

Introduction to VITESS

Klaus Lieutenant

V irtual
I nstrumentation
T ool for the
E uropean
S palliation
S ource



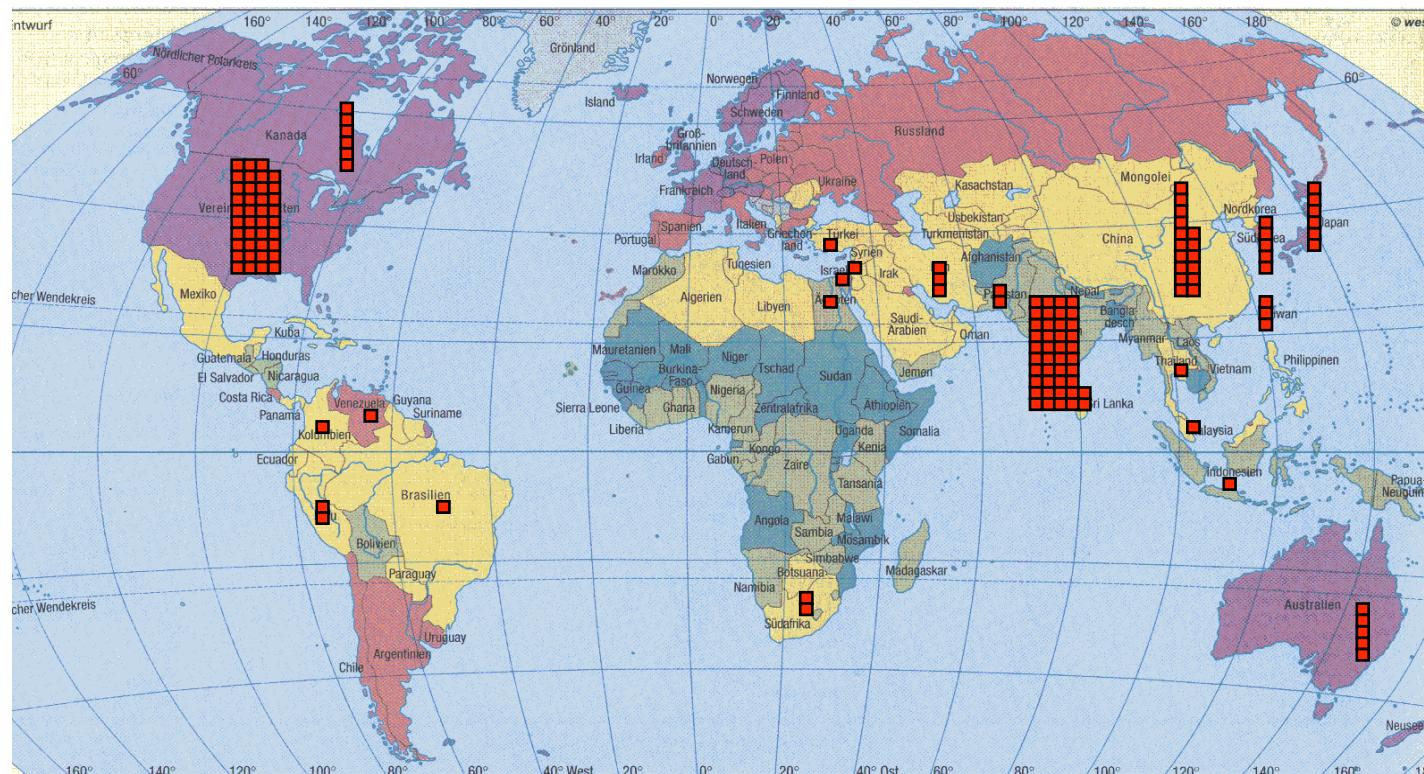
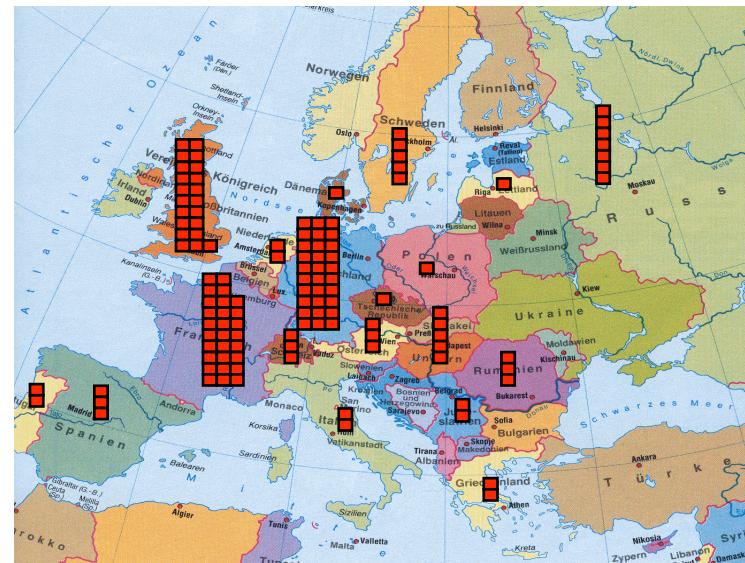
History of VITESS

Idea of Ferenc Mezei to realize a package to simulate all kinds of neutron scattering instruments especially on neutron spallation sources because of the European spallation source (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 (followed by MCNSI in FP6)
 - (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 instruments on other sources
- 2005: VITESS group at HMI closed
- 2006: VITESS released under GNU license
 - larger developer team, all working only partly on VITESS
- 2008: Version 2.8 released
- 2009: Latest version 2.9 released

Distribution of Downloads in 2003



Present Status

Staff

Michael Fromme (HMI; GUI and release of new versions)
Sergey Manoshin (JINR; development of new modules)
Klaus Lieutenant (IFE; module development)
Andreas Houben (RWTH Aachen, module development)
Phillip Bentley (ANSTO; optimisation routine)
Geza Zsigmond (PSI; maintenance of his modules)

Program

Executables for Windows/DOS, Unix (SunOS: versions from 5.6, OSF1 V4.0) and Linux (versions from 2.0.35), Macintosh on demand

free of charge

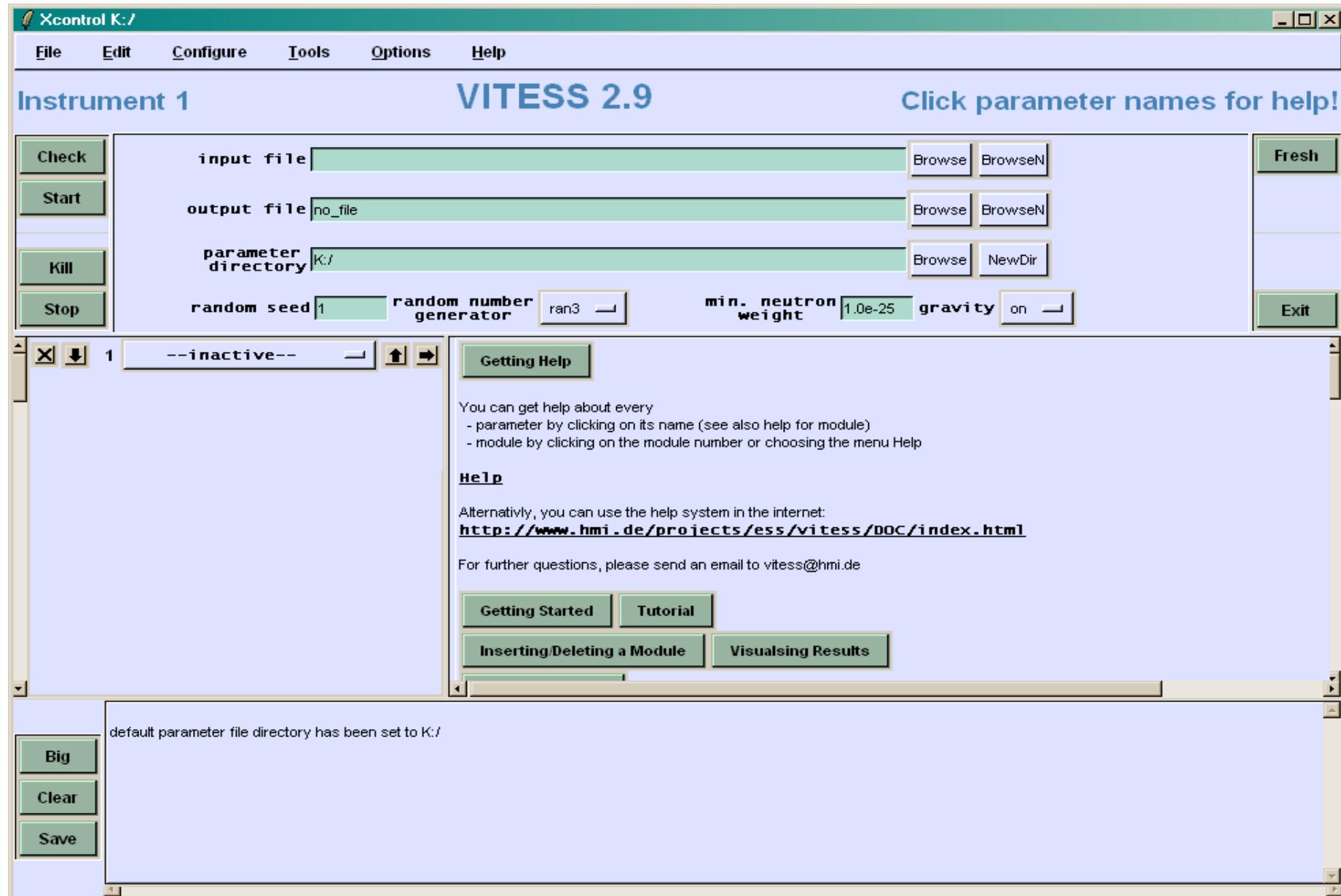
Can be downloaded from internet address <http://www.helmholtz-berlin.de/vitess/>

Home Page 'www.helmholtz-berlin.de/vitess'

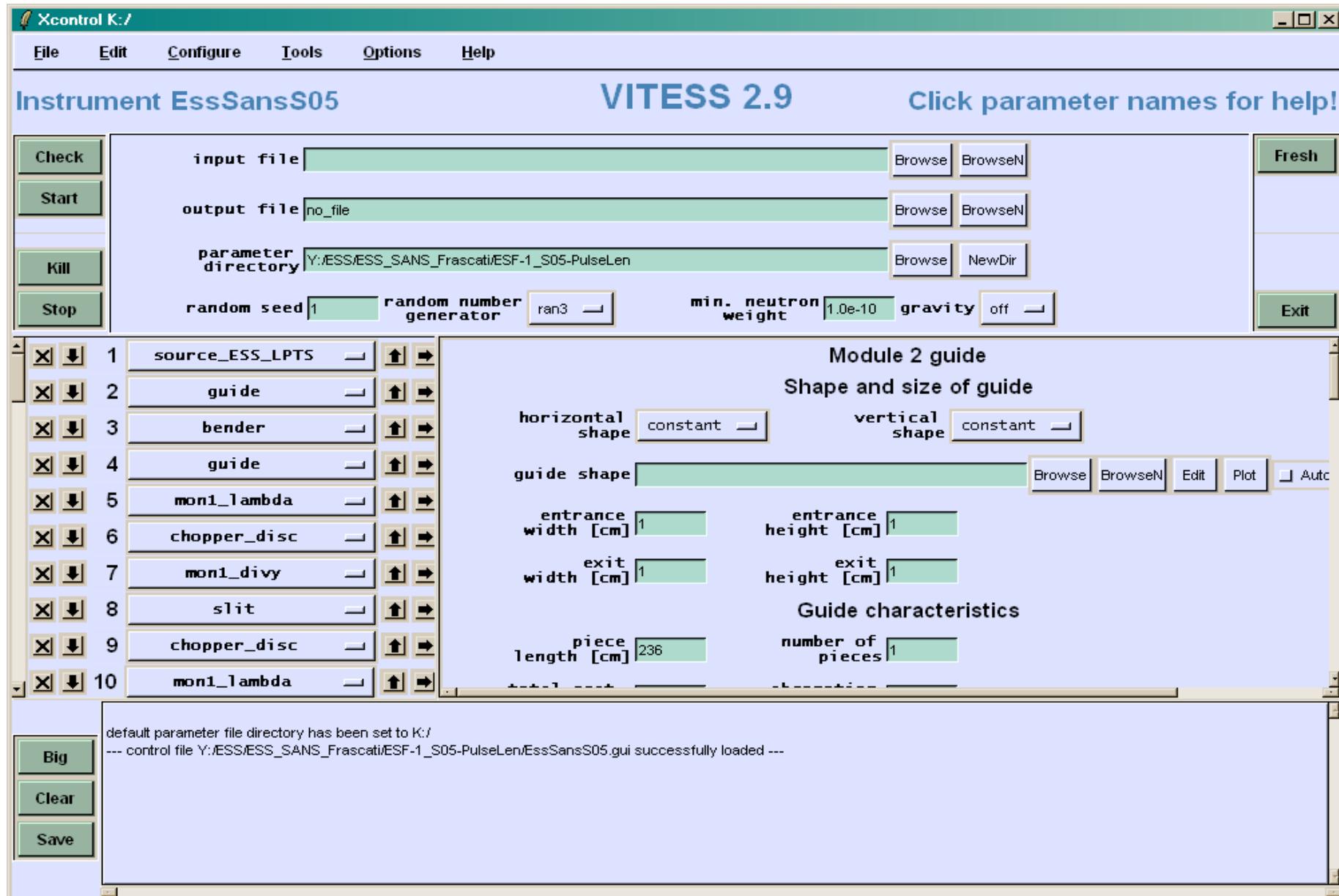
→

The screenshot shows a Mozilla Firefox window with the title bar 'VITESS - Mozilla Firefox'. The address bar displays the URL 'http://www.helmholtz-berlin.de/forschung/grossgeraete/neutronenstreuung/projekte/vitess/index_de.html'. The page content is the Vitess project page, featuring the Vitess logo (a stylized 'n' inside a blue circle) and a brief description of the tool. A sidebar on the left contains a navigation menu with links like 'Das Zentrum im Überblick', 'Forschung', 'Großgeräte', 'Methoden und Instrumente der Neutronenstreuung', 'Projekte/Kooperationen', 'VITESS', 'Nutzerdienst', 'Angebote', and 'Aktuell'. On the right, there are sections for 'Vitess 2.9' and 'Vitess 2.8', each listing a Windows Installer and a Linux Tar-Ball file with their respective MD5 checksums.

GUI after program start

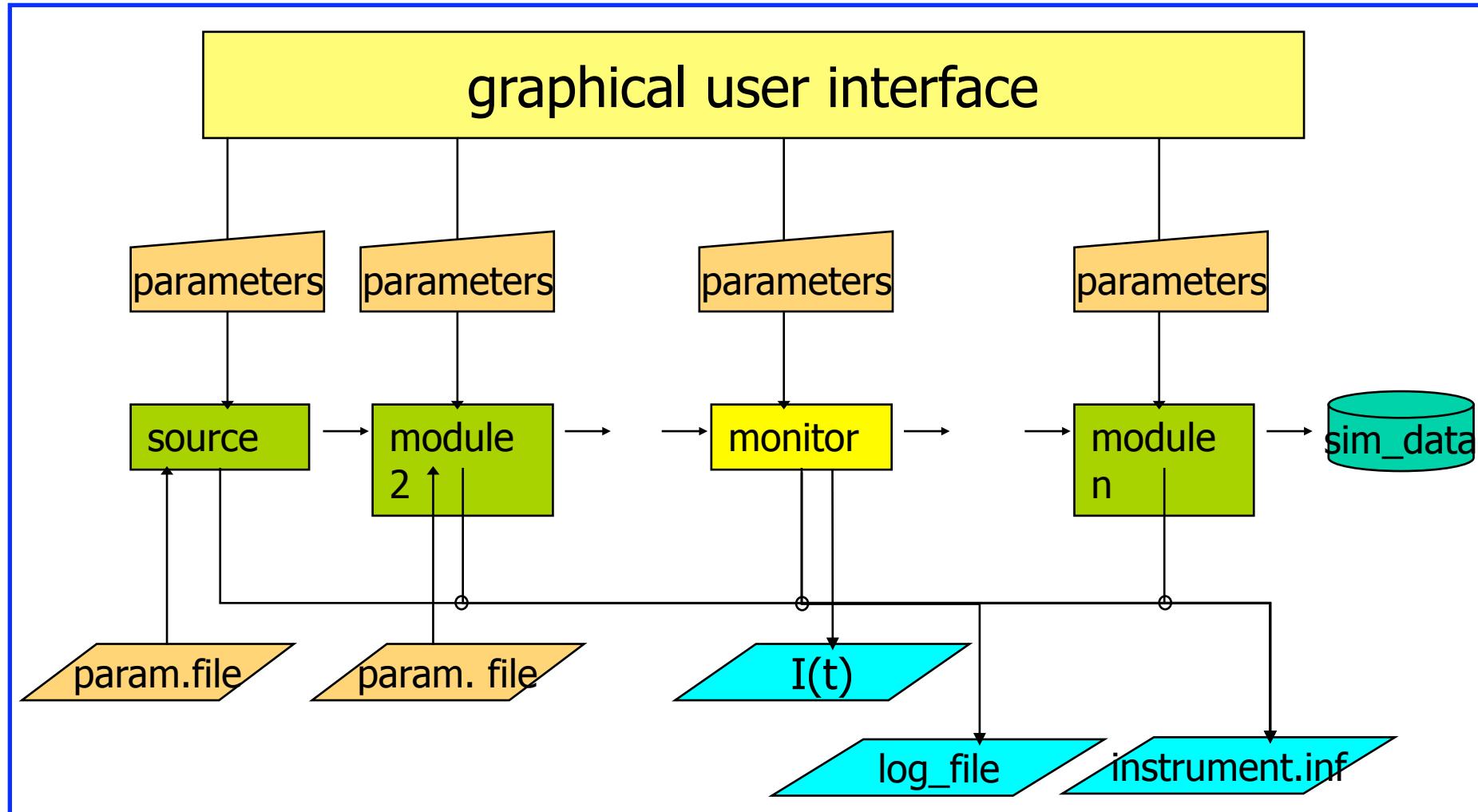


GUI after loading an instrument



Concept of VITESS

Ven 2010
essworkshop.org



Parameter set transferred

Right-handed system
x: along the beamline
y: to the left
z: (vertically) up

ID

criterion ‘ray tracing’

‘colour’

Time of flight t [ms]

wavelength λ [\AA]

count rate p [n/s]

location of neutron x [cm]

location of neutron y [cm]

location of neutron z [cm]

flight direction $v_x/|v| = \cos \alpha$

flight direction $v_y/|v| = \cos \beta$

flight direction $v_z/|v| = \cos \gamma$

Spin P_x

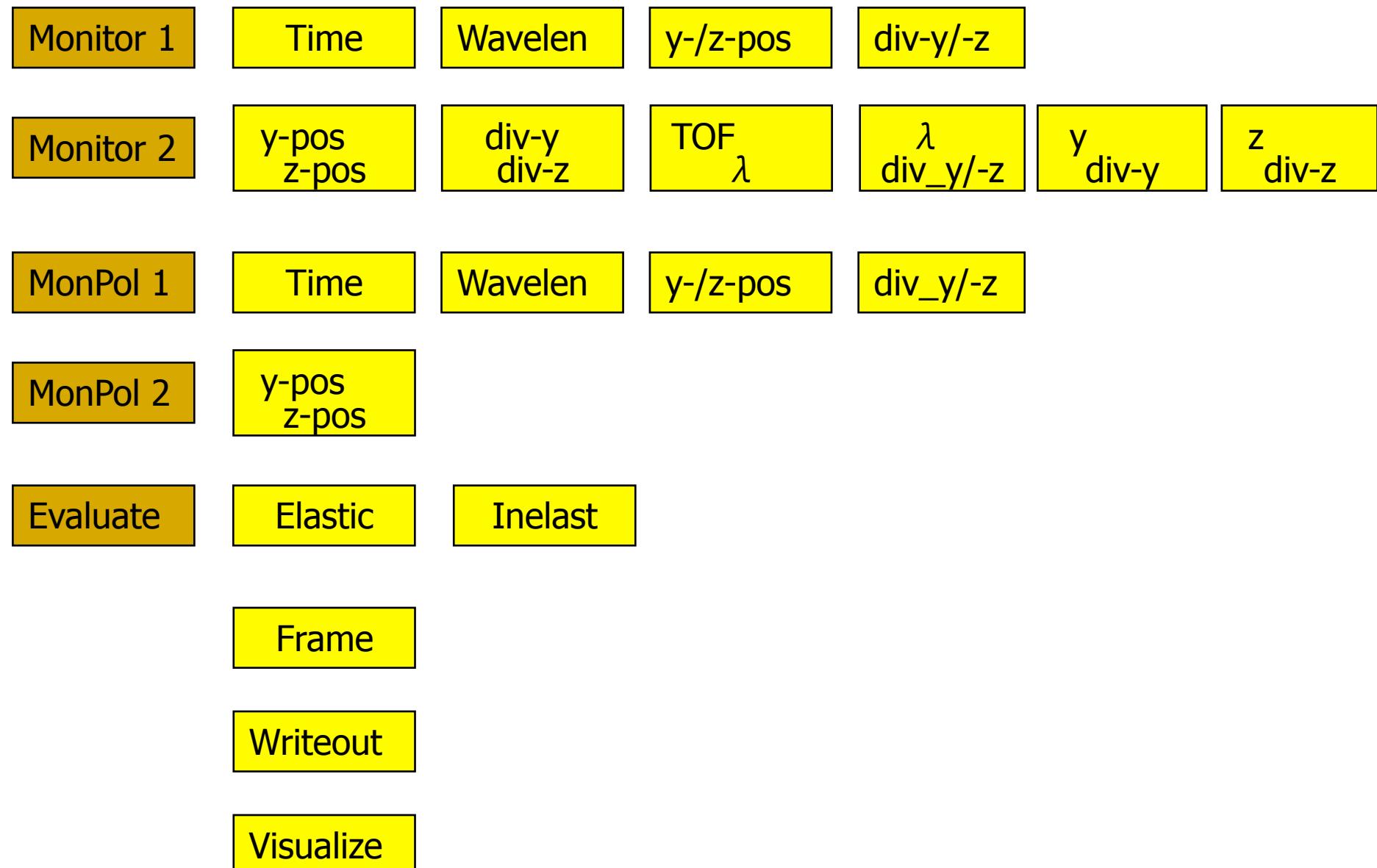
Spin P_y

Spin P_z

Modules representing Hardware

Sources	reactor	SPSS	LPSS		
Space + Windows	space	slit	window/ beamstop	multiple windows	grid
Choppers	disk	Fermi str.	Fermi cur		
Mono/Ana	flat	focus	foc.user		
Modules f. Polaris.	³ He-pol.	coil flip.	prec.field	sesansfield	pol. mirror
	SM-polar.	grad.flip.	rot. field	res.Drabkin	
Samples	elast.isot.	powder	SANS	reflecto.	
	inelastic	sngl.crys.	S(Q)	environm	
Collimat.	coll.simpl	coll.soller	coll.radial		
	guide	bender	vel.select	SM-ensmbl	detector

Modules for Data Evaluation



Input Data: Parameter File

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essworkshop.org

Edit IFEtherm.src

Moderator 1

shape

moderator diameter or width [cm] moderator height [cm] spatial order

center of moderator X [cm] center Y [cm] center Z [cm]

total flux at moderator [n/(cm*s)] neutron current [n/s]

user wavelength dist. file

moderator temperature [K] colour

Moderator 2

second moderator

shape

moderator diameter or width [cm] moderator height [cm] spatial order

center of moderator X [cm] center Y [cm] center Z [cm]

total flux at moderator [n/(cm*s)] neutron current [n/s]

user wavelength dist. file

moderator temperature [K] colour

Output Data: Log File and Instrument Data

VITESS Output

```

Starting simulation
C:/Programme/VITESS_2.5.1/MODULES/source.exe -S1 --Z5 --G1 --U1.0e-25 --B10000
| C:/Programme/VITESS_2.5.1/MODULES/guide.exe --Z5 --G1 --U1.0e-25 --B10000 --
| C:/Programme/VITESS_2.5.1/MODULES/guide.exe --Z5 --G1 --U1.0e-25 --B10000
C:/Programme/VITESS_2.5.1/MODULES/veselect.exe --Z5 --G1 --U1.0e-25 --B10000
C:/Programme/VITESS_2.5.1/MODULES/monitor1.exe -k1 --Z5 --G1 --U1.0e-25 --B1
C:/Programme/VITESS_2.5.1/MODULES/guide.exe --Z5 --G1 --U1.0e-25 --B10000 --
C:/Programme/VITESS_2.5.1/MODULES/spacewindow.exe --Z5 --G1 --U1.0e-25 --B10
C:/Programme/VITESS_2.5.1/MODULES/spacewindow.exe --Z5 --G1 --U1.0e-25 --B10
C:/Programme/VITESS_2.5.1/MODULES/sample_sans.exe --Z5 --G1 --U1.0e-25 --B10
C:/Programme/VITESS_2.5.1/MODULES/spacewindow.exe --Z5 --G1 --U1.0e-25 --B10
C:/Programme/VITESS_2.5.1/MODULES/detector.exe --Z5 --G1 --U1.0e-25 --B10000
C:/Programme/VITESS_2.5.1/MODULES/mon2_pos.exe --Z5 --G1 --U1.0e-25 --B10000
C:/Programme/VITESS_2.5.1/MODULES/eval_elast.exe --Z5 --G1 --U1.0e-25 --B100
simulation (f00 e80 1d0 104 f7c 33c ac fd4 1b0 2b4 25c fac a8c ) (3840 3712 46
.....
```

VITESS version 2.5 module Source and Window 1.11

> Simulation of constant wave source <

moderator temperature : 45.000 K
total neutron flux (in 2*pi) : 3.0000e+013 n/(cm²s)
moderator position :(0.000 0.000 0.000) cm
moderator size (W x H) : 7.500 cm x 7.000 cm
divergence defined by propagation window
time averaged neutron current: 1.6054e+011 n/s in 0.000640 str
wavelength band used : 6.000 Ang - 10.000 Ang

window (W x H) : 3.000 cm x 5.000 cm
in a distance of : 1.530 m
with a declination of : 0.000°
polarization : 0.000 % X: 1.000 Y: 0.000 Z: 0.000
Center of beam at window :(153.000 0.000 0.000) cm
Average TOF : 2.829 ms

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

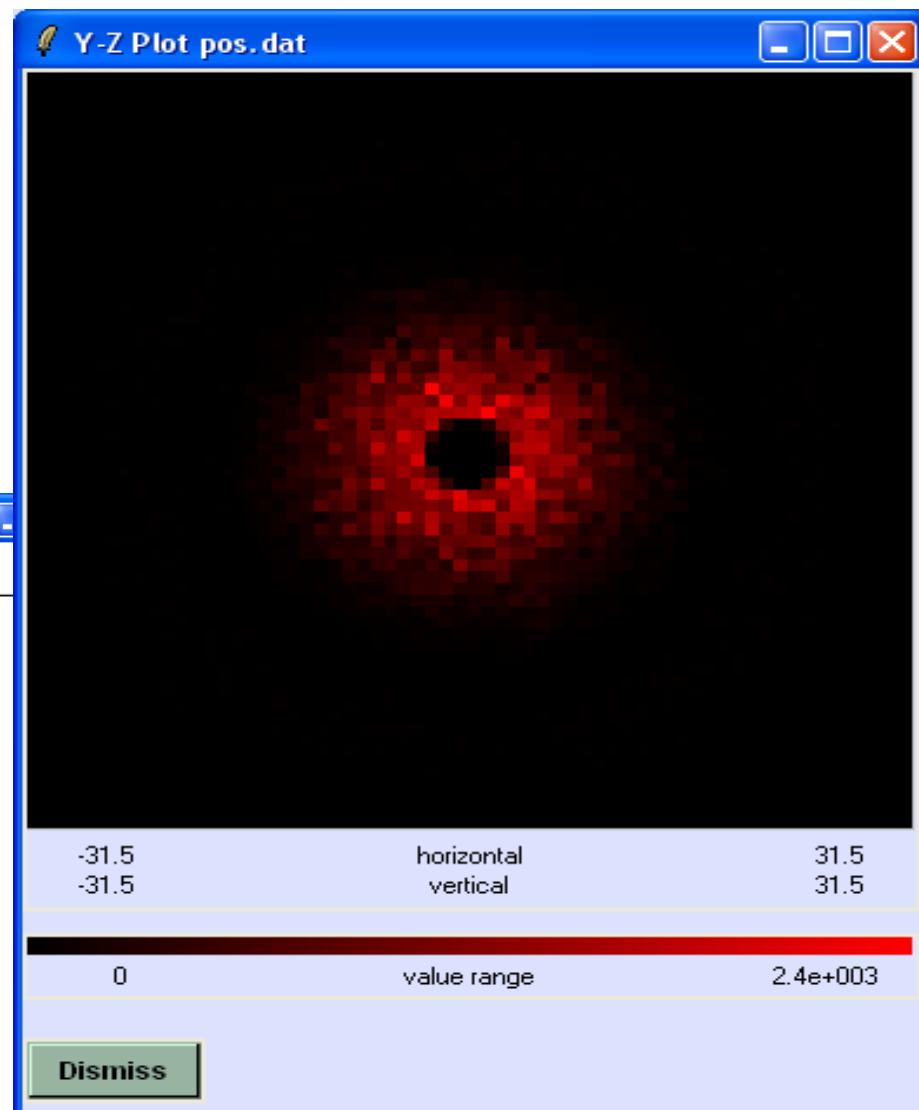
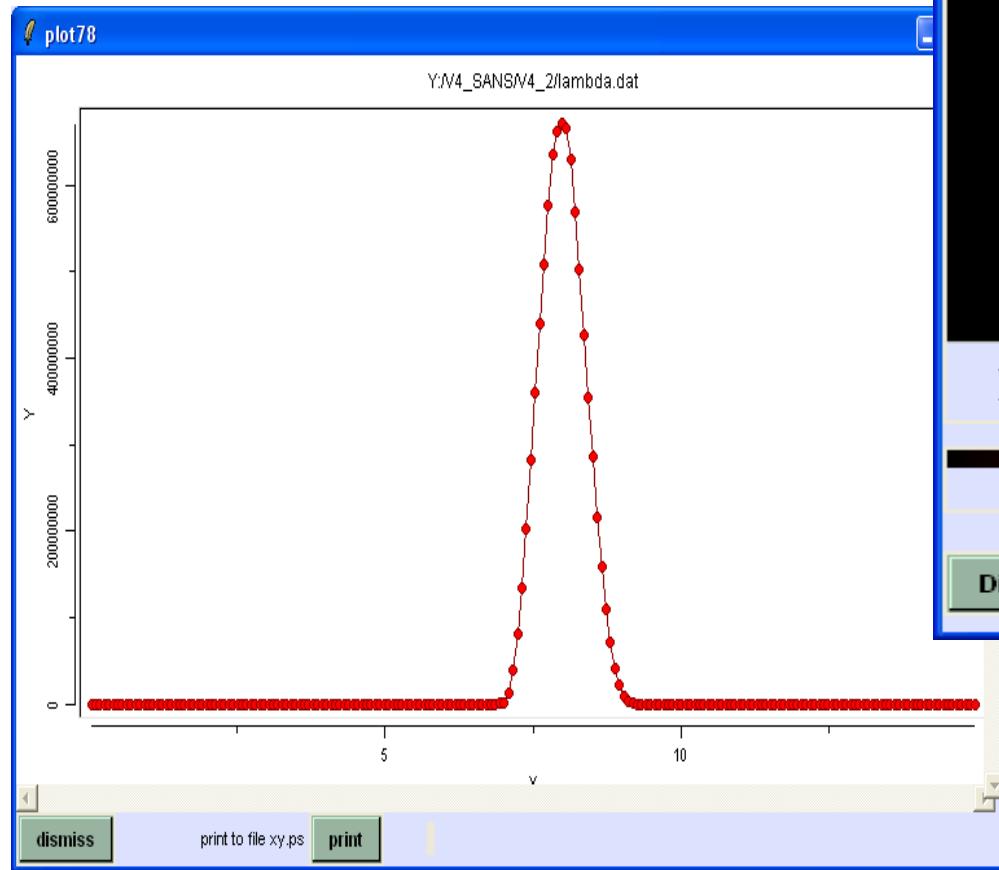
number of trajectories started : 22000000
1 number of trajectories read : 0
number of trajectories written : 21999977
(time averaged) neutron count rate : 1.5724e+010 n/s

VITESS version 2.5 module

NOTE: coating of top wall
Horizontal: curved, radius
Vertical : constant height

#	No	ID	module	len [m]	x [m]	y [m]	z [m]	hor. [deg]	ver.	W-Par.	H-Par.	R-Par	number	type	Descrip:
0	1	Source and Window	0.000	0.000	0.000	0.000	0.000	7.5000e+000	0.0000e+000	0.0000e+000	0.0000e+000	0.0000e+000	1	1	45.0 K
1	1	Source and Window	1.530	1.530	0.000	0.000	0.000	3.0000e+000	0.0000e+000	0.0000e+000	0.0000e+000	0.0000e+000	0	0	
2	11	guide	21.530	21.529	0.150	0.000	0.859	0.000	3.0000e+000	3.0000e+000	1.3000e+003	40	20		
3	11	guide	25.530	25.529	0.210	0.000	0.859	0.000	3.0000e+000	3.0000e+000	0.0000e+000	1	0		
4	41	veselect	25.780	25.779	0.214	0.000	0.859	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0		
5	101	monitor1	25.780	25.779	0.214	0.000	0.859	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	1		
6	11	guide	37.780	37.778	0.394	0.000	0.859	0.000	3.0000e+000	3.0000e+000	0.0000e+000	1	0		
7	21	Window	37.780	37.778	0.394	0.000	0.859	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0		
8	21	Window	41.780	41.778	0.454	0.000	0.859	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0		
9	87	sample_sans	41.790	41.788	0.454	0.000	0.859	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	2		
10	21	Window	45.740	45.738	0.513	0.000	0.859	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0		
11	71	detector	49.740	49.738	0.573	0.000	0.859	0.000	6.4000e+001	1.0000e+000	4.0000e+002	1	2		
12	102	mon2_pos	49.740	49.738	0.573	0.000	0.859	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	0		
13	111	eval_elast	49.740	49.738	0.573	0.000	0.859	0.000	0.0000e+000	0.0000e+000	0.0000e+000	1	2		

Graphical output from Monitors



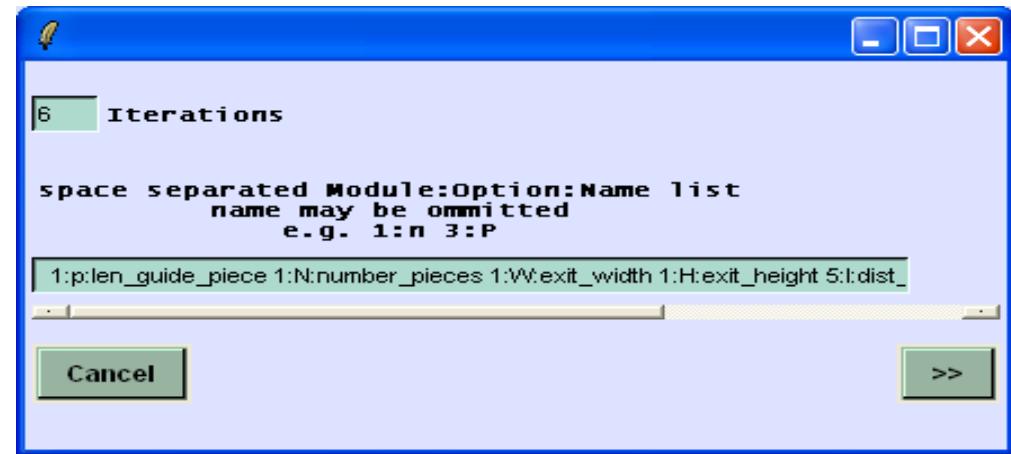
Generate Series

Generate Series

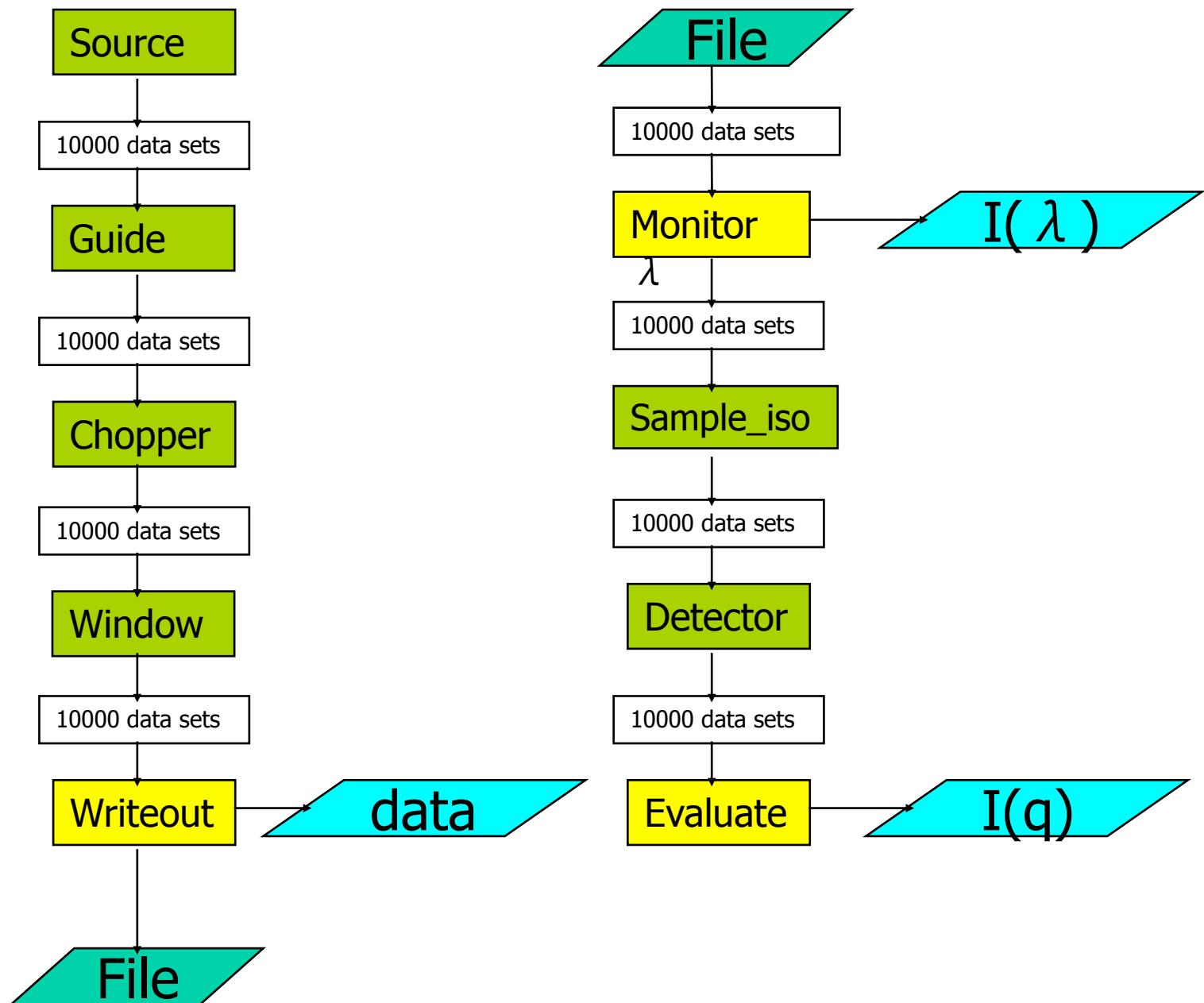
Name	len_guide	number_pi	exit_width	exit_height	dist_orig	max_width	max_height
Option	1:p	1:N	1:W	1:H	5:l	1:y	1:z
delta							
1.	150	3	4.878	7.956	500		
2.	150	2	5.403	8.848	650		
3.	125	6	3	5	200	76.14	75.72
4.	125	3	5.133	8.544	575	76.14	75.72
5.	375	2	3	5	200	75.31	73.50
6.	375	1	5.120	8.490	575	75.31	73.50

Parameter Directory: Y:/NLH2/Exed7
 Files to be copied: sample.wdz sample.wdy sample.myz sample.mtl sample.stl
 Copy Target Directory: Y:/NLH2/Exed7/NumPieces

<< Cancel Save Series Start Series



Splitting of the Simulation



Tools

- Most are used to calculate input data

AsciiToBinary

GenerMirrorFile

ChopPhases

DefineDirection

GenerSurfFile

ChopSystem

Direct View

StdDeviation

CrysAnalySpec

GenerateBatch

LatticeDist.

- Others to visualize output

DistTimePlot

VisualOutput

Computer Grids

File|‘Save as Grid Command’

saves the command line in a form that it can be used on computer clusters

Multi-core Processors

Ongoing development

Tests made for

Guide

Fermi chopper

supermirror ensemble

polariser supermirror

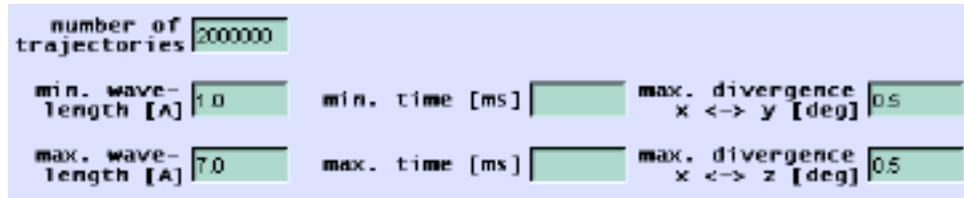
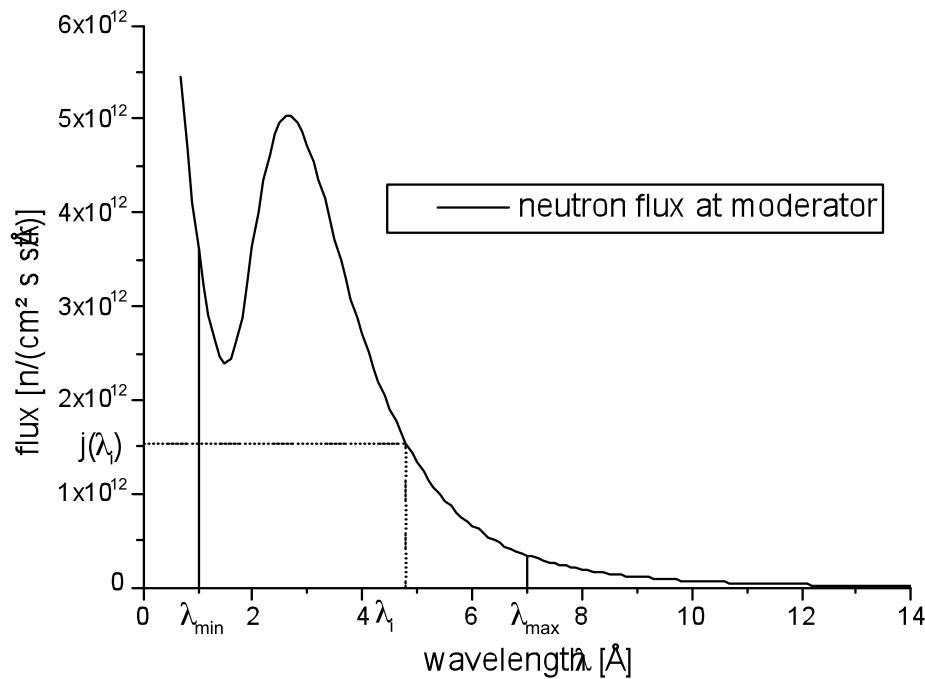
Support

Address to Michael Fromme (fromme@helmholtz-berlin.de)



Thank you for your attention !

Absolute Flux Values



- $I_{CW} = \int j(\lambda) d\lambda$
 $\approx (\lambda_{max} - \lambda_{min})/N \sum_i j(\lambda_i)$
- $I_{SS} \approx (\lambda_{max} - \lambda_{min})(t_{max} - t_{min})/N \sum j(\lambda_i, t_i)$

- Each trajectory represents a package of a certain number of neutrons with the same starting conditions
- By statistical processes like reflection, the number of neutrons in the package decreases, while the number of trajectories remains unchanged
- If the neutron package does not pass a module regularly, the trajectory is taken out of consideration
- A neutron count rate can be calculated from the number of neutrons in a package
- Summing of the count rates of all packages gives the neutron count rate at any point of the instrument