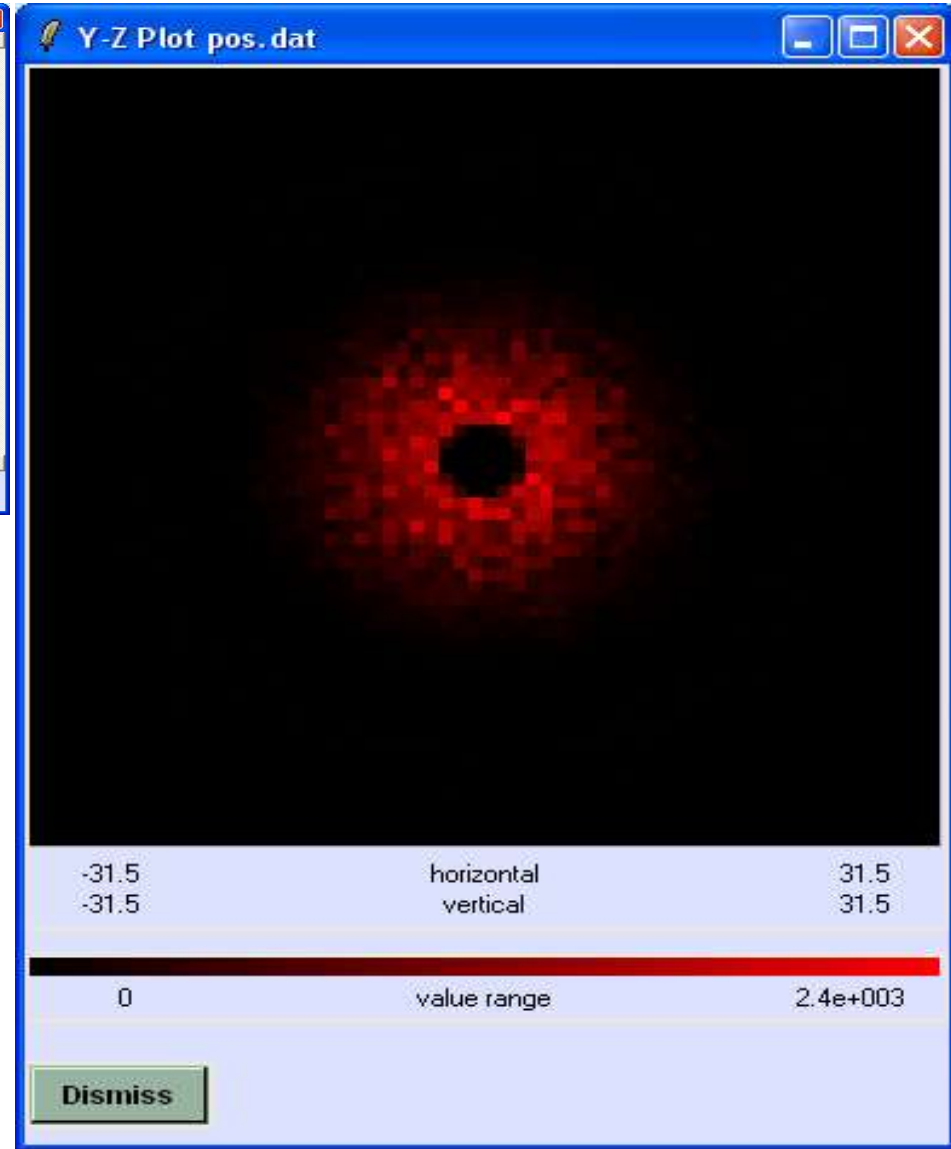
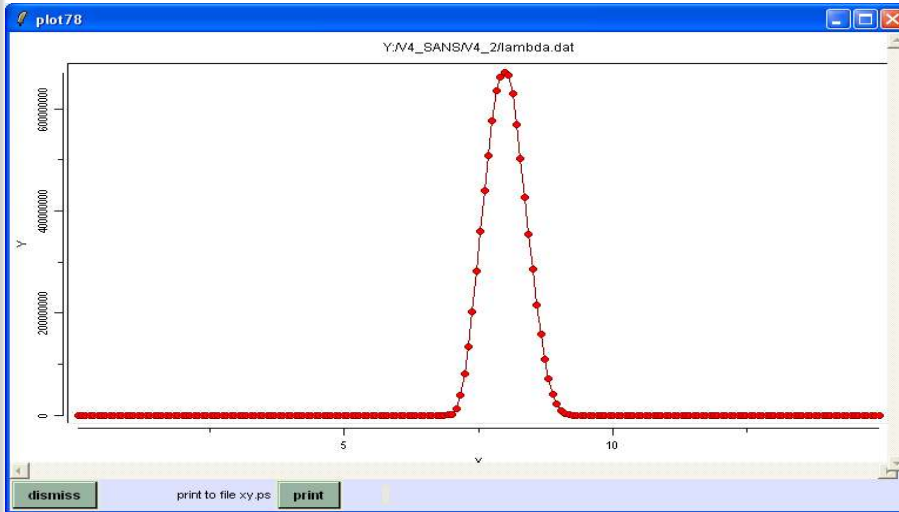
Edit Instrument File

#	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	

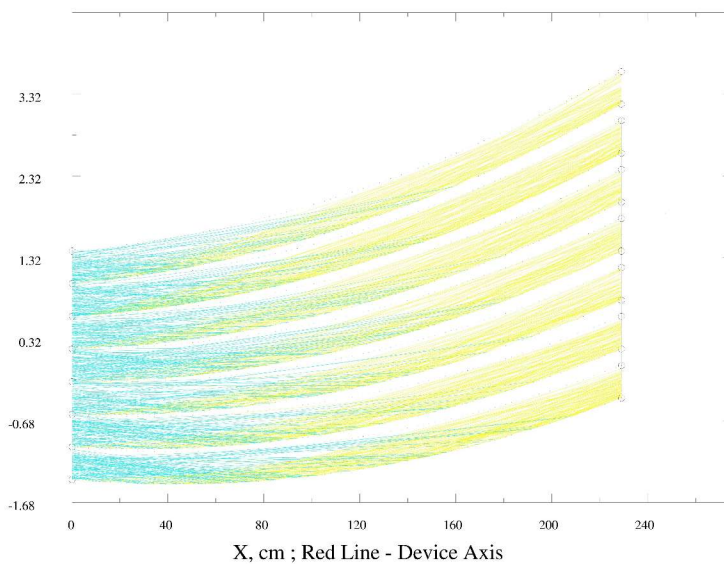
Modules for Monitoring



Graphical output



Y, cm Bender Surfaces Visualisation WITHOUT crosstalk between channels



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

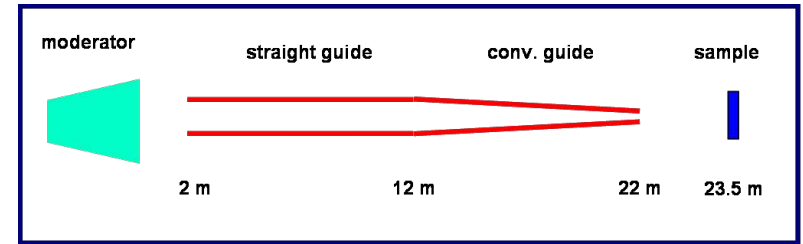
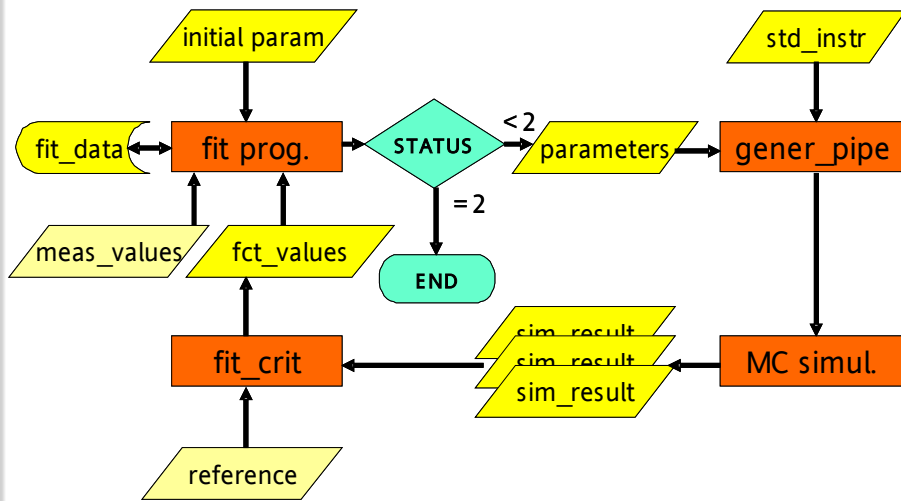
Y:/C3PO/C3PO_6_Detector/SeriesA

Import Table File Series Start Series

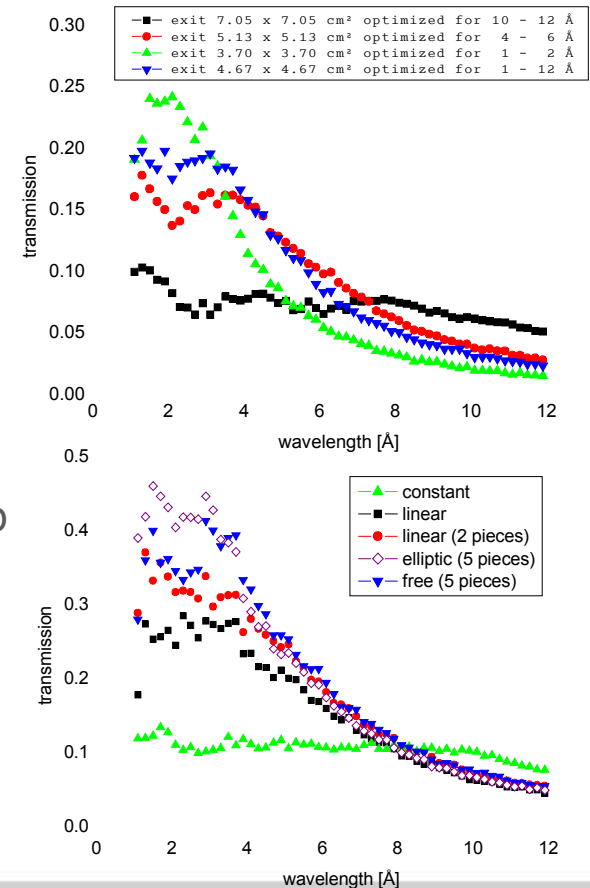
Additional Features

- Tools can be used
 - to generate input files
 - to visualize output data
 - to help designing the instrument
- Splitting of the simulation possible
- Treatment of dependent parameters possible
- Special ray tracing options (to follow individual trajectories)
- Option to mark and identify trajectories by 'colour'

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.

New features in VITESS 2.7

- Numerical optimization
- Double (or single) focusing monochromator with slabs in a flat plane
- ISIS source improved
- Virtual propagation window

To come soon

- 3D instrument visualisation
- Time dependent magnetic fields
- Modules for ultra-cold neutrons

- We continue with
 - A demonstration of the new tool to visualize the instrument by Phillip Bentley
 - Examples of using polarized neutrons by Sasha Ioffe and Sergey Manoshin