Introduction to VITESS

- 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, 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

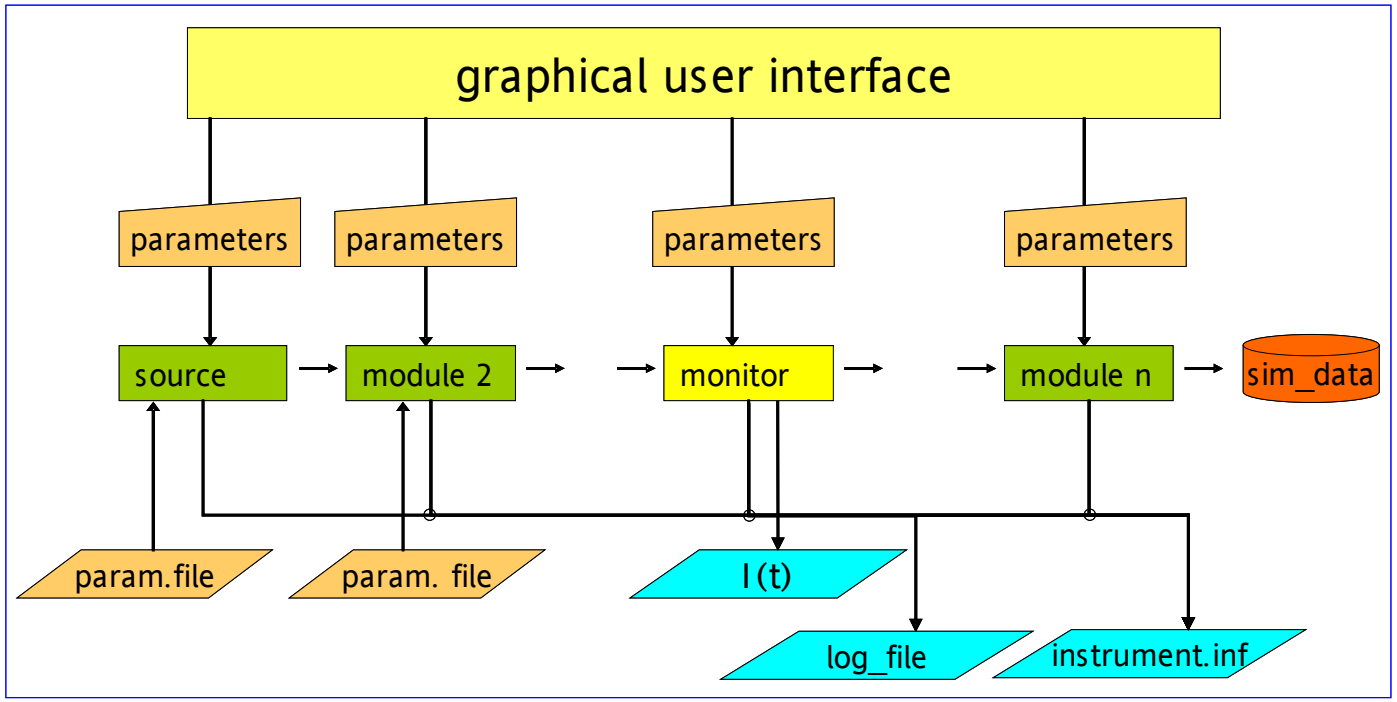
Some general features

- 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

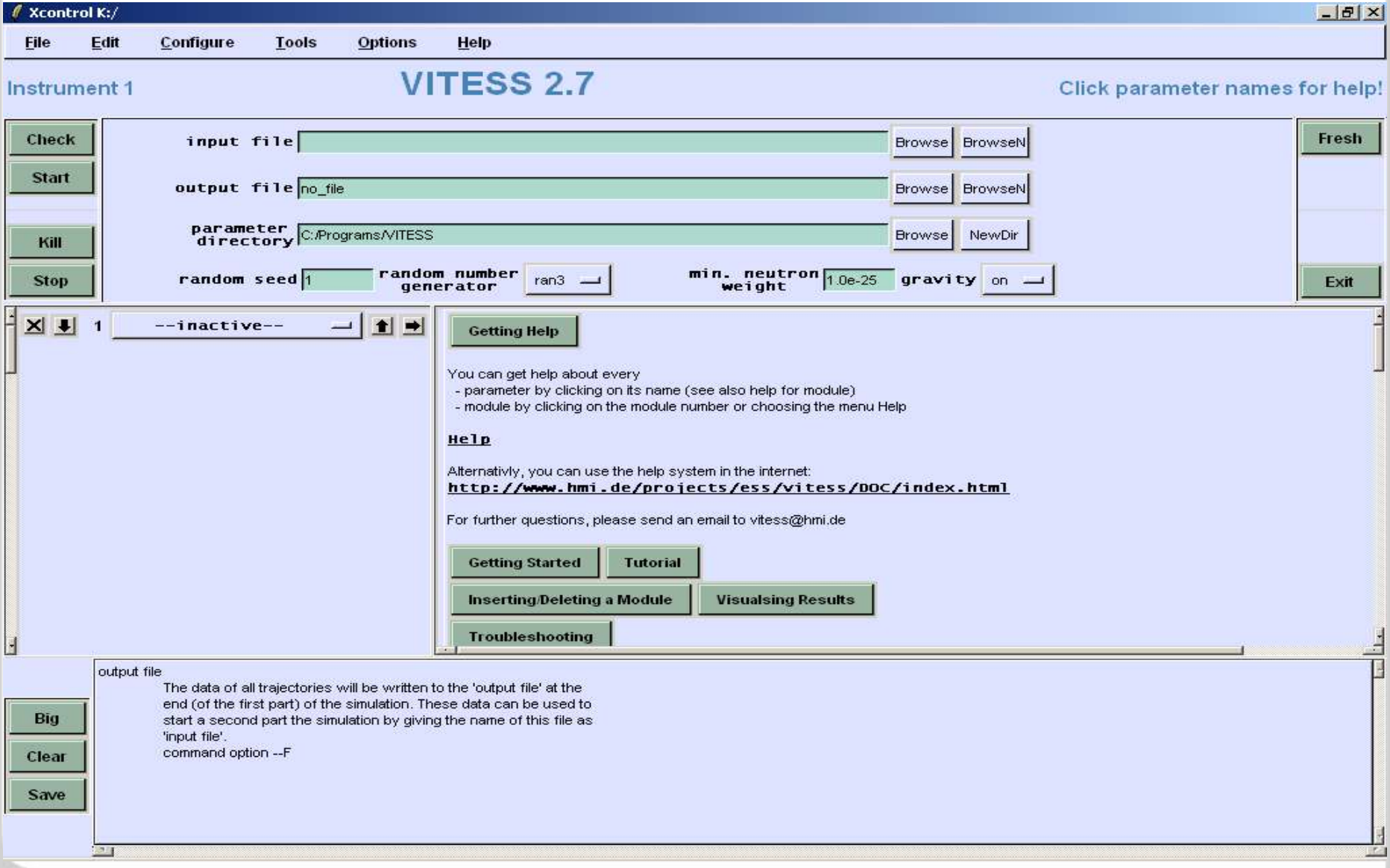


- Advantages of the piping concept:
  - No need of large memories
  - Shorter calculations times
  - Instrument can easily be split
- Disadvantages
  - Little information about the whole instrument
  - No calculation of dependent parameters (from some independent parameters)

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



Help

Module Source - Microsoft Internet Explorer

File Edit View Favorites Tools Help

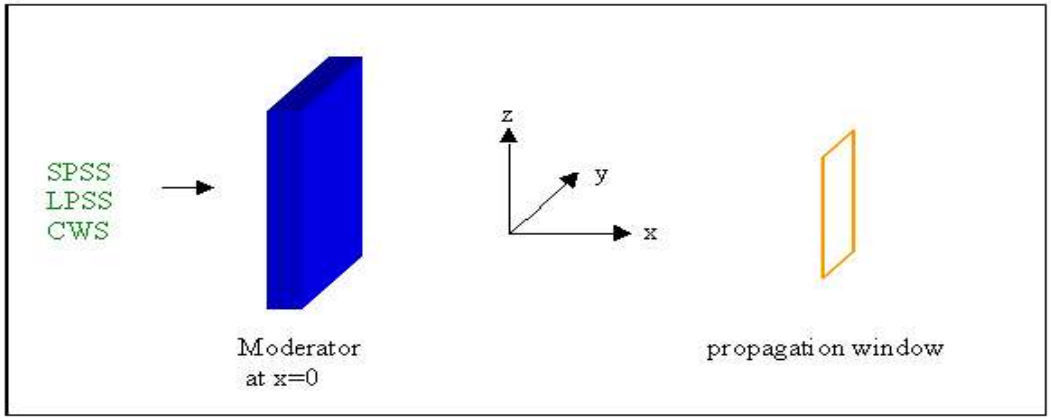
Back Search Favorites

Address K:\WWW\source.html Go Links

VITESS Module Source

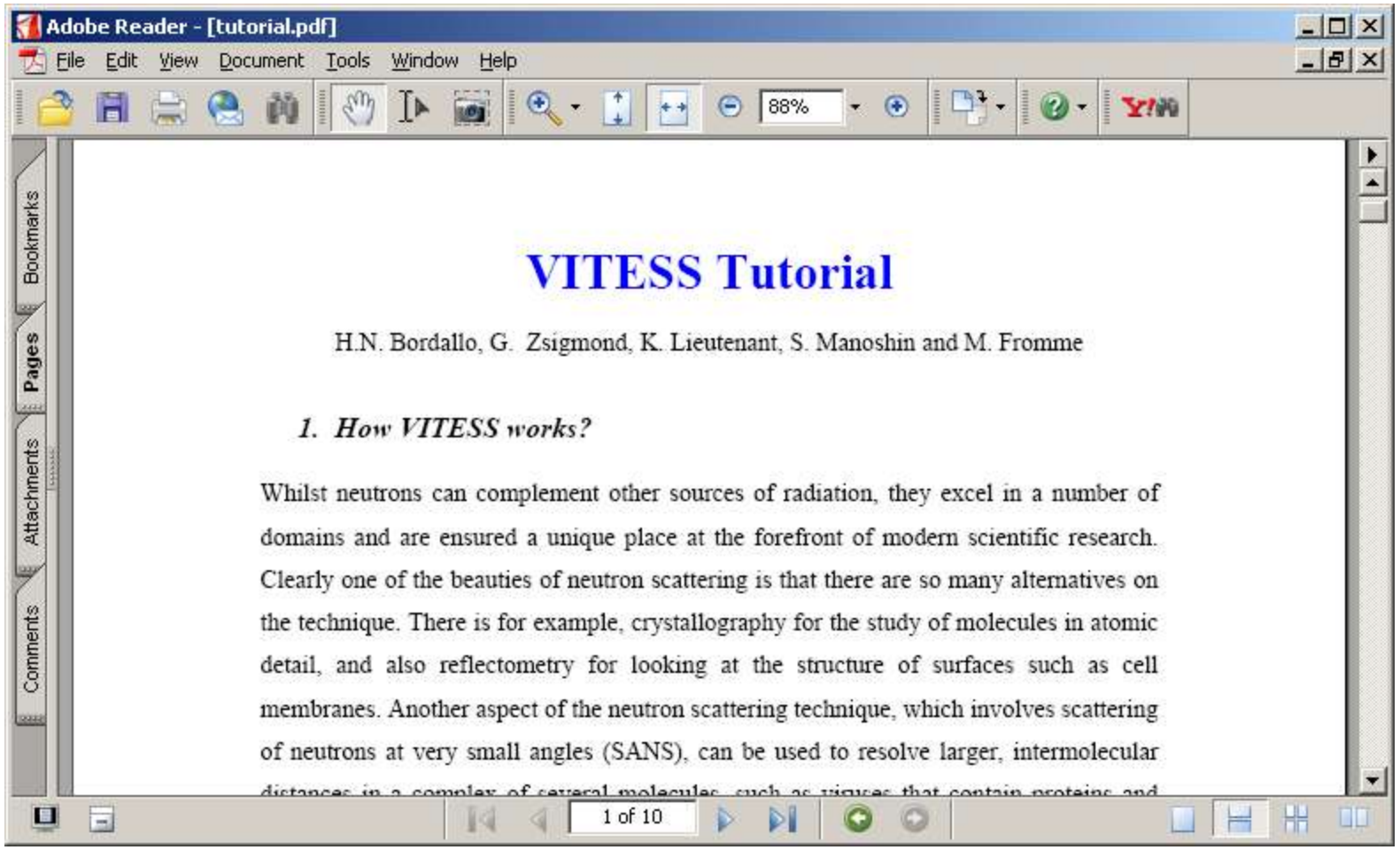
The module **source** initialises neutrons originated at a short pulsed (SPSS), long pulsed (LPSS), or a continuous source (CWS). Their starting positions are randomly distributed over a rectangular moderator surface. Further parameters like wavelength, divergence and time at the moderator are determined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


Adobe Reader - [tutorial.pdf]
File Edit View Document Tools Window Help
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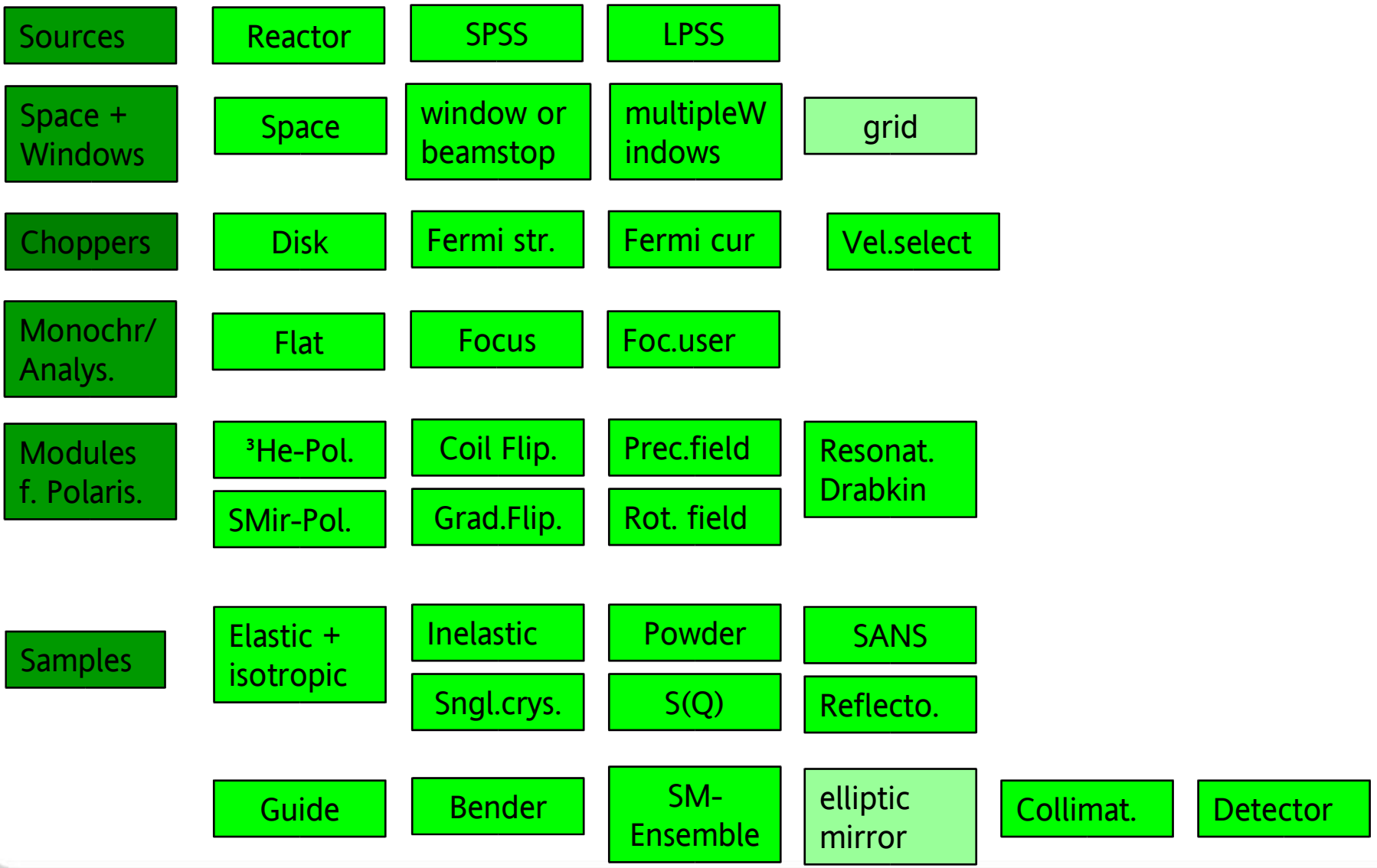
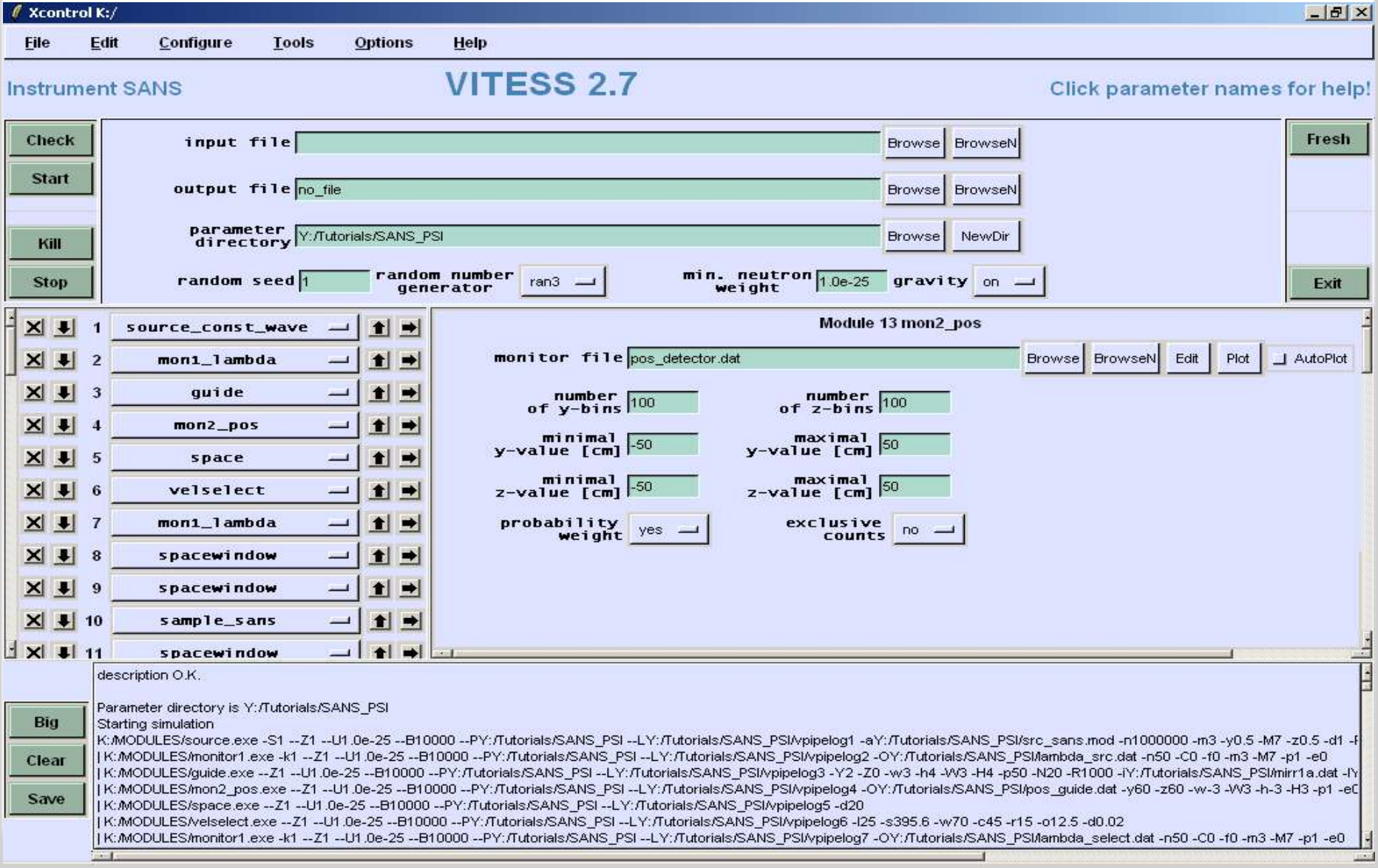
Attachments
Comments
VITESS Tutorial
H.N. Bordallo, G. Zsigmond, K. Lieutenant, S. Manoshin and M. Fromme
1. How VITESS works?
Whilst neutrons can complement other sources of radiation, they excel in a number of domains and are ensured a unique place at the forefront of modern scientific research. Clearly 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
1 of 10

Modules representing Hardware

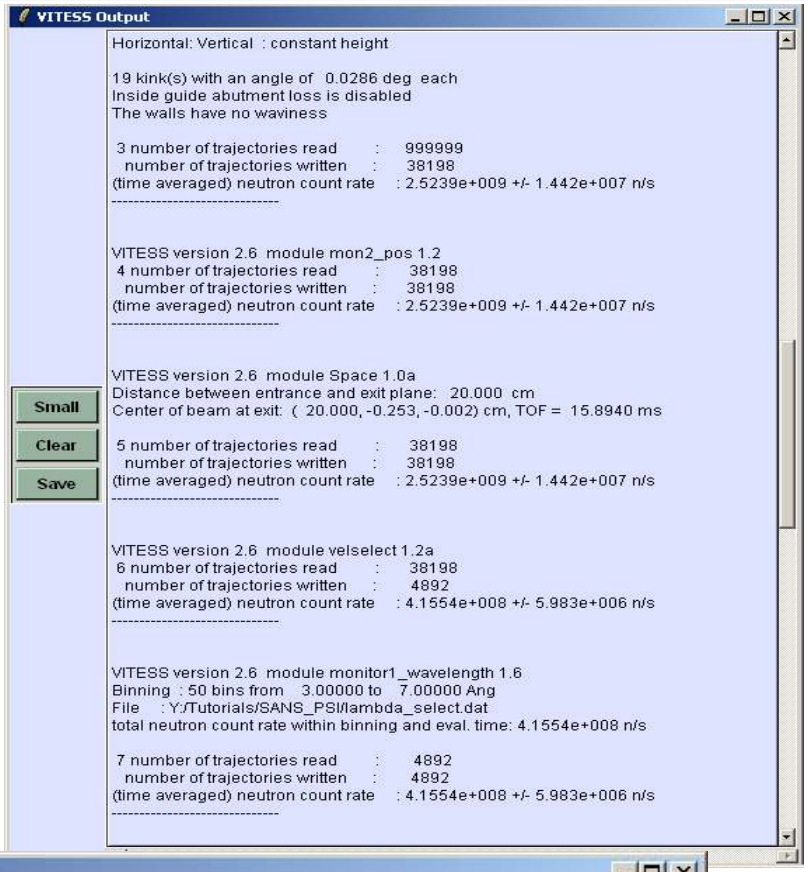


GUI after loading of an instrument



Output

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



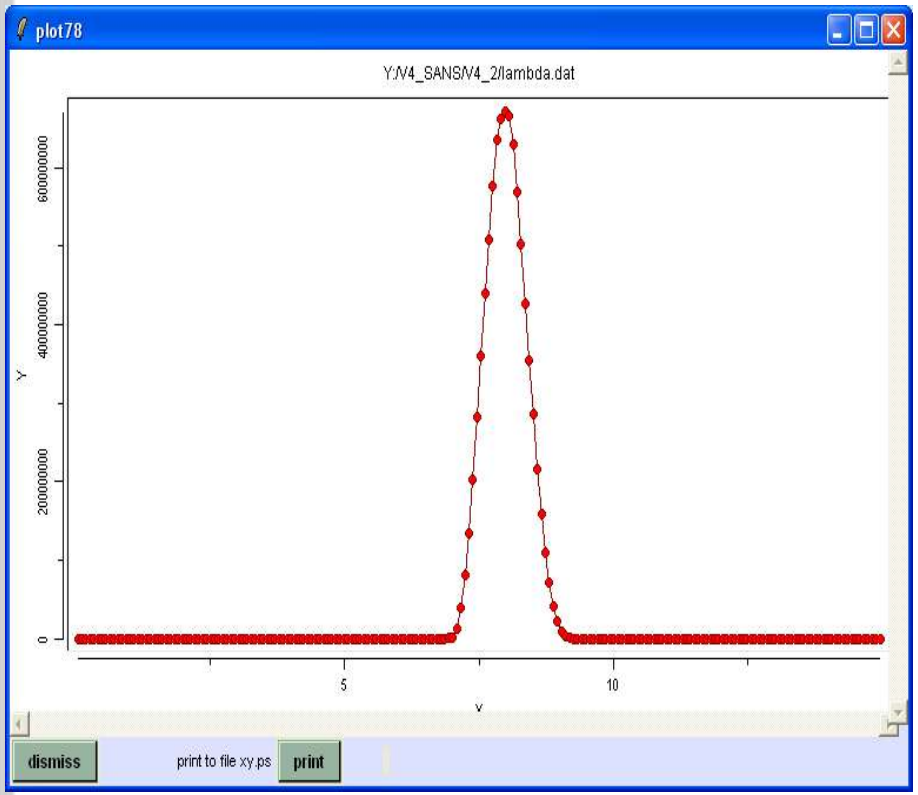
Edit Instrument File

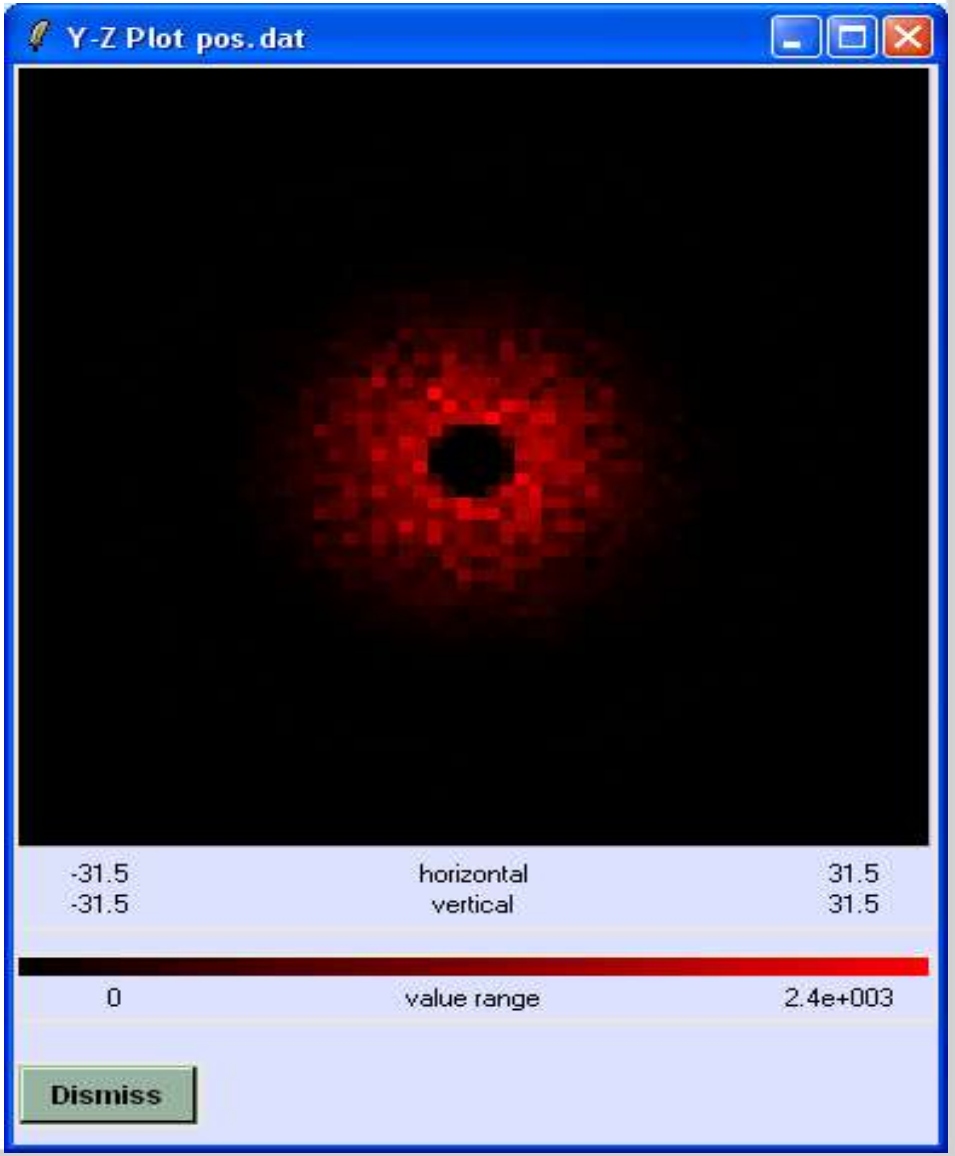
# No	ID	module	len [m]	x [m]	y [m]	z [m]	hor. [deg]	ver.	W-Par.	H-Par.	R-Par	number	type	Descr
0	1	Source and Window	0.000	0.000	0.000	0.000	0.000	0.000	1.8000e+001	0.0000e+000	0.0000e+000	1	1	30.0 K
1	1	Source and Window	2.000	2.000	0.000	0.000	0.000	0.000	3.0000e+000	0.0000e+000	0.0000e+000	0	0	
2	101	monitor1_wavelengt	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_wavelengt	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 F	1	0	
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

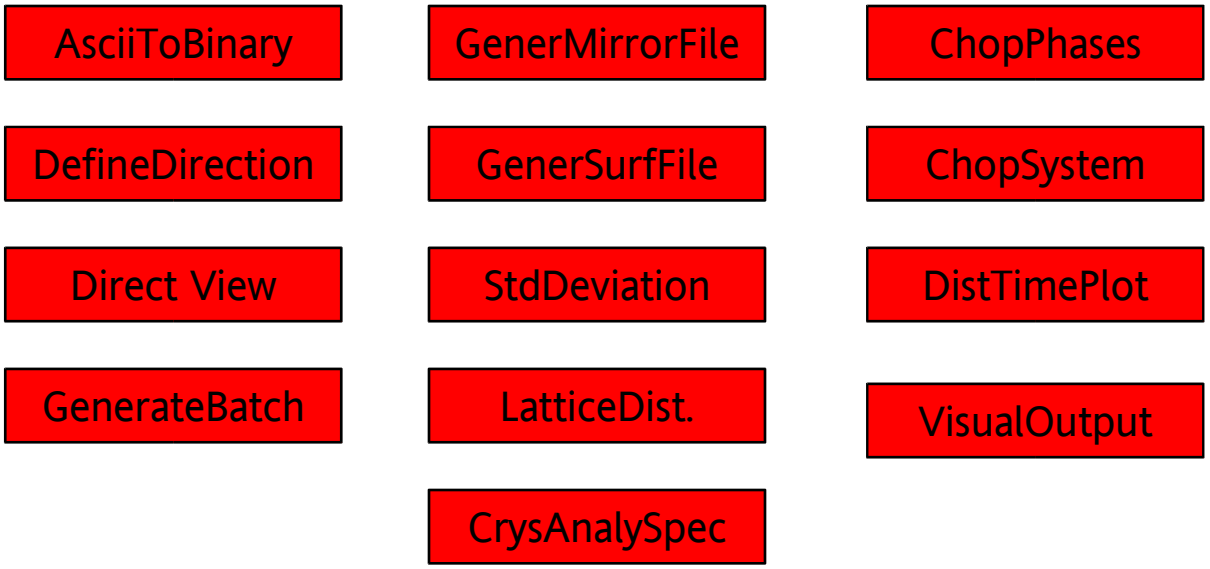
Monitor 1	Time	Wavelen	y-/z-pos	div-y/-z		
Monitor 2	y-pos z-pos	div-y div-z	TOF λ	λ div_y/-z	y div-y	z div-z
MonPol 1	Time	Wavelen	y-/z-pos	div_y/-z		
MonPol 2	y-pos z-pos					
Evaluate	Elastic	Inelast				
	Frame					
	Writeout					
	Visualize					

Graphical output





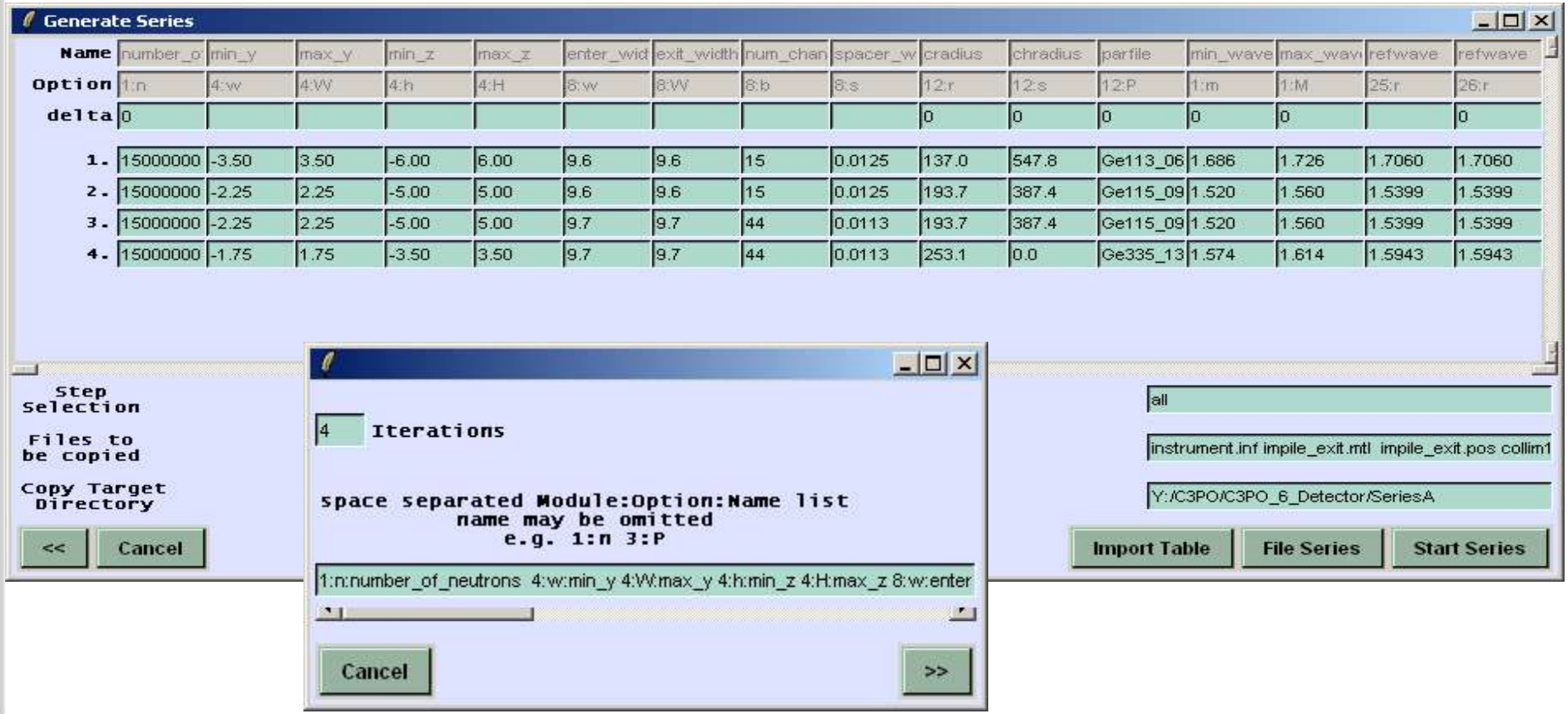
Tools



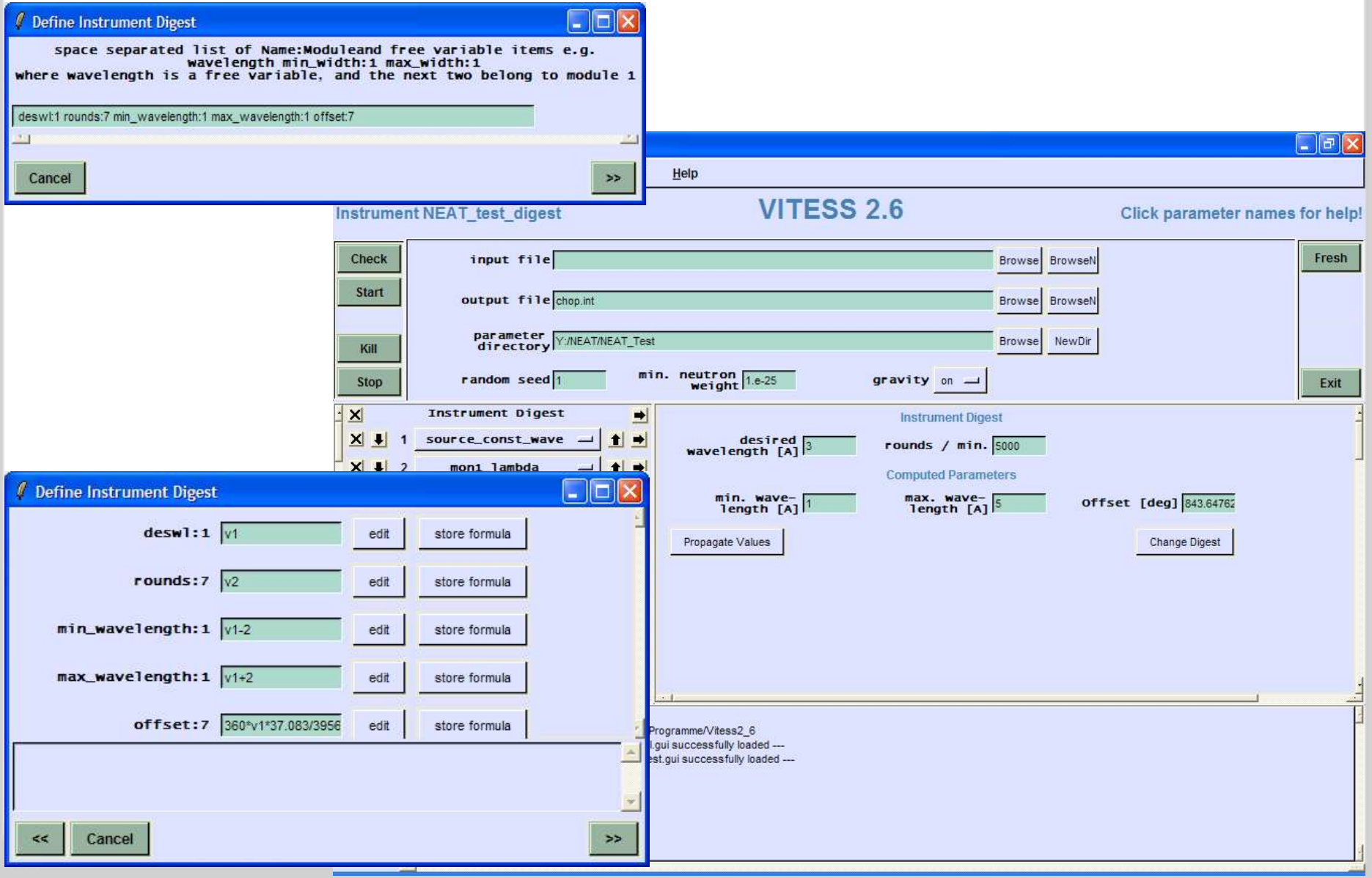
- Tool can be used
  - to generate input files
  - to visualize output data
  - to help designing the instrument

Series of Simulations

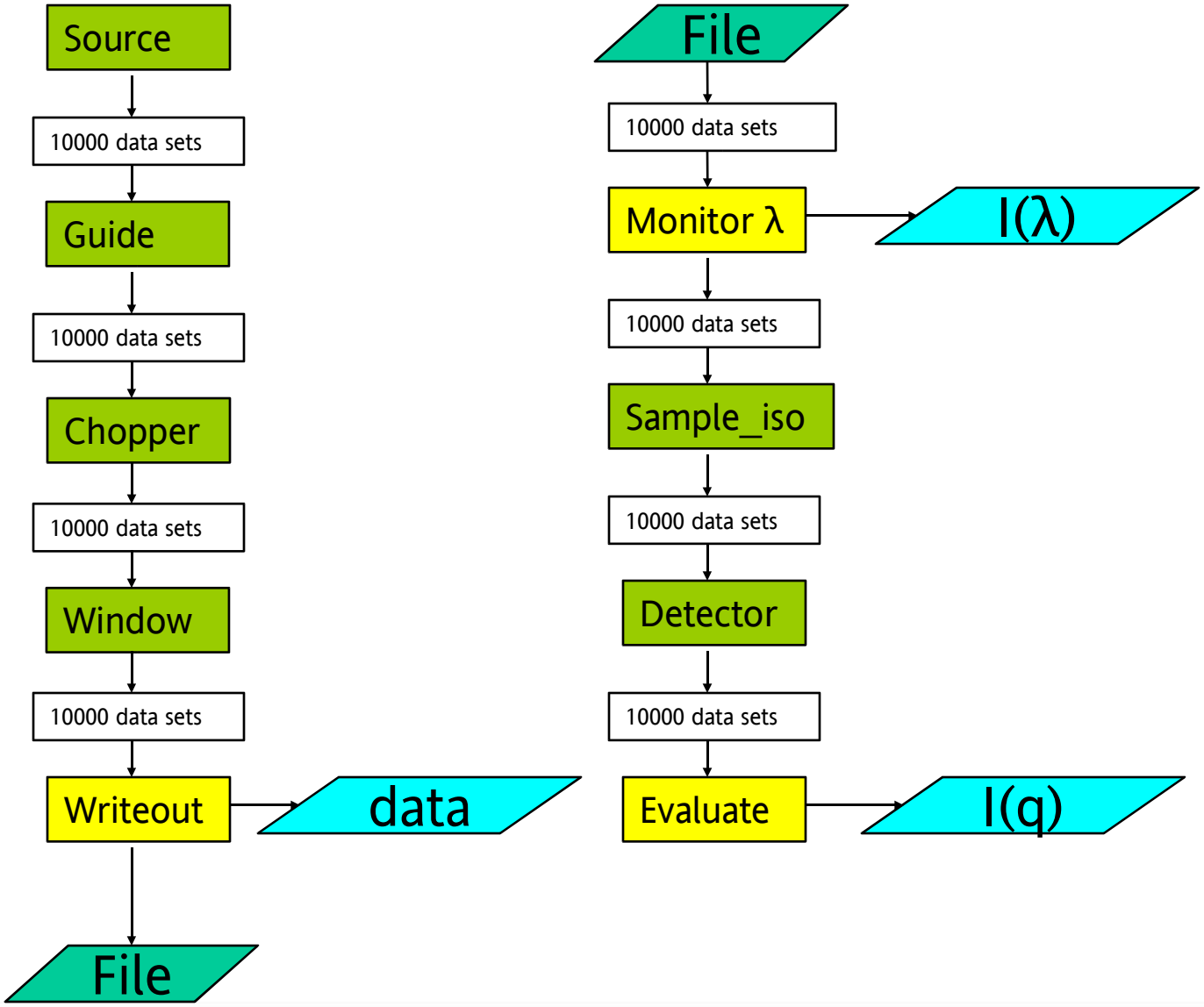
L_eff [cm]	take-off [deg]	h	k	l	coll 1 [min]	num traj.	impile window 2				coll. 1				mono.			lambda		
137.0	60.0	1	1	3	30.0	15000000	-3.50	3.50	-6.00	6.00	9.6	9.6	15	0.0125	137.0	547.8	Ge113_060.par	1.686	1.726	1.7060
137.0	90.0	1	1	5	30.0	15000000	-2.25	2.25	-5.00	5.00	9.6	9.6	15	0.0125	193.7	387.4	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



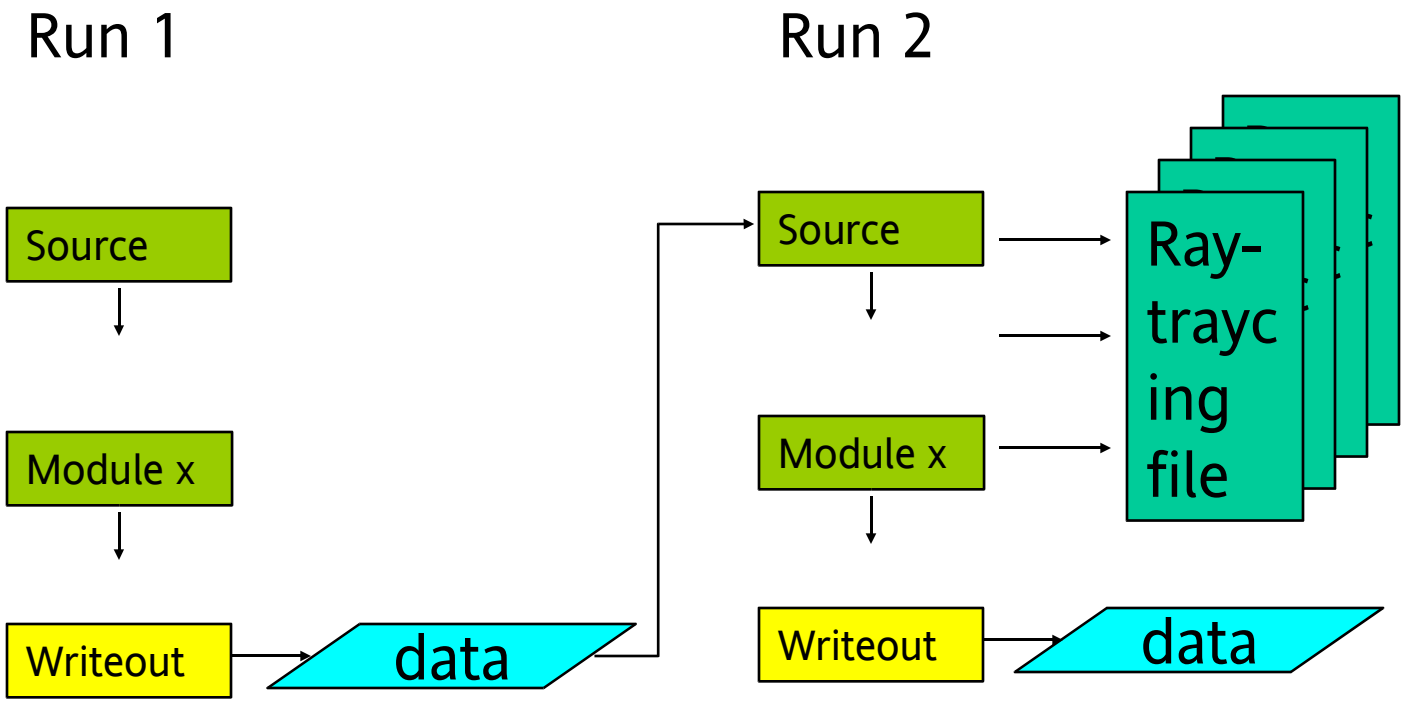
'Instrument Digest'



Splitting of the Simulation



Ray tracing


Run 1
Source
Module x
Writeout
data
Run 2
Source
Module x
Writeout
data
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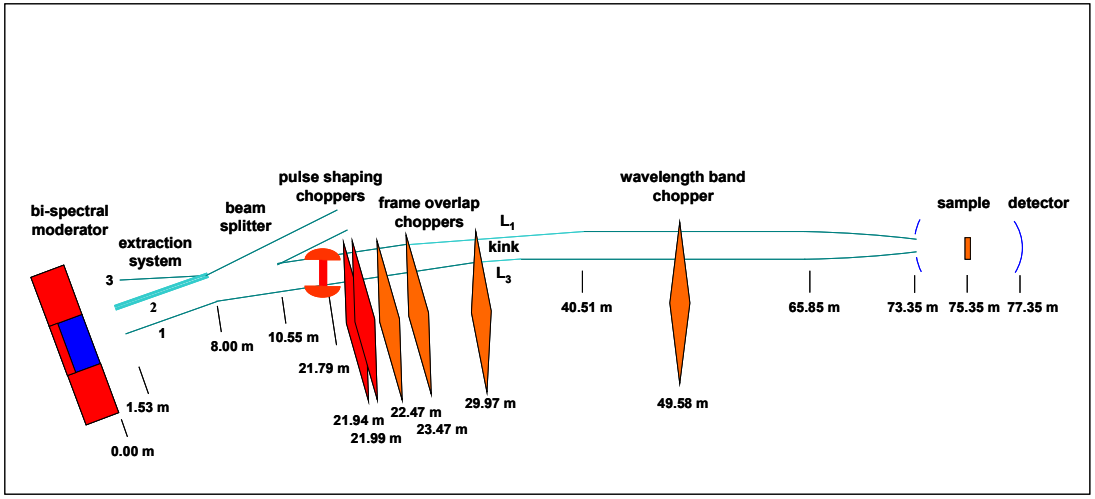
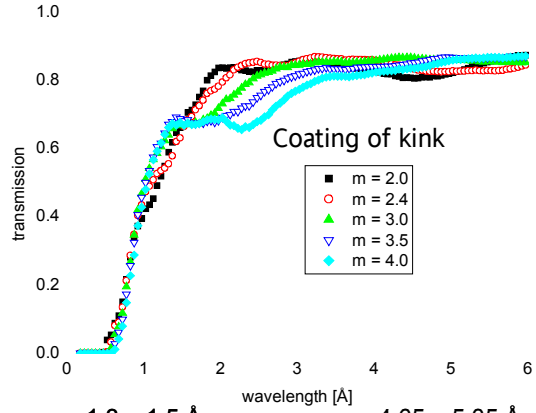
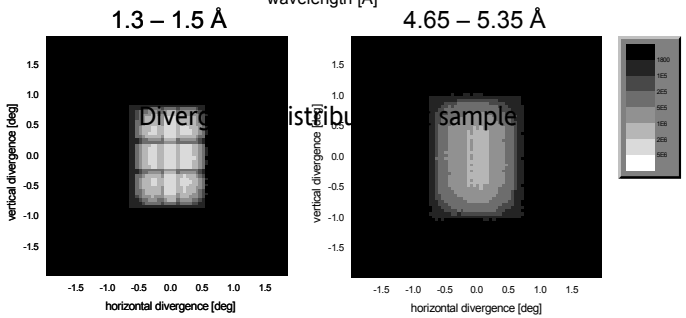
file

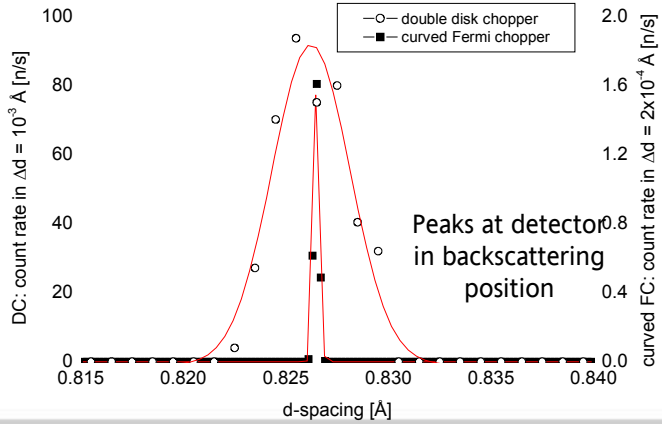
TOF powder diffractometer EXED at HMI





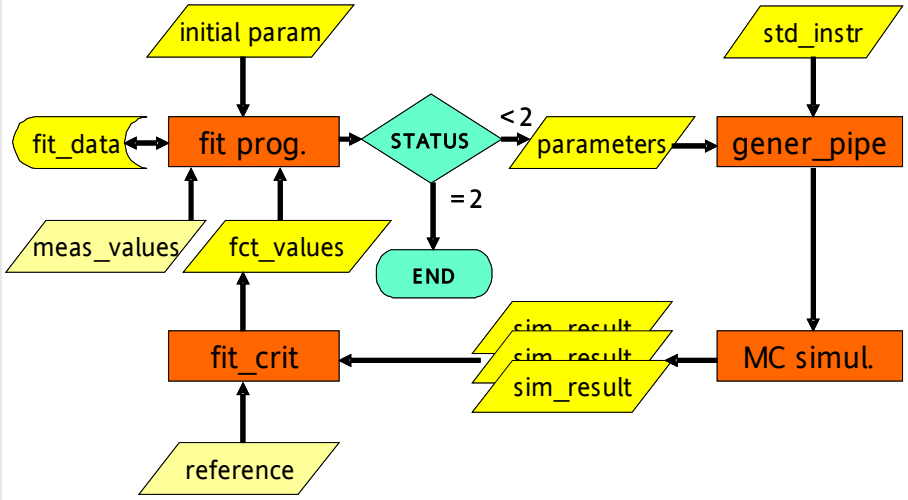


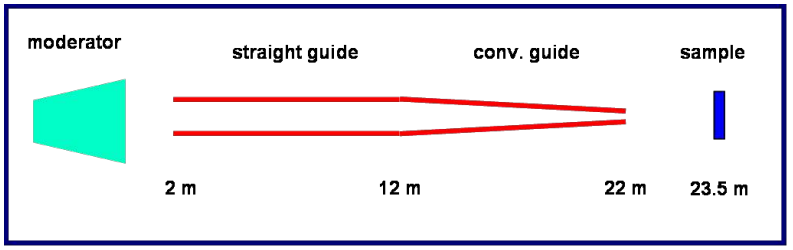
- Concept of EXED
  - TOF diffractometer
  - beam extraction system to use neutrons of cold and thermal moderator
  - kink to suppress hot neutrons
  - pulse generation by double chopper system or Fermi chopper
  - elliptic tapered guide
- Whole instrument simulated and optimized
- Results
  - resolution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

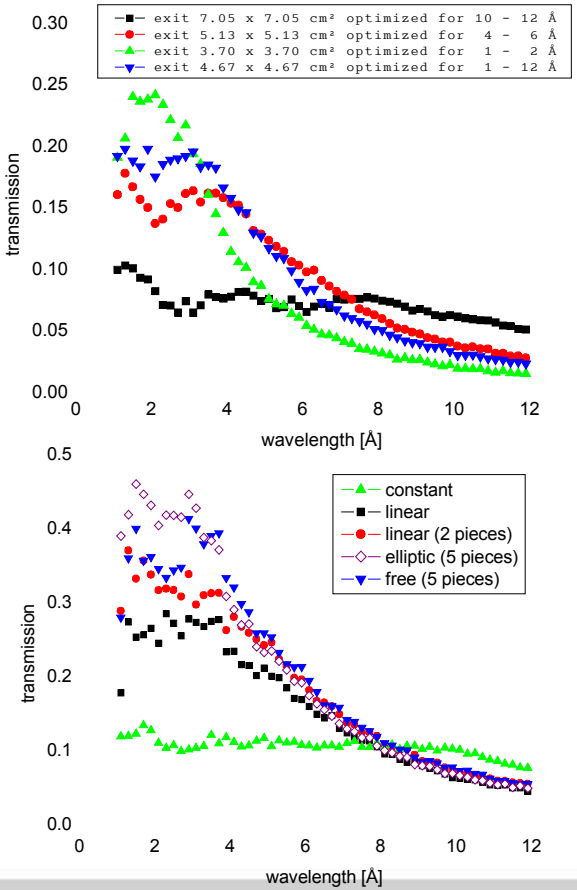


J. Peters, K. Lieutenant, D. Clemens, F. Mezei, Z. Kristall. (accepted for publication)
K. Lieutenant, J.Peters, F. Mezei, J. Neutron Res. (submitted for publication)

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. Matter17 (2005) S167-S174.

Task in Tutorial: Simulation of a SANS Instrument

VITESS tutorial – MC workshop at PSI 02. oct 2006

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 $1x10^{13}$ n/(cm^2s). It is described by a Maxwellian distribution of 30 K.

- Monitor the wavelength distribution in a window of 3 x 4 cm^2 (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 cm^2 (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 cm^2 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^{10} cm^{-2}, for the surrounding it is 1×10^{10} 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

2

6. Beamstop (module 'spacewindow')

Put a beam-stop of 5 x 6 cm^2 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 m^2 size, 2 cm thickness, 1 x 1 cm^2 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 $Å^{-1}$ to 0.1 $Å^{-1}$ logarithmically.
  Hint: don't forget to give the wavelength used

Thank you for your attention !