VITESS software for Monte-Carlo simulations

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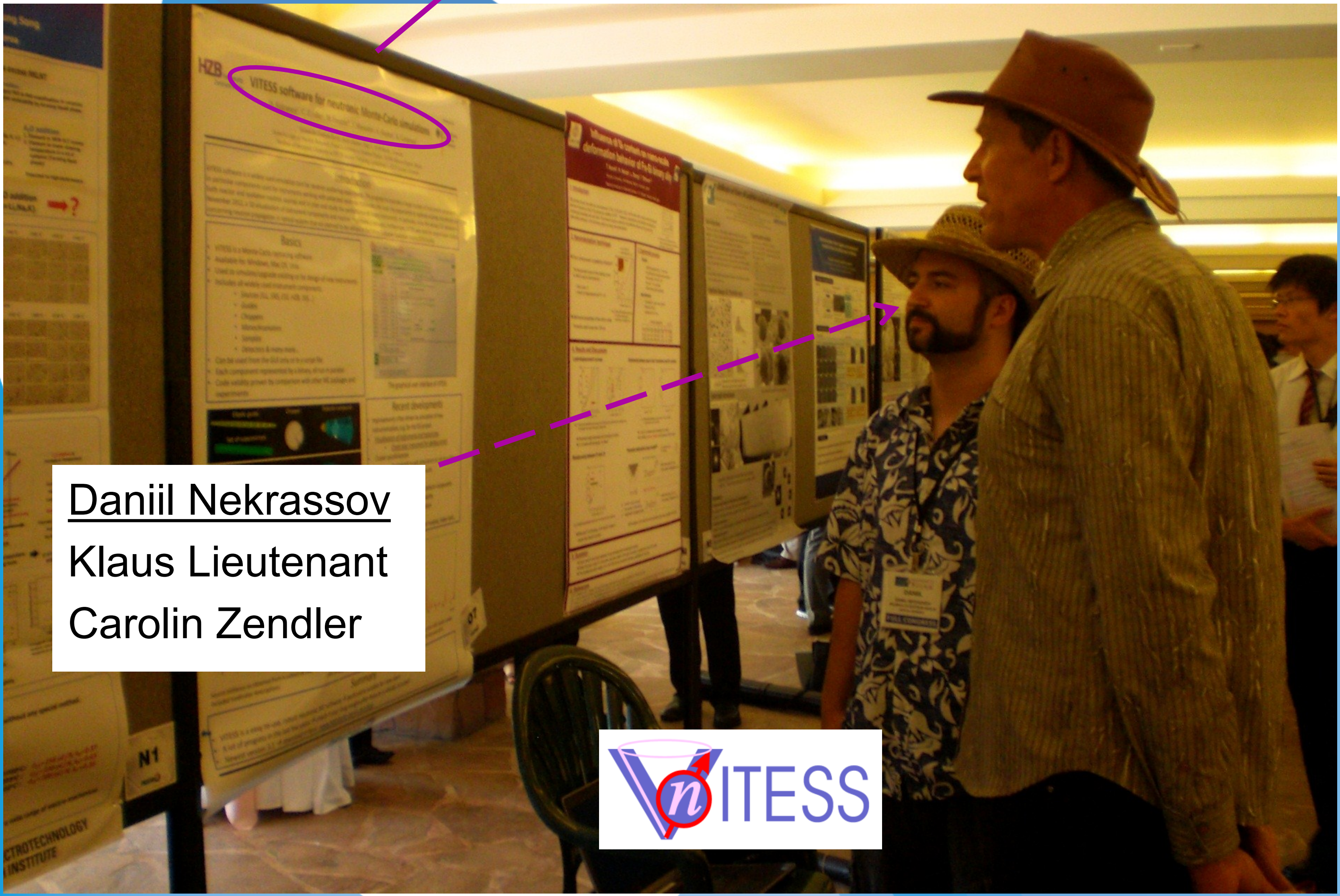

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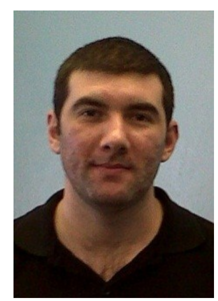

Raul Erhan

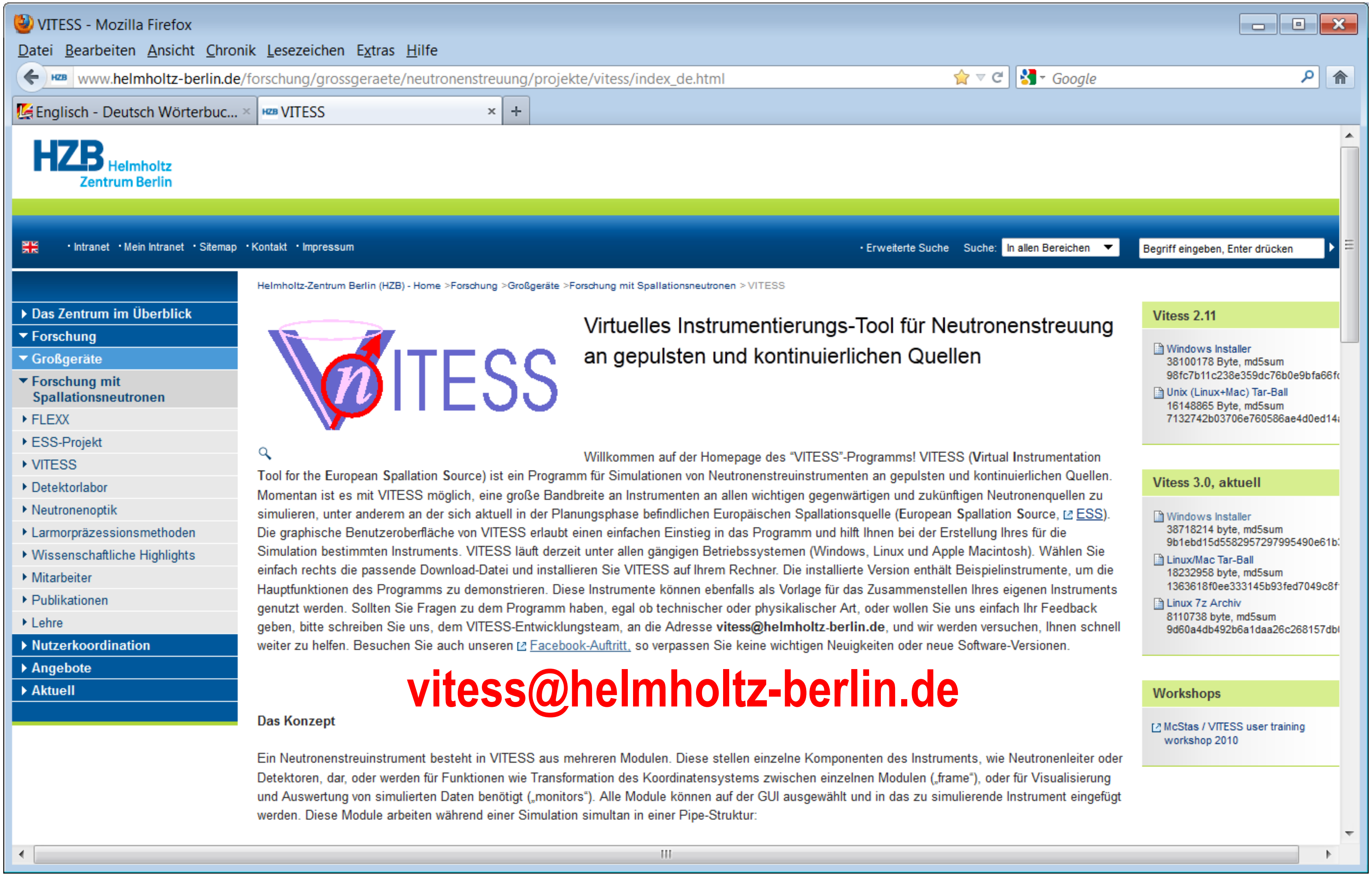
Outline

- History
- Characteristics of the VITESS simulation package
  - Concept
  - GUI, help system, output
  - Ways to use it
  - Instrument visualization
- Examples for instrument design and basic research

History of VITESS

- Initiative:
  - Idea of Ferenc Mezei to realize a package well suited to simulate instruments on neutron spallation sources, as European spallation source (ESS) has been planned
- Important dates
  - 1999: Release of VITESS 1.0 (First complete instruments simulated)
  - 2000: SCANS collaboration started, in FP6 and FP7 continued as MCNSI (McStas, VITESS, …)
  - 2001: Release of VITESS 2.0 containing polarisation, absolute flux values, improved GUI (several ESS instruments simulated)
  - 2005: HMI stops support of VITESS
  - 2006: VITESS released under GNU license (more developers all working only part time on VITESS)
  - 2010: VITESS again supported by HZB (permanent position for simulations)
  - 2012: VITESS 3.0 released
  - 2013: VITESS 3.1 released
  - 2013: *VITESS 3.2 will be released!*

The VITESS Package:
Home Page ‘www.helmholtz-berlin.de/vitess’



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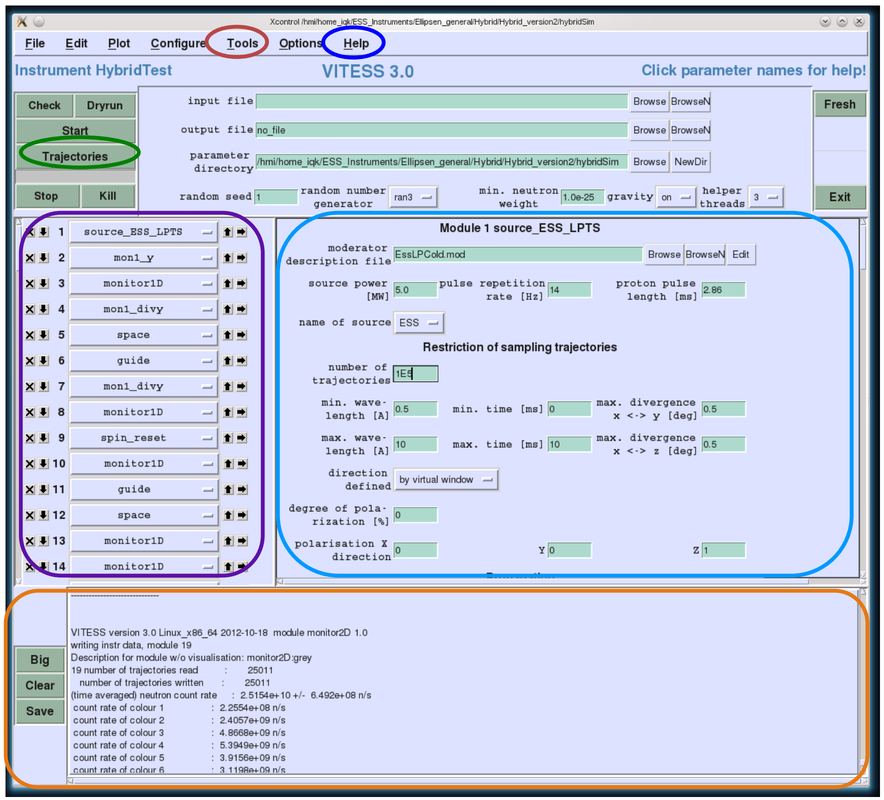
VITESS concepts

- Monte Carlo raytracing technique
  - neutrons modeled as trajectories through instrument components
  - each interaction (reflection, scattering) modifies probability weight (**= intensity**), correct flux independent of simulated number of neutrons
  - trajectories are created in source modules
  - 12 trajectory parameters: time, λ, probability weight, position (x, y, z), direction (cos(alpha), cos(beta), cos(gamma)) and Spin (S_x, S_y, S_z)
- Modular structure
  - component represented by modules (executables) run successively in a pipe: source | guide | sample | detector
  - modules are independent, can run in parallel
  - flexible usage (add/shift components, divide instrument, ...)
- Validity
  - delivered results in good agreement with experiments and other software packages (McStas, Restrax, …)

How to use VITESS

- Easy to install: available for Windows, Linux, Macintosh
  - download from VITESS website: www.helmholtz-berlin.de
  - Mac users need to install libgd, gnuplot: recipe included



- Easy to use: graphical user interface (GUI)
  - component list
  - parameter describing component
  - short help: click on names
  - long help: documentation
  - helper tools
  - visualization
  - log-file and pipe command
- Can also be run from the command line
  - export pipe in batch/tcl/python/perl script

Concept of VITESS

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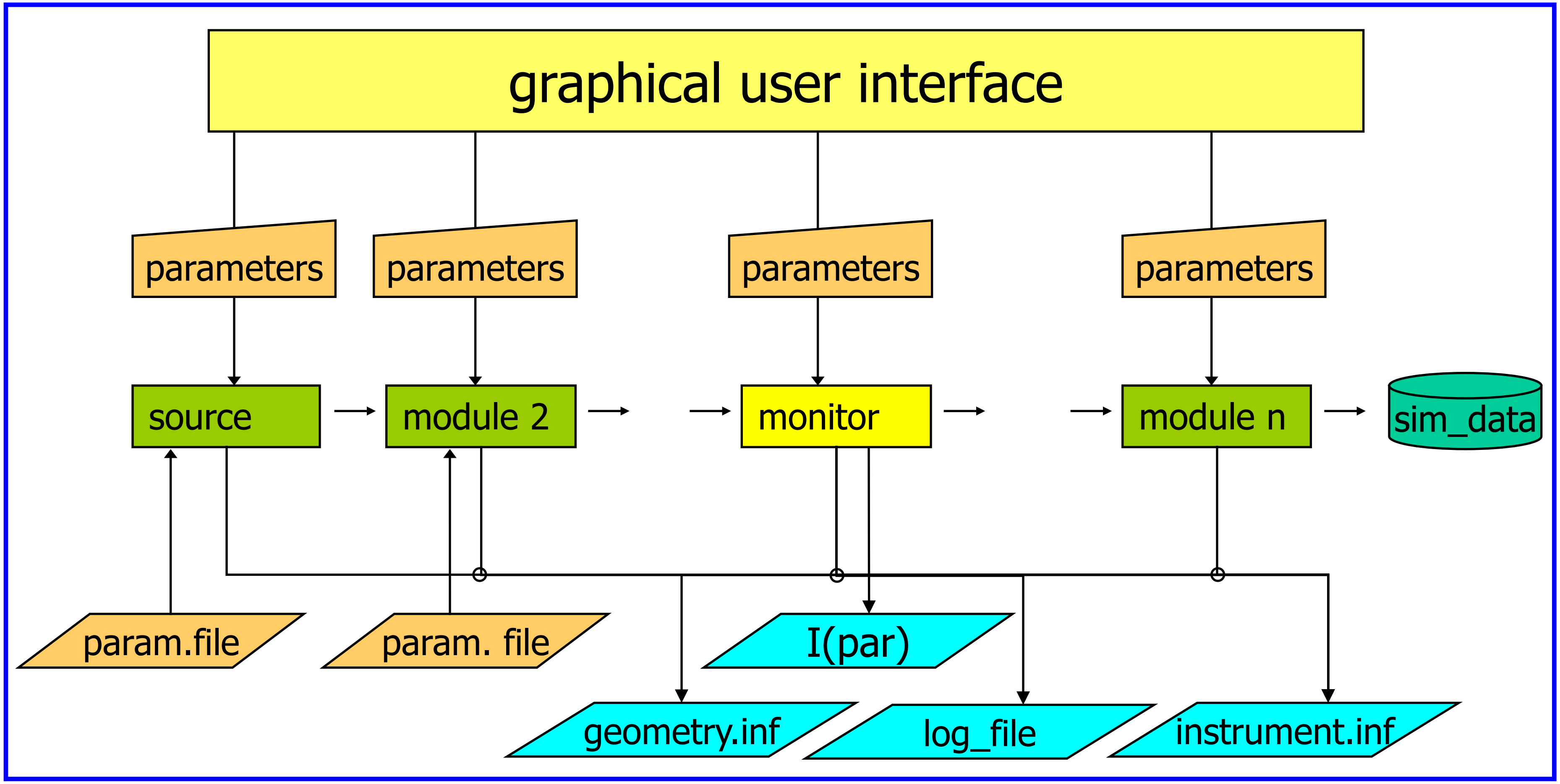

- **Runs on Windows, Linux/Unix and Macintosh systems**
- **Package contains everything need for simulation and basic output visualization**

Components for Neutron Scattering Instruments

- Transport
  - Guides
  - Benders
- Optics
  - Slits
  - Collimators
  - Lenses
  - Prisms
- Monochromatization
  - Disc choppers
  - Fermi choppers
  - Crystal monochromators
- Polarization
  - Polarizers
  - Flippers
  - Magnetic fields

Modules representing Hardware

Sources	reactor	SPSS	LPSS			
Space + Windows	space	slit	window/ beamstop	multiple windows	grid	beamstop
Choppers	disk	Fermi str.	Fermi curv.		vel.select	
Mono/Ana	flat	focus	foc. user		detector	
Modules f. Polaris.	^{3}He-polar.	coil flipper	prec. field	4-ang.field	pol. mirror	
	SM-polar.	grad. flipper	rot. field	res. Drabkin		
Samples	elast. isotr.	powder	SANS	reflectom.		
	inelastic	sngl.crys.	S(Q)	environm.		
Collimator	simple coll.	Soller coll.	radial coll.			
Optics / Transport	guide	ellipt. guide	bender	SM ensemb	lens	ellipt. mirror

Modules for Data Evaluation

Monitor 1	monitor1D	time	waveleng	y-/z-pos	div-y/-z	brilliance
Monitor 2	monitor2D	y-pos z-pos	div-y div-z	k-y k-z	y z div-y div-z	r div-r
		TOF λ	λ div-y/-z			
MonPol 1	Time	Wavelen	y-/z-pos	div_y/-z		
MonPol 2	y-pos z-pos					
Evaluate	elast	elast2	inelast	sans		
Geometr.	frame					
Trajector.	writeout	read_in				
	capt_flux	visualize	spin_reset			

Structure of Functions and Classes

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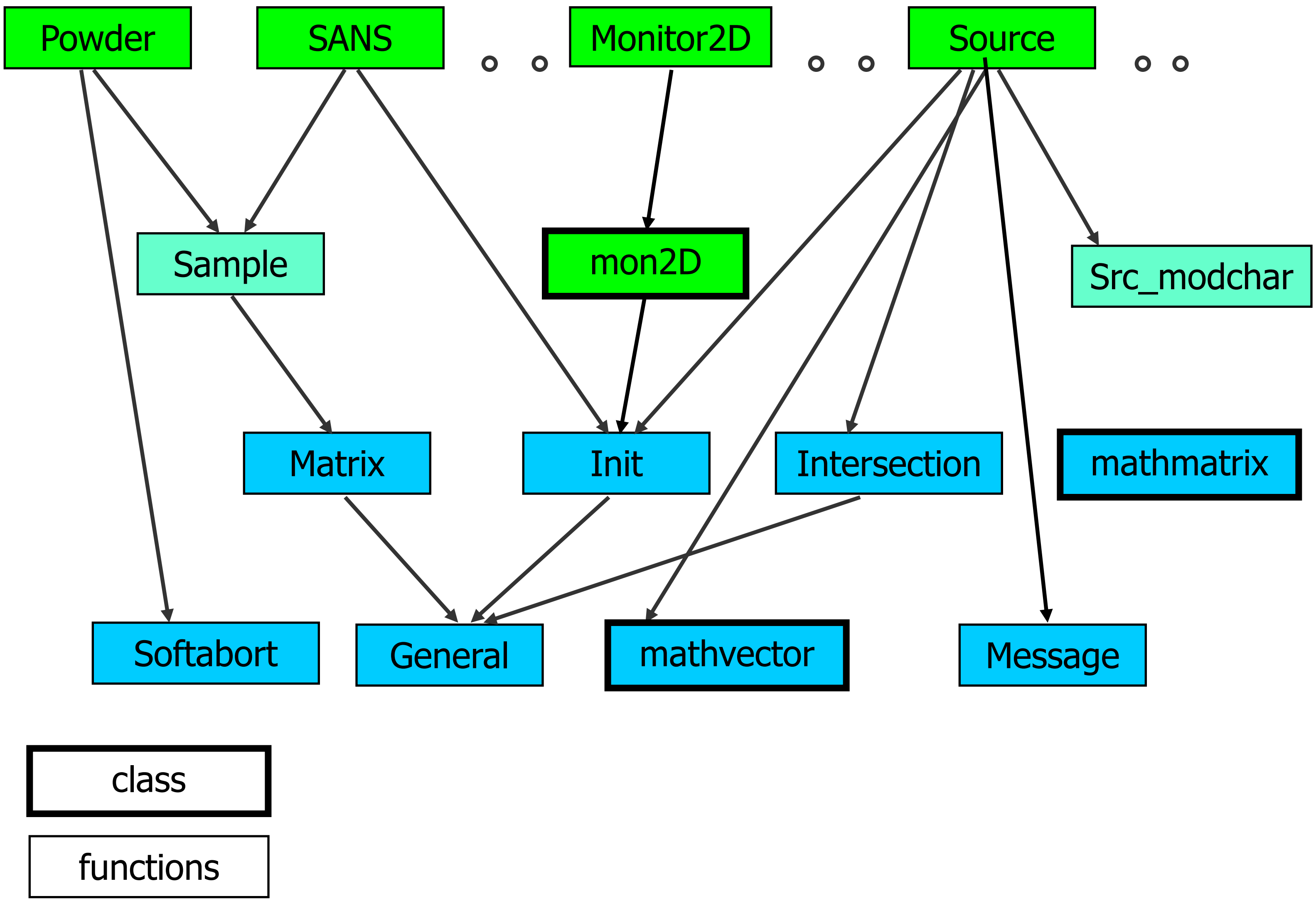


main
C functions
of a module

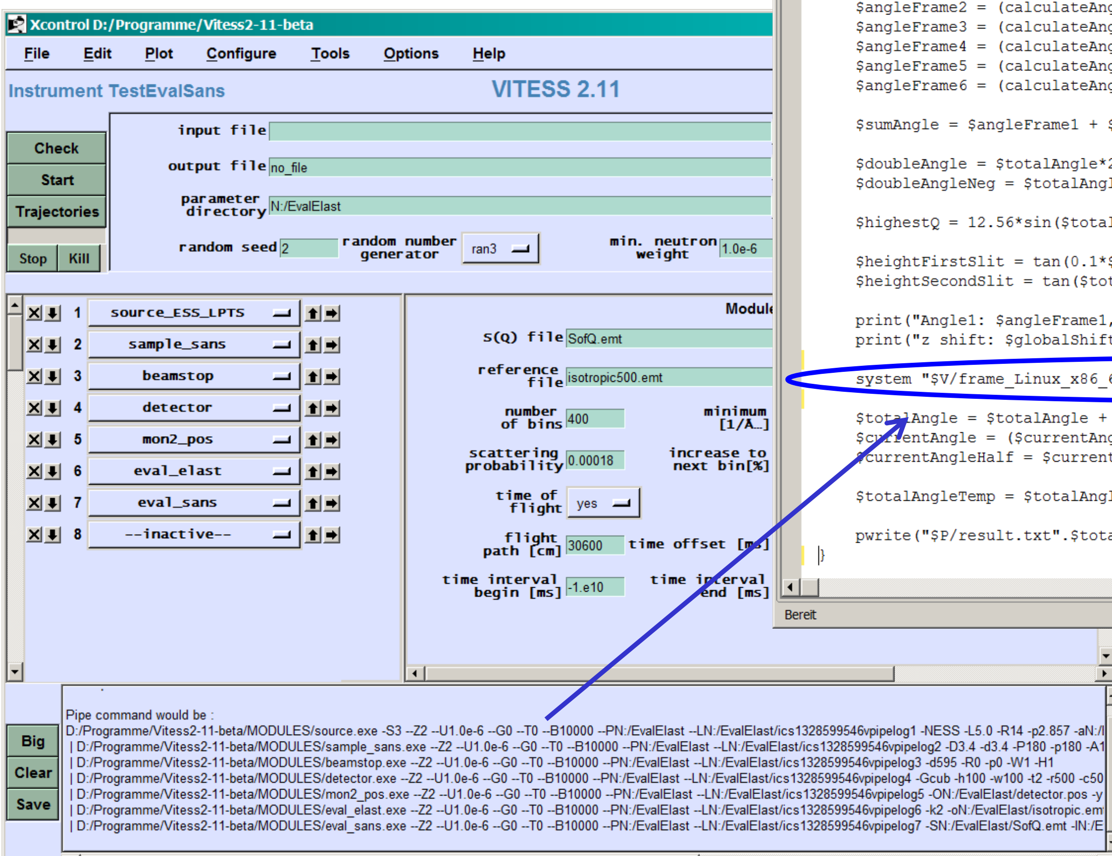
application
specific
C functions

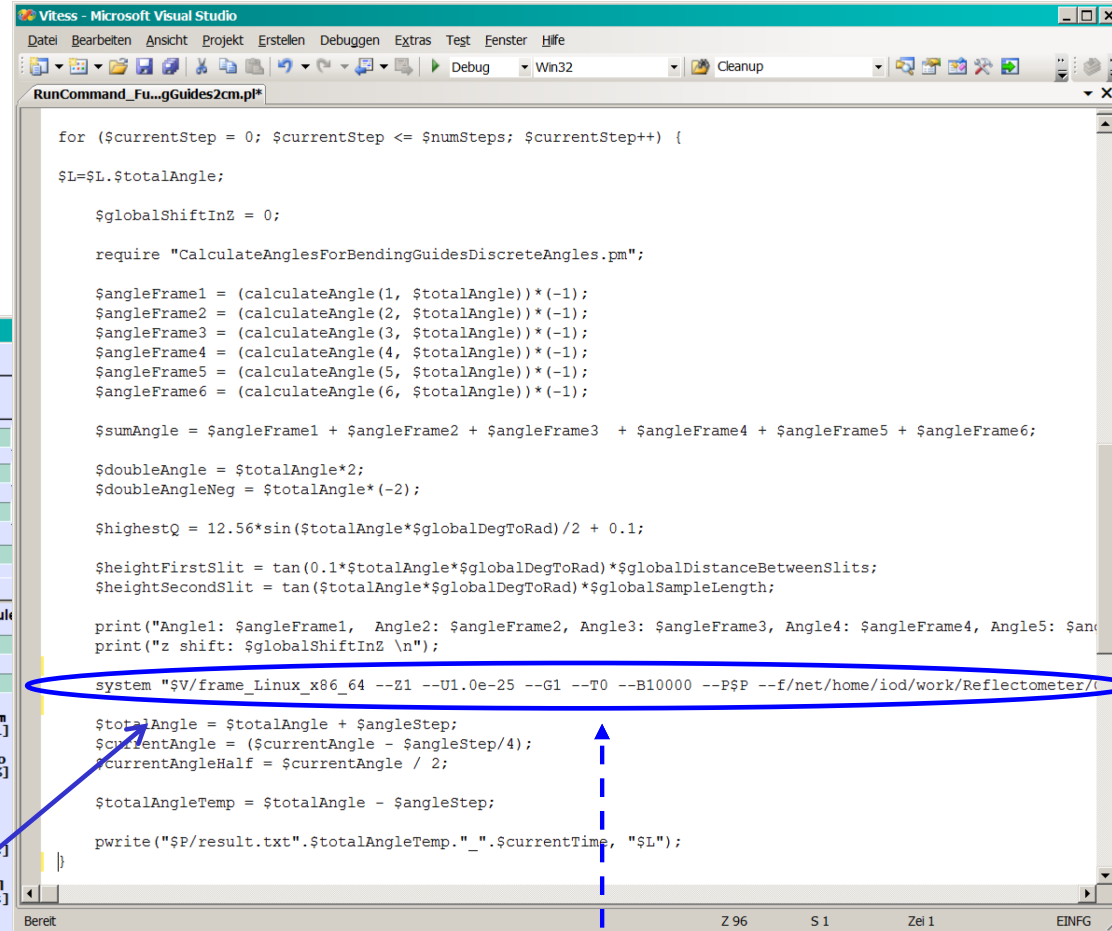
general
(complex)
C functions

basic
C functions
and classes

GUI and Script

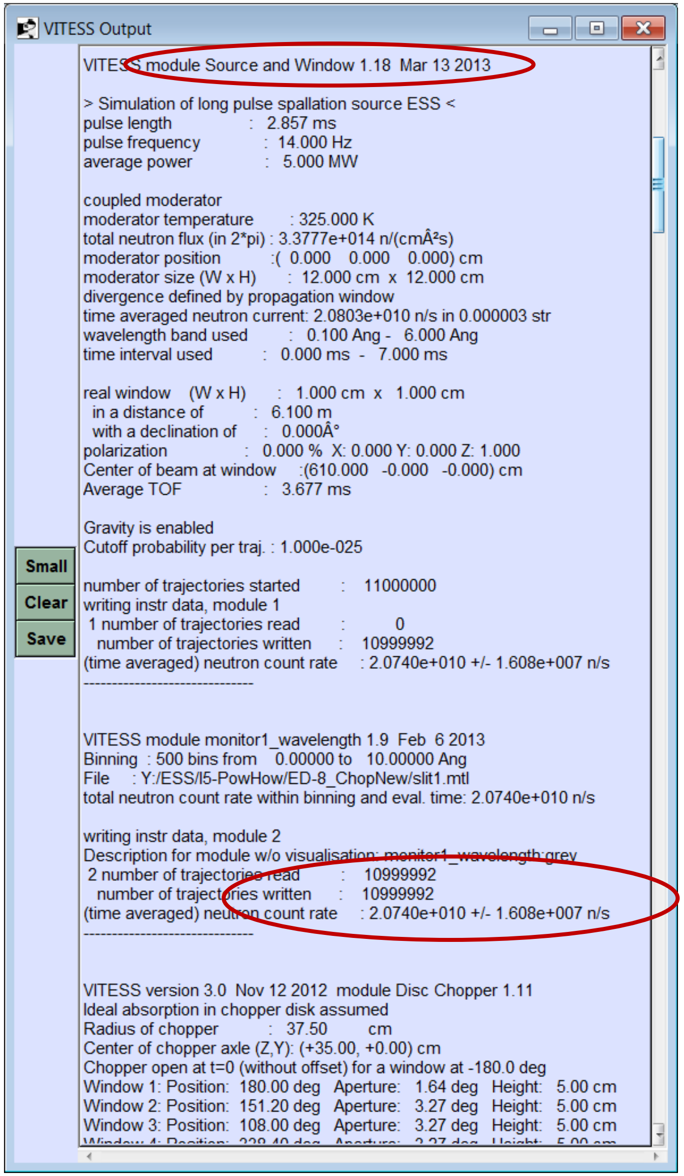
- Scripts
  - Python
  - Perl
  - Shell script
  - Tcl script





Command to run simulation

VITESS Log File and Monitor Output


VITESS Output

VITESS module Source and Window 1.18 Mar 13 2013

> Simulation of long pulse spallation source ESS <
pulse length : 2.857 ms
pulse frequency : 14.000 Hz
average power : 5.000 MW

coupled moderator
moderator temperature : 325.000 K
total neutron flux (in 2*pi) : 3.3777e+014 n/(cmÂ²s)
moderator position :(0.000 0.000 0.000) cm
moderator size (W x H) : 12.000 cm x 12.000 cm
divergence defined by propagation window
time averaged neutron current: 2.0803e+010 n/s in 0.000003 str
wavelength band used : 0.100 Ang - 6.000 Ang
time interval used : 0.000 ms - 7.000 ms

real window (W x H) : 1.000 cm x 1.000 cm
in a distance of : 6.100 m
with a declination of : 0.000Â°
polarization : 0.000 % X: 0.000 Y: 0.000 Z: 1.000
Center of beam at window :(610.000 -0.000 -0.000) cm
Average TOF : 3.677 ms

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

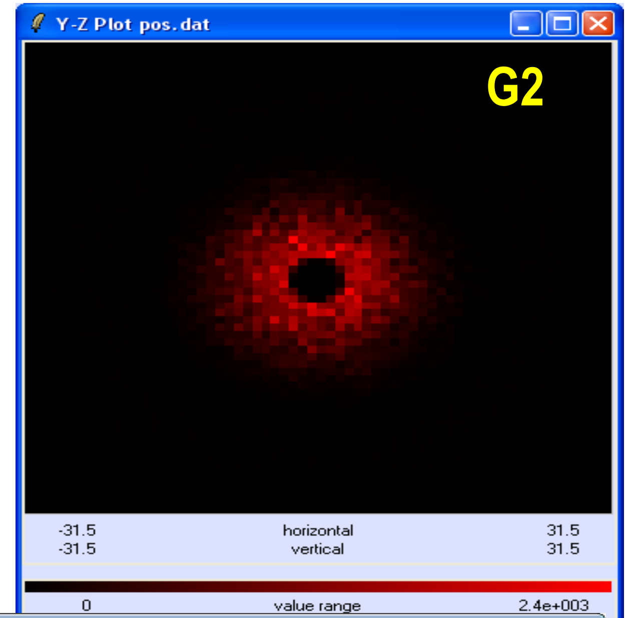
number of trajectories started : 11000000
writing instr data, module 1
1 number of trajectories read : 0
number of trajectories written : 10999992
(time averaged) neutron count rate : 2.0740e+010 +/- 1.608e+007 n/s

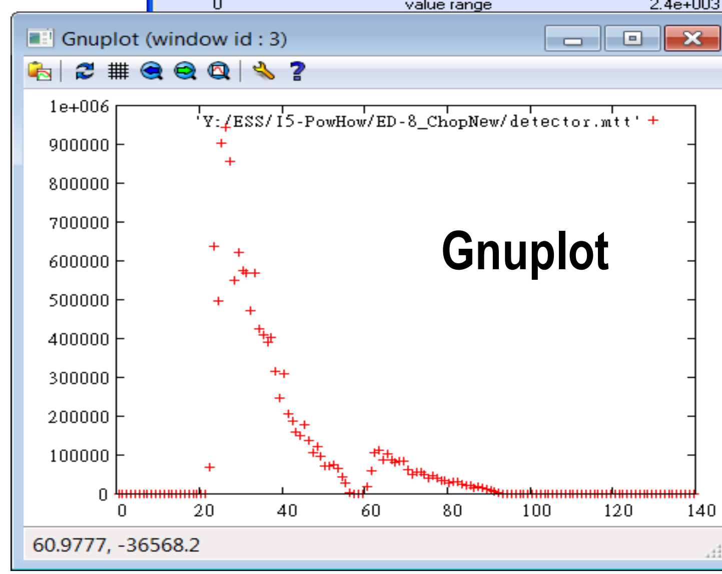
VITESS module monitor1_wavelength 1.9 Feb 6 2013
Binning : 500 bins from 0.00000 to 10.00000 Ang
File : Y:/ESS/I5-PowHow/ED-8_ChopNew/slit1.mtl
total neutron count rate within binning and eval. time: 2.0740e+010 n/s

writing instr data, module 2
Description for module w/o visualisation: monitor1_wavelength:grey
2 number of trajectories read : 10999992
number of trajectories written : 10999992
(time averaged) neutron count rate : 2.0740e+010 +/- 1.608e+007 n/s

VITESS version 3.0 Nov 12 2012 module Disc Chopper 1.11
Ideal absorption in chopper disk assumed
Radius of chopper : 37.50 cm
Center of chopper axle (Z,Y): (+35.00, +0.00) cm
Chopper open at t=0 (without offset) for a window at -180.0 deg
Window 1: Position: 180.00 deg Aperture: 1.64 deg Height: 5.00 cm
Window 2: Position: 151.20 deg Aperture: 3.27 deg Height: 5.00 cm
Window 3: Position: 108.00 deg Aperture: 3.27 deg Height: 5.00 cm

- Monitor output in ASCII format
- 2-dim monitors write matrix or xyz file





Visualization of Instruments and Trajectories

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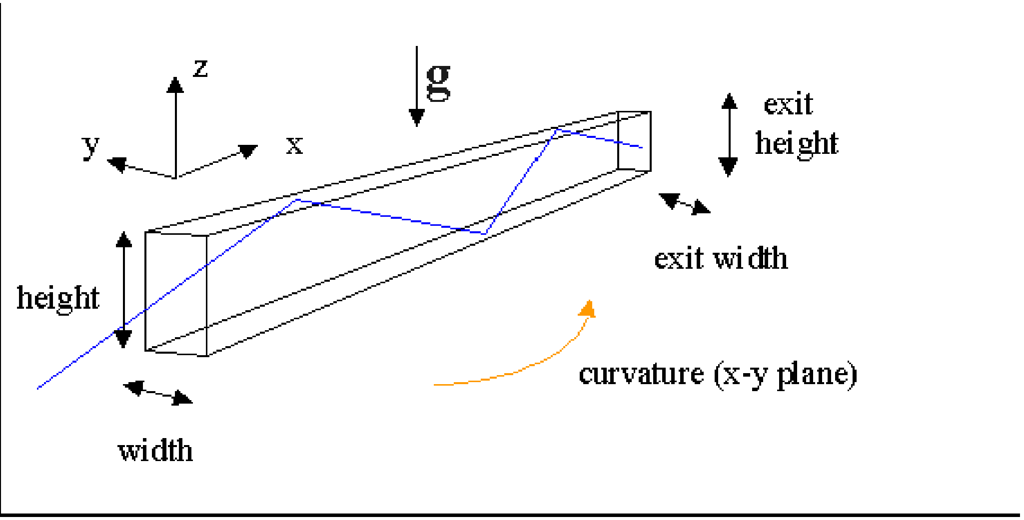
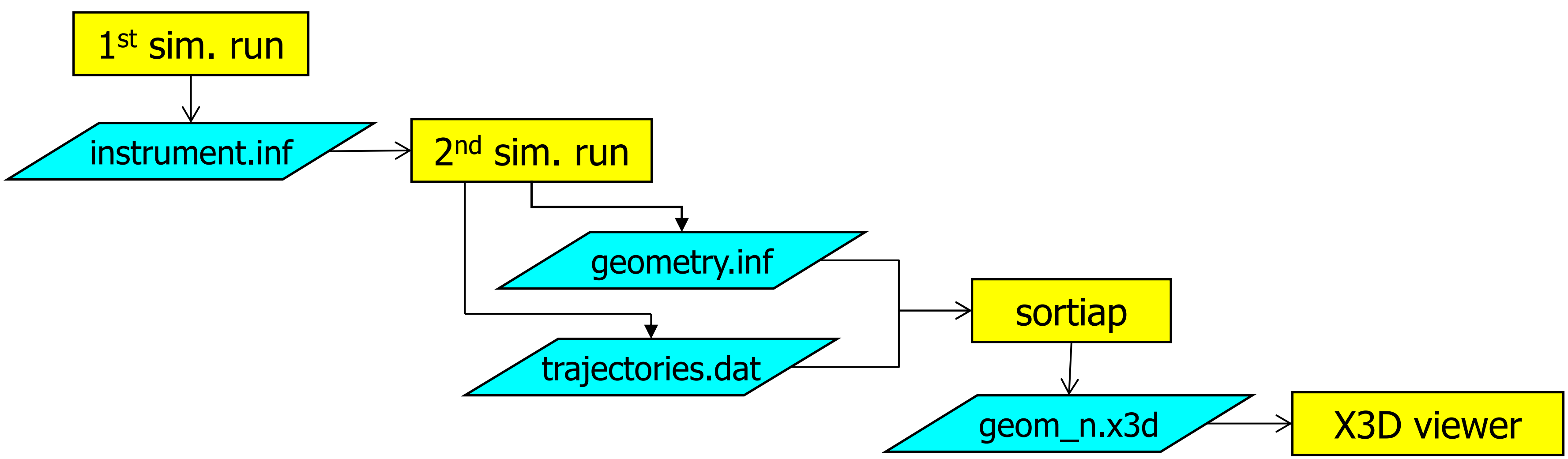


- **Idea**: 3D visualization of instrument and trajectories
- **Problem**: no information about the absolute co-ordinate systems exists in the VITESS modules
- **Solution**: A preliminary run creating the file '*instrument.inf*' containing absolute positions of the components
- The simulation output files '*geometry,inf*' and '*trajectories.dat*' contain positions in an absolute co-ordinate system
- This is then transferred to a file in x3d format to be read by a X3D viewer



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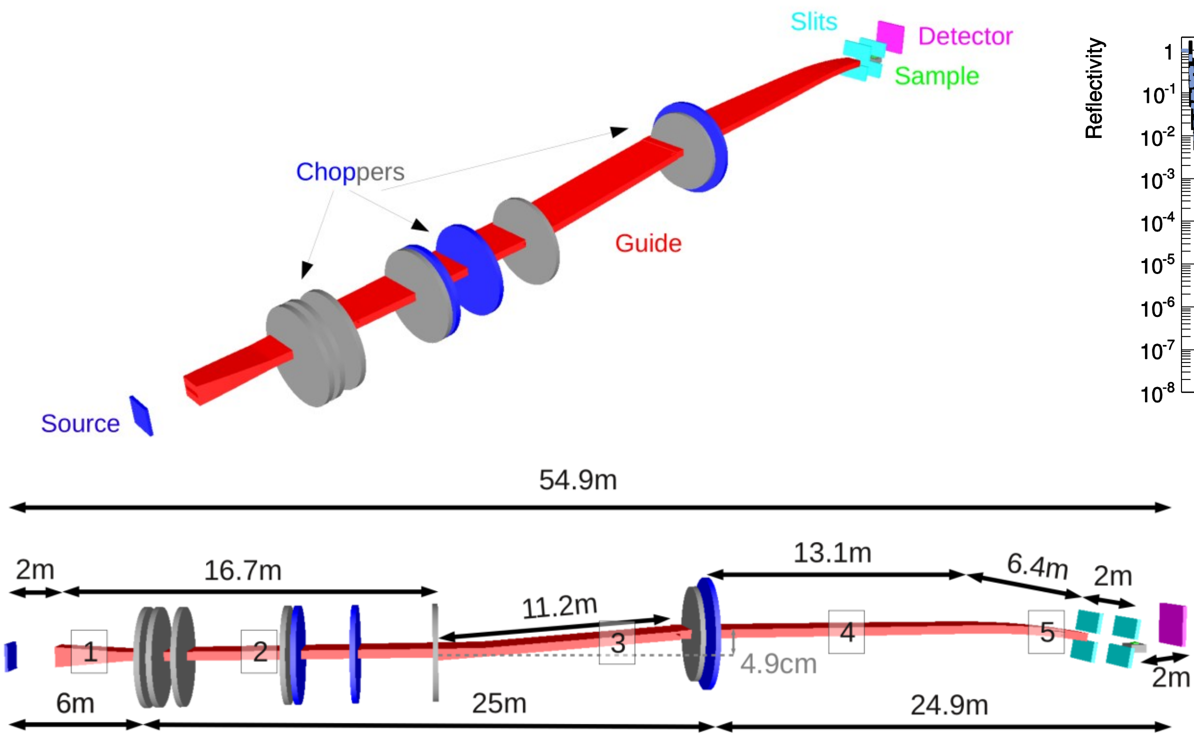
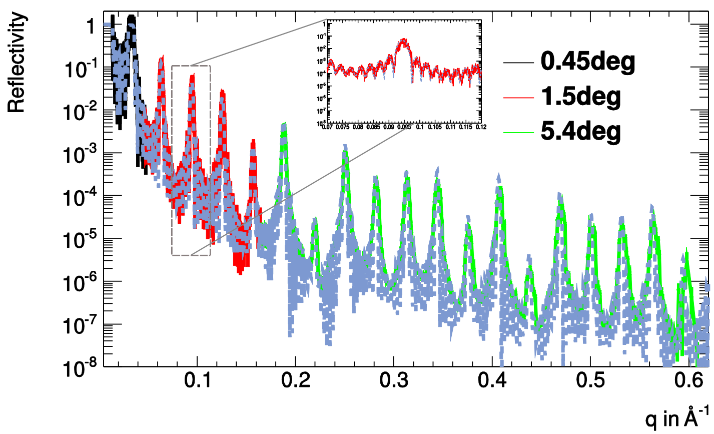
- Goals
  - Q-range up 0.9 Å^{-1} from both sides
  - 1% to 10% resolution
  - Low background

Bending guides: 5
Coating: m=5
Angles: 0.3° < θ < 9°





TOF powder diffractometer EXED at HMI

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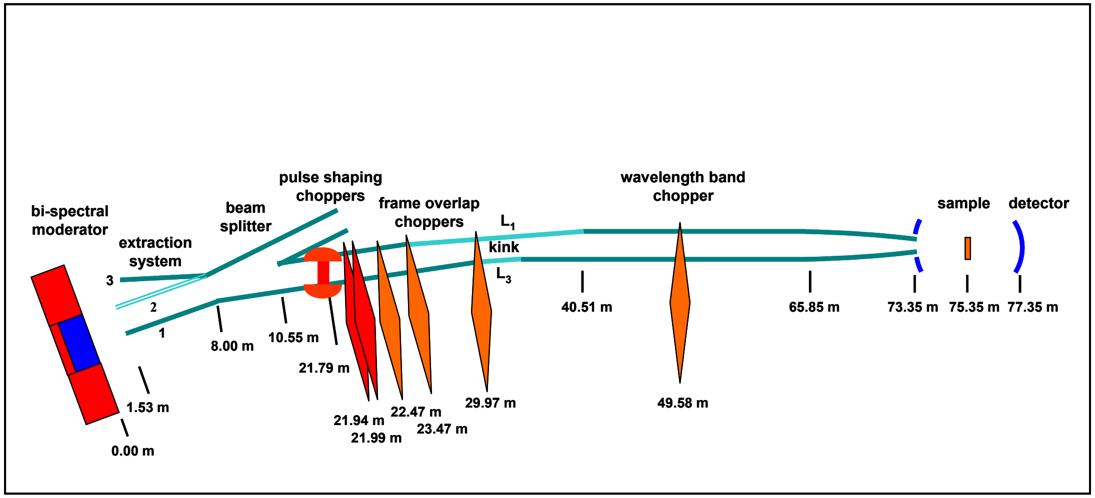
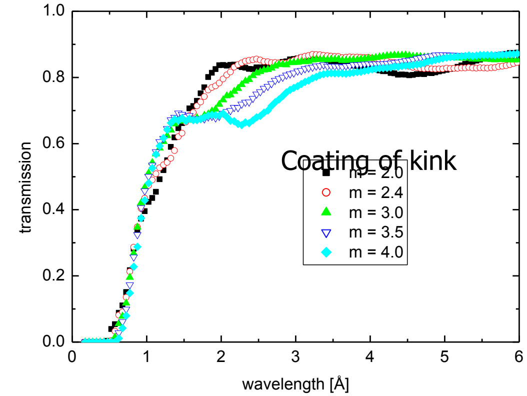
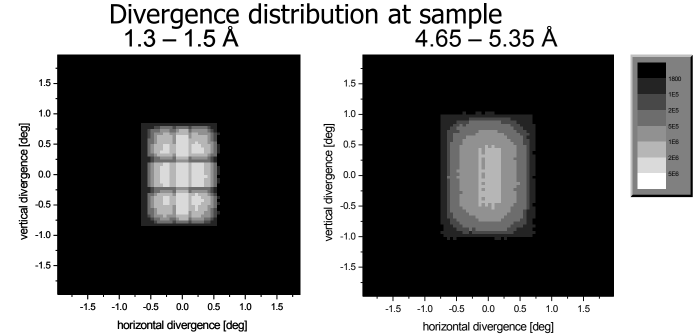
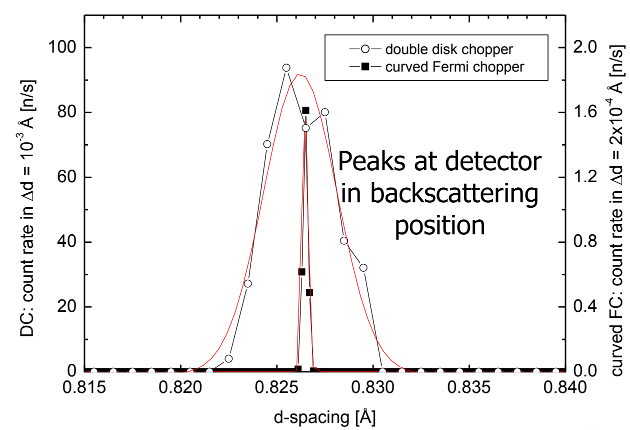




Divergence distribution at sample



- 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
- Results
  - resolution of $2x10^{-4}$ possible
  - large gain by elliptic focusing guide



J. Peters, K. Lieutenant, D. Clemens, F. Mezei, Z. Kristallogr. Suppl. 23 (2006) 189-194.
K. Lieutenant, J.Peters, F. Mezei, J. Neutron Res. 14.2 (2006) 147-165.

Numerical Optimization of whole Instruments

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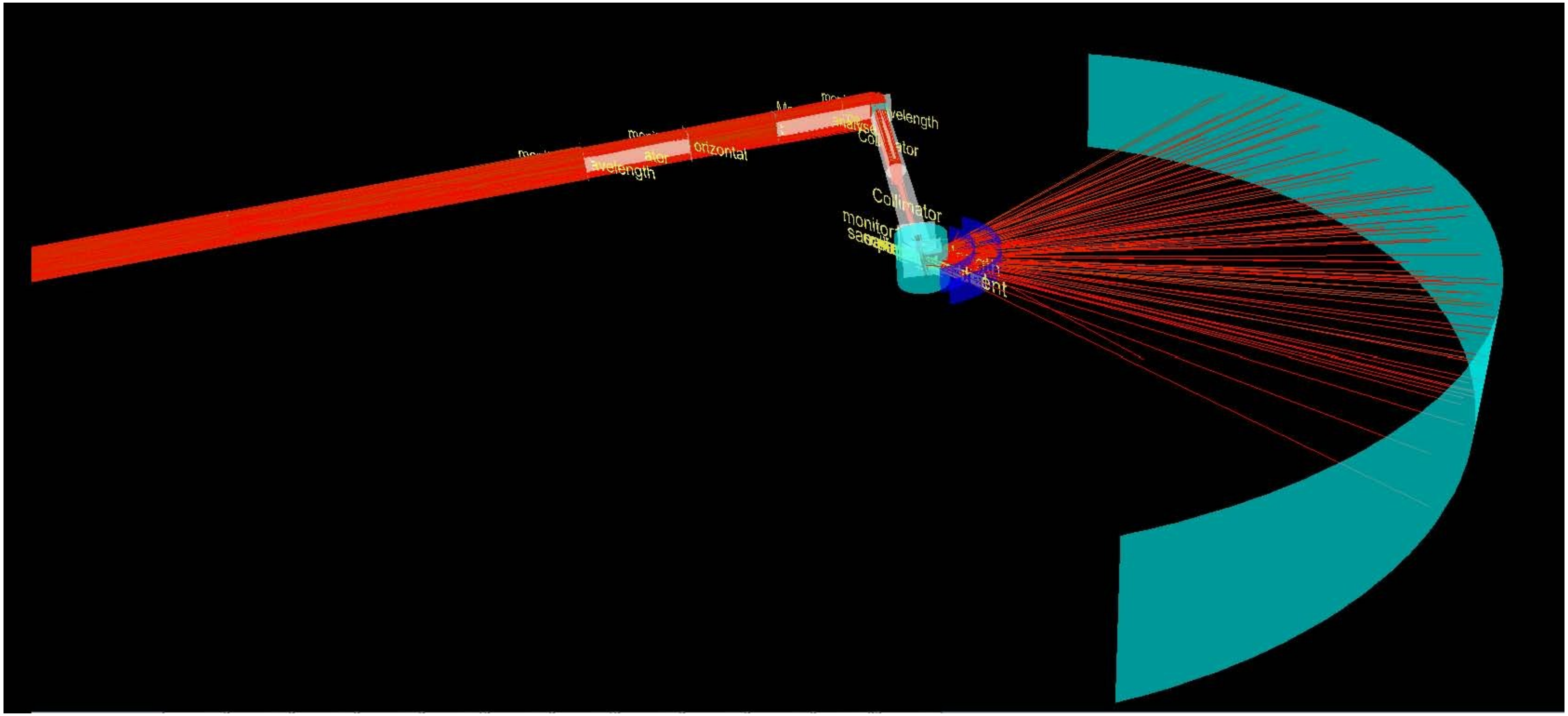


Diffractomer ODIN at IFE

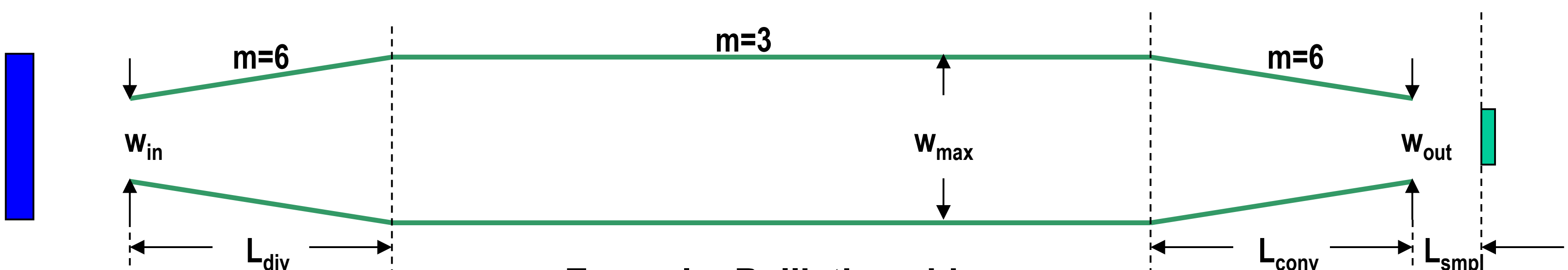
Diffractometer ODIN at IFE – Swarm Algorithm

take off angle	deg						60 deg				120 deg		
number of lines							15				23		
scatterig range	deg						10 - 100				10 - 145		
parameter		min	fixed	max	best FoM	2nd FoM	3rd FoM			best FoM	2nd FoM	3rd FoM	
ID					28.37	17.41	8.31	4.47	1.07	49.17	40.49	34.31	
collimation (channels)	min	5.0		120.0	124 (1)	124 (1)	124 (3)	120 (5)	26 (23)	21 (28)	24 (25)	21 (28)	
slit width	cm	0.50		8.00	7.73	7.76	7.70	8.00	6.17	7.58	7.48	7.32	
slit height	cm	3.00		18.40	10.53	11.34	11.34	10.38	10.64	18.28	16.90	16.03	
hor mosaicity	min		12.0										
vert mosaicity	min		24.0										
vert focus radius	m	1.50		20.00	20.00	20.00	20.00	20.00	20.00	8.30	11.72	11.98	
hor focus radius	m	2.00		20.00	20.00	20.00	20.00	19.91	20.00	14.70	14.87	15.20	
monochr - sample dist	cm		180.0										
detector radius	cm		190.0										
detector rows		3		30	29	29	30	28	29	29	30	30	
detector height	cm		$2.54 x N_{rows}$		73.7	73.7	76.2	71.1	73.7	73.7	76.2	76.2	
count rate	n/s				180.2	175.4	177.3	160.1	113.6	38.7	41.2	36.0	
resolution x 1000	$Å^{-2}$				4.354	4.319	4.379	4.309	3.785	2.587	2.642	2.527	
$sigma_{pos}$	deg				0.00500	0.00500	0.00507	0.00500	0.00500	0.0060	0.0060	0.0060	limit 0.006
1/FoM [10^{-10} $Å^{-2}$ deg^2 s/n]					6.039	6.157	6.354	6.730	8.331	2.077	2.081	2.084	1/FoM = $sigma^{1.5} R^3 / I$

- Optimization
  - Method: swarm algorithm
  - Some parameters are strongly correlated, not all can be determined simultaneously
  - Therefore: sizes and monochromator mosaicity fixed
- Results
  - Optimal detector height is very large (later fixed to 50 cm)
  - The focusing should be weak

Long Guide Systems – Optimization

- Idea: optimize all types of guides for highest flux at sample (1 x 1 cm²)
  - constant – ballistic – elliptic - parabolic
- Indepently for all combinations of
  - 50 m, 100 m, 150 m, 300 m total instrument length
  - 0.5° and 2.0° max. divergence
  - 1.5 and 5.0 Å average wavelength
    (range as is accessible at ESS for baseline parameters: 16.7 Hz, 2 ms)
- Optimization split between DTU (K. Klenø, McStas) and HZB (K. Lieutenant, VITESS)
  Final runs with both packages
- Fixed parameters
  - Moderator size 12 x 12 cm² (all sizes symmetric in width and height)
  - Coating and waviness
  - Distance moderator – sample 1.5 m
- Optimized parameters
  - Maximal, entrance and exit width/height of guide (max. width 40 cm)
  - Lengths of diverging and converging section, max. 30 % of total length
  - End position of guide (min. distance 0.5 m)

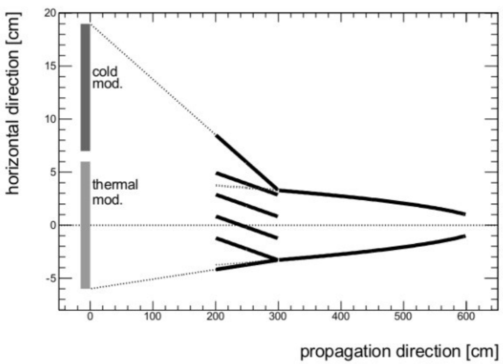


Example: Ballistic guide

Instrumentation research with VITESS

VITESS is being used for basic research of neutron instrumentation

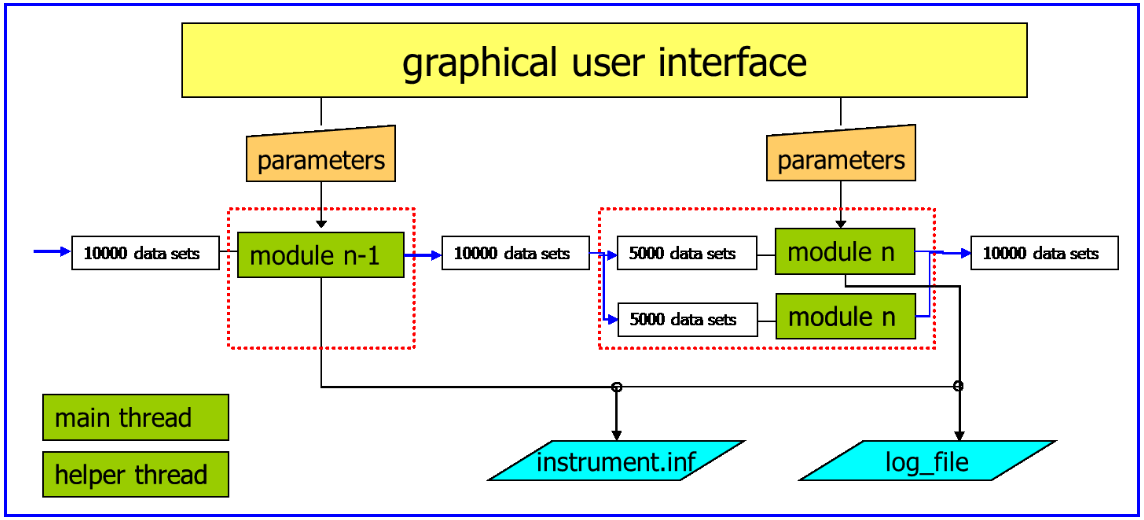
- Fundamental study of neutron propagation through elliptic guides
  - Aberrations, multiple scattering, guide segmentation
  - L. Cussen et al, NIM A 705 (2013) 121-131
- Extraction of neutrons from two moderators with a supermirror system



C. Zendler et al., NIM A: 704, 2013, 68-75

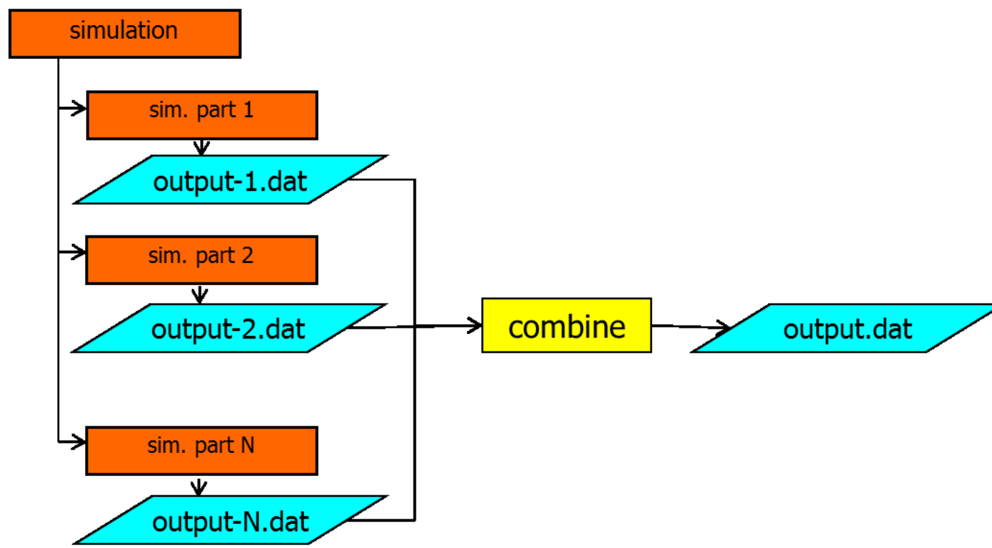
- The depende of gravity effects in elliptic neutron guide on the size of the feeding source
  - To appear in proceedings of the NOP & D 2013

Parallelisation



- Helper threads for multi-core processors
  - In addition to the main thread, n 'helper threads' can be defined
  - The main thread gives 1/(n+1) of the trajectories to each helper thread and treats the same number it self
  - All threads work on the same memory
  - At the end, the main thread collects the resulting data and takes care of the output

- Split of whole simulation for clusters
  - Whole simulation is split into N individual runs
  - At the end, the results are collected and combined to the final result
- Will be available in VITESS 3.1



Acknowledgement

We like to thank the BMBF for their support through the contribution to the ESS update phase.
Work package K7: Simulationscode-Entwicklung, Helpdesk work package

Thank you for your attention

New Optimization Concept for VITESS 3.1

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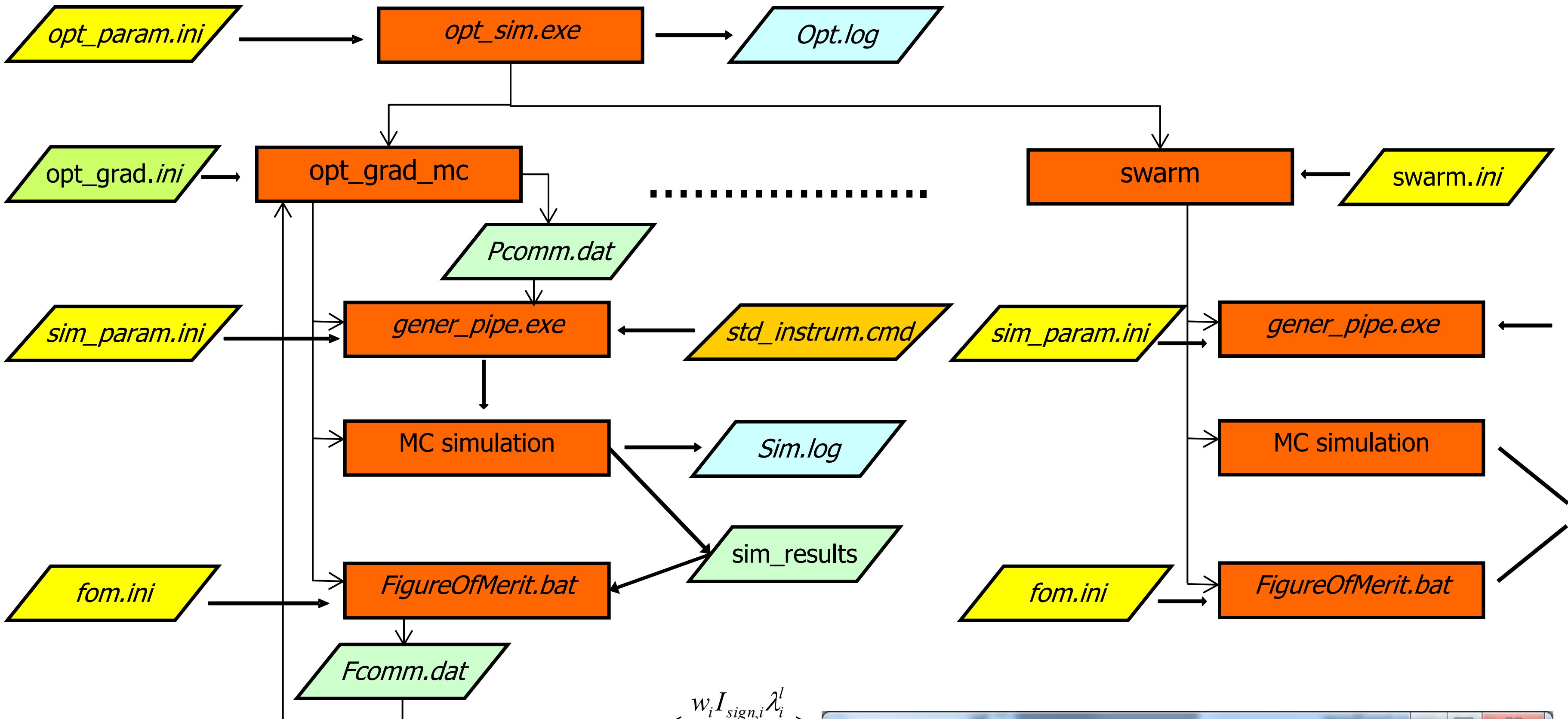


opt_param.ini - Editor

Datei Bearbeiten Format Ansicht ?

```
fit_grad
#    start     min      max     delta    description
1   43.7     10.0    120.0     0.1    #  temperature of cold
2    1.2e05   0.1e05   9.9e05  10.0    #  intensity of cold pa
3 137.2     50.0    300.0     0.1    #  temperature of therm
4    1.787    0.1     20.0     0.001  #  intensity of thermal
```

$$FoM = \frac{\left\langle \frac{w_i I_{sign,i} \lambda_i^l}{I^m_{ref,i}} \right\rangle}{\left\langle I^n_{noise,i} \right\rangle}$$

or

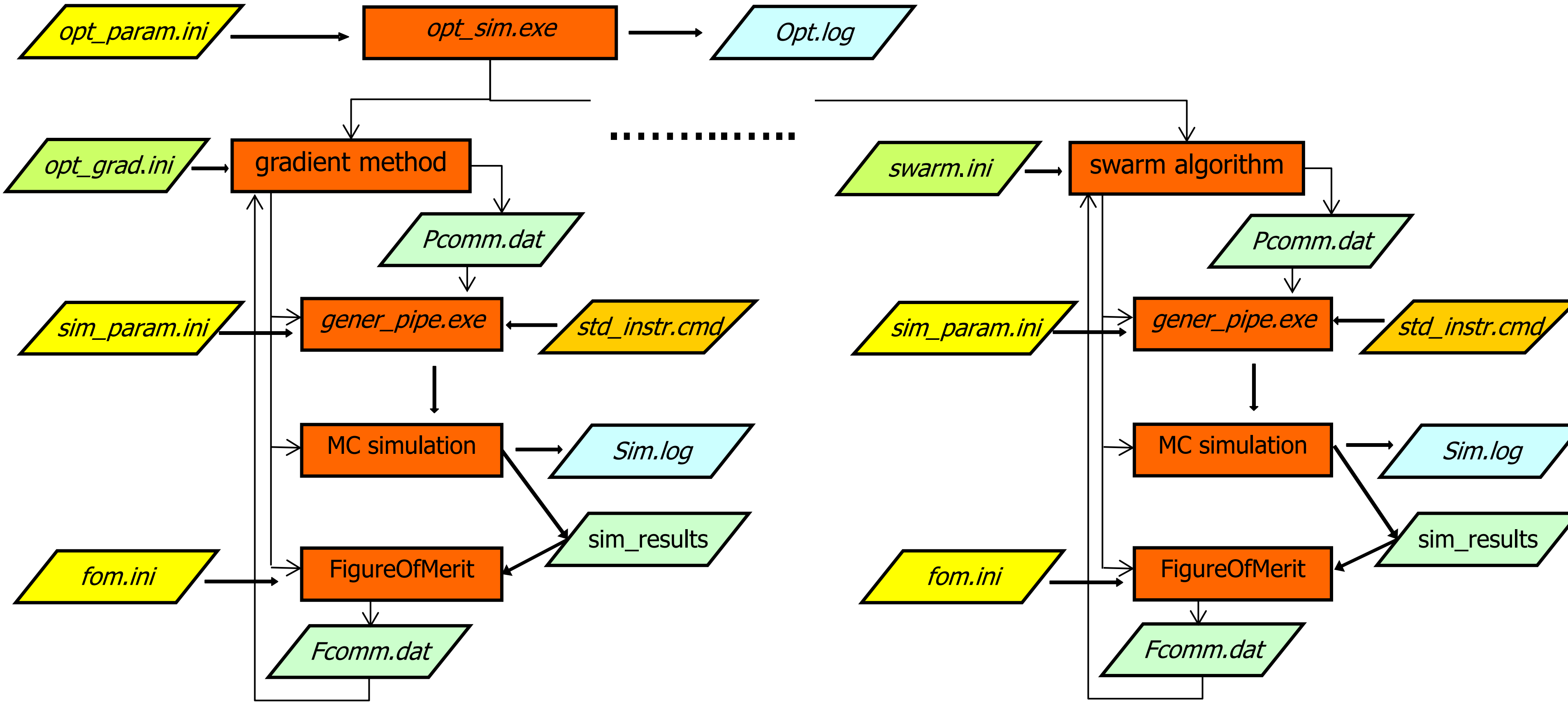
$$FoM = \frac{\sum_i \frac{w_i I_{sign,i} \lambda_i^l}{I^m_{ref,i}}}{\sum_i I^n_{noise,i}}$$

fom.ini - Editor

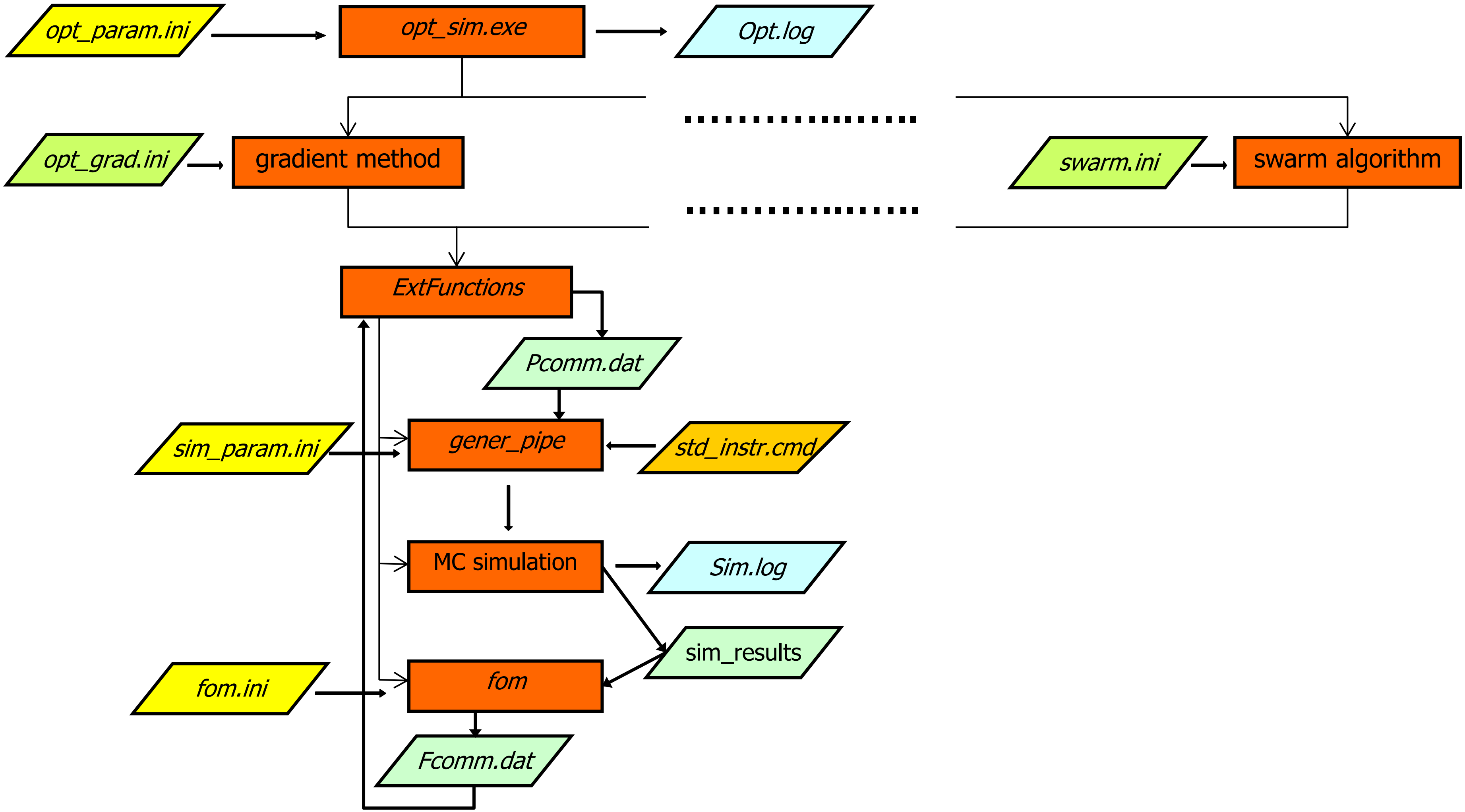
Datei Bearbeiten Format Ansicht ?

```
A= 0           # criterion: sum (A=0) or average (A=1)
l= 0.0         #       Sum\Average(I_sig/I_ref^m * Lambda^l)
m= 0.0         #  FoM = -------------------------------------
n= 0.0         #           Sum\Average(I_noise)^n
f= 1.0e09      # normalization factor for output value: f/FoM
S=slit.mtl     # signal file for 'FigureOfMerit'
R=no_file      # reference file
N=no_file      # noise file
W=no_file      # weight file
```

New Optimization Concept for VITESS 3.1



New Optimization Concept for VITESS 3.1



Example: Optimization of guide trumpet

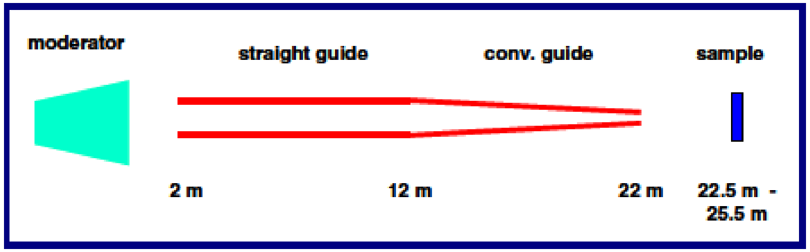


Table 3. Properties of a converging guide with elliptic shape obtained in runs with different initial values using the least-square fitting method and the Metropolis algorithm.

Method	Run	Long axis (m)	Short axis (cm)	Shift (m)	Exit size (cm)	Average transmission (%)	Flux on sample (n cm^{-2} s^{-1})
Least-square	1	13.75	6.50	−1.14	3.81	18.3	2.01×10^9
Least-square	2	13.77	7.48	−1.30	4.28	18.2	1.95×10^9
Least-square	3	11.90	6.46	0.47	3.87	18.7	2.05×10^9
Least-square	4	8.63	6.46	3.09	3.87	20.2	2.21×10^9
Least-square	5	7.80	6.58	3.83	4.03	20.5	2.28×10^9
Metropolis[a]	1	10.61	6.33	1.68	3.93	19.2	2.10×10^9
Metropolis[b]	1	7.94	6.60	3.69	4.00	20.6	2.28×10^9
Metropolis[c]	1	7.96 ± 0.23	6.54 ± 0.09	3.66 ± 0.18	4.00	20.6	2.28×10^9

[a] Best parameter set within first 1000 steps.
[b] Best parameter set during run (stopped after 4100 steps).
[c] Average over the last 388 executed steps (limit of maximum set to 20%, see text).

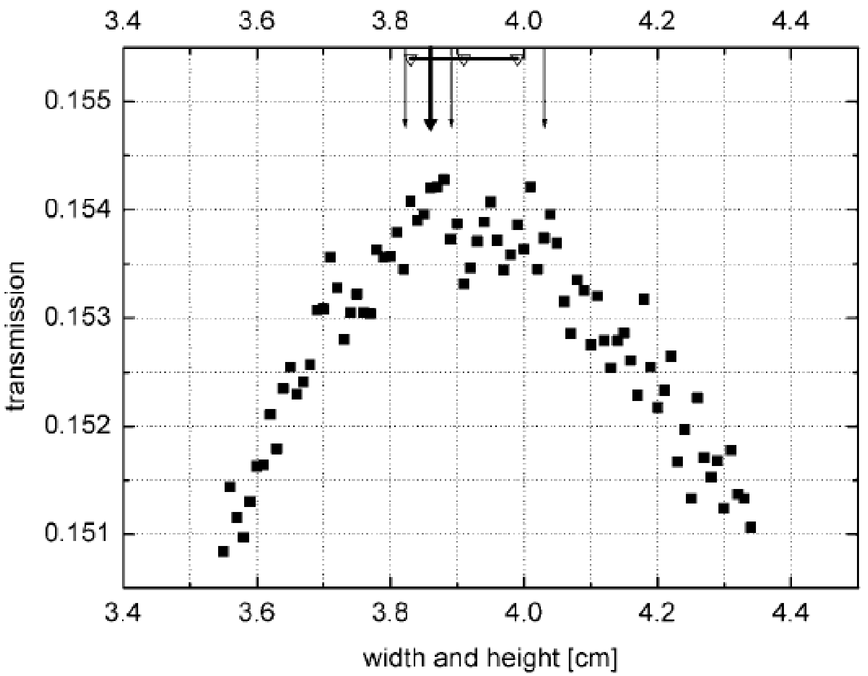


Figure 3. Transmission as a function of exit width (full squares). The arrows mark the sizes found in optimization runs using least-square fits (thin arrows) and Metropolis algorithm (thick arrow). The indicated range shows average value and standard deviation (for the size) of the random walk within the maximum using the Metropolis algorithm.

K. Lieutenant, J.Phys.:Condens.Matter 17 (2005) S167

- Statistical effect of the Monte Carlo method make numerical optimization difficult
- But it is feasible

Visualization of Instruments and Trajectories

geometry.inf - Editor

Datei Bearbeiten Format Ansicht ?

```
DEF grey=<Material diffuseColor='.6 .6 .6' emissiveColor='.6 .6 .6' transparency='.4'/>
DEF black=<Material diffuseColor='.01 .01 .01' emissiveColor='.01 .01 .01' transparency='.4'/>
DEF white=<Material diffuseColor='.99 .99 .99' emissiveColor='.99 .99 .99' transparency='.4'/>
#
#units
#  [m]  position, length, width, height, radius
# [deg] angels
#
Circle          0.00000   0.00000   0.00000    1.00000   0.00000   0.00000    0.08000   0.00000  360.00000   source:yellow
Rectangle       4.14500   0.00000   0.00000    1.00000   0.00000   0.00000    0.08300   0.16700    0.00000 source:yellow
Cylinder        0.36500   0.00000   0.00000    1.00000   0.00000   0.00000    0.00000   0.07100   space window
Rectangle       1.34500   0.00000   0.00000    1.00000   0.00000   0.00000    0.07000   0.14000    0.00000 slit:cyan
Rectangle       2.84500   0.00000   0.00000    1.00000   0.00000   0.00000    0.07000   0.14000    0.00000 slit:cyan
Rectangle       2.84500   0.00000   0.00000    1.00000   0.00000   0.00000    0.15000   0.15000    0.00000 monitor1_wavelength:grey
Cylinder        3.09500   0.00000   0.00000    1.00000   0.00000   0.00000    0.50000   0.05000   Collimator:white
Rectangle       3.34500   0.00000   0.00000    1.00000   0.00000   0.00000    0.15000   0.15000    0.00000 monitor1_horizontal :grey
Rectangle       3.79500   0.00000   0.00000    1.00000   0.00000   0.00000    0.08300   0.16700    0.00000 slit:cyan
Cylinder        4.07000   0.00000   0.00000    1.00000   0.00000   0.00000    0.55000   0.05000   Monochr_analyser:white
Rectangle       4.34500   0.00000   0.00000   -0.25882  -0.96593   0.00000    0.15000   0.15000    0.00000 monitor1_wavelength:grey
```

- Each Module adds lines to the geometry file that describe the component geometry
- Each event of a neutron creates a line in the trajectories file
  - Entering, passing or exiting a component
  - Reflection, scattering or absorption

TrajTest.dat - Editor

Datei Bearbeiten Format Ansicht ?

```
# Trajectories
#
# units
#   [m]   position
# [Ang]  lambda
# [n/s]  weight
#
#     ID       color  lambda     weight       pos_x      pos_y      pos_z  spin  rsn
AA000000001     0   1.18148  0.000e+000   0.00000    0.00992    0.04881    1   0
AA000000001     0   1.18148  0.000e+000   1.00000    0.00298    0.04477    1   3
AA000000002     0   3.24376  0.000e+000   0.00000    0.00236    0.01234   -1   0
AA000000002     0   3.24376  0.000e+000   1.00000   -0.02073   -0.02954   -1   3
AA000000003     0   3.09758  0.000e+000   0.00000   -0.01849    0.05891   -1   0
AA000000003     0   3.09758  0.000e+000   1.00000   -0.01399    0.01327   -1   3
AA000000004     0   5.78118  0.000e+000   0.00000   -0.04933   -0.00452   -1   0
AA000000004     0   5.78118  0.000e+000   1.00000   -0.00009    0.00136   -1   3
AA000000005     0   6.49735  0.000e+000   0.00000    0.04891   -0.03406    1   0
AA000000005     0   6.49735  0.000e+000   1.00000    0.02124    0.00462    1   3
AA000000006     0   2.23889  0.000e+000   0.00000    0.01437   -0.05372    1   0
AA000000006     0   2.23889  0.000e+000   1.00000    0.02818    0.00052    1   3
AA000000007     0   3.99686  0.000e+000   0.00000    0.06738    0.03288    1   0
AA000000007     0   3.99686  0.000e+000   1.00000   -0.02421   -0.03183    1   3
```

Components with visualization in VITESS 3.0

HZB Helmholtz Zentrum Berlin

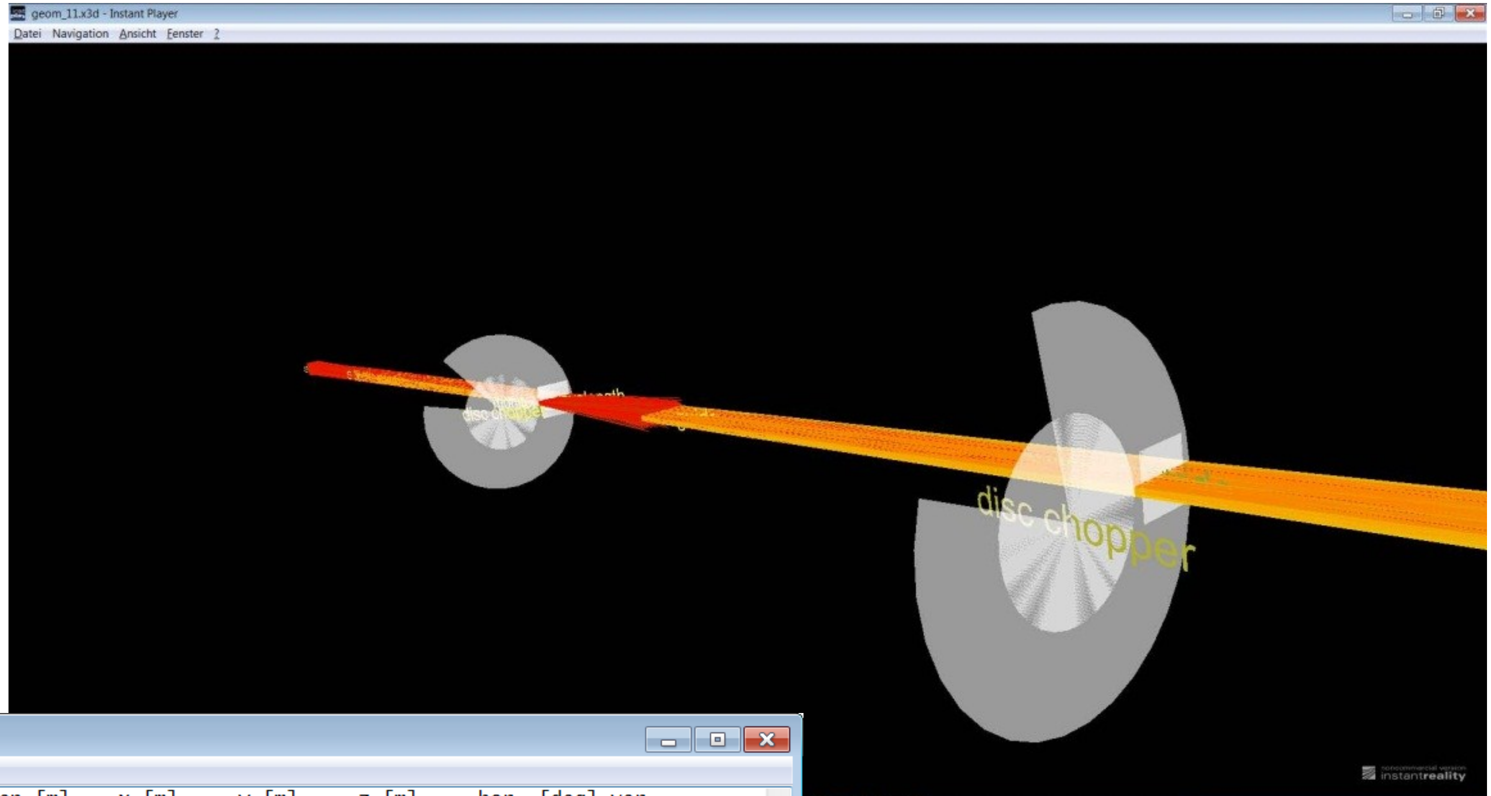
Sources	**reactor**	**SPSS**	**LPSS**			
Space + Windows	**space**	**slit**	**window/ beamstop**	multiple windows	grid	beamstop
Choppers	**disk**	Fermi str.	Fermi curv.		vel.select	
Mono/Ana	**flat**	**focus**	**foc. user**		**detector**	
Modules f. Polaris.	³He-polar.	coil flipper	prec. field	4-ang.field	pol. mirror	
	SM-polar.	grad. flipper	rot. field	res. Drabkin		
Samples	elast. isotr.	powder	SANS	reflectom.		
	inelastic	sngl.crys.	S(Q)	**environm.**		
Collimator	simple coll.	Soller coll.	**radial coll.**			
Optics / Transport	**guide**	**ellip. guide**	bender	**SM ensemb**	lens	ellipt. mirror

All Monitors work by default settings

comp1	**trajectories and component**
comp2	**trajectories**
comp3	**not yet implemented**

Instrument visualization and information about component positions

HZB Helmholtz Zentrum Berlin



instrument.inf - Editor

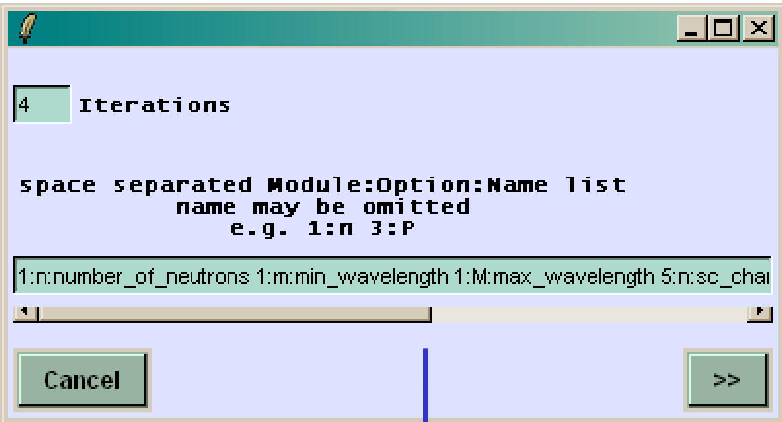
Datei Bearbeiten Format Ansicht ?

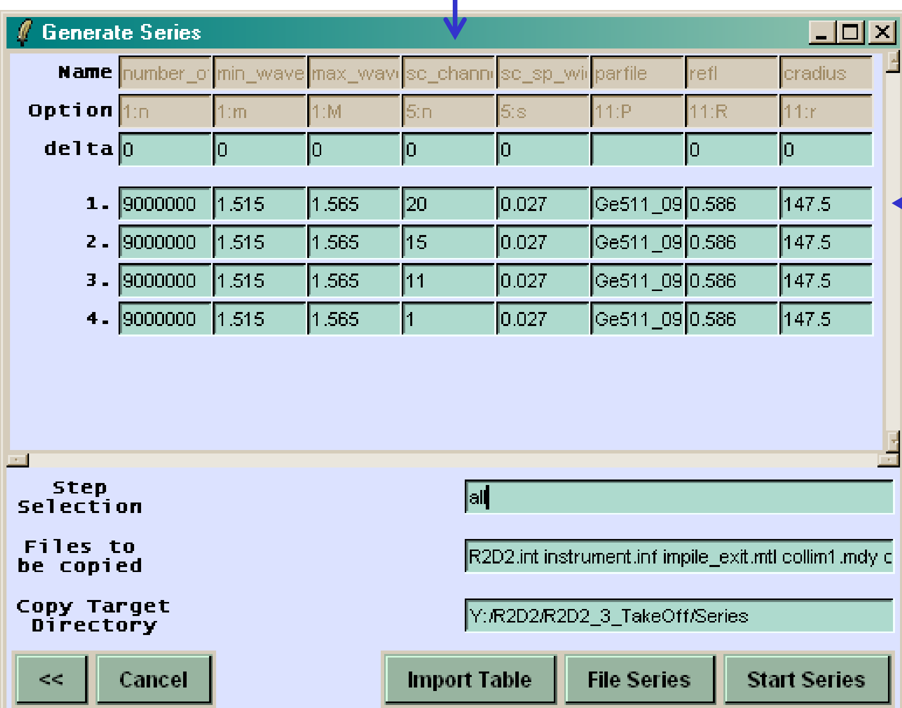
# No	ID	module	len [m]	x [m]	y [m]	z [m]	hor. [deg]	ver.
0	1	Source and Window	0.00000	0.00000	0.00000	0.00000	0.000	0.000
1	1	Source and Window	2.00000	2.00000	0.00000	0.00000	0.000	0.000
2	11	guide_parallel	6.00000	6.00000	0.00000	0.00000	0.000	0.000
3	101	monitor1_wavelengt	6.00000	6.00000	0.00000	0.00000	0.000	0.000
4	31	Disc Chopper	6.00000	6.00000	0.00000	0.00000	0.000	0.000
5	101	monitor1_wavelengt	6.00000	6.00000	0.00000	0.00000	0.000	0.000
6	20	Space	7.00000	7.00000	0.00000	0.00000	0.000	0.000
7	11	guide_parallel	9.00000	9.00000	0.00000	0.00000	0.000	0.000
8	31	Disc Chopper	9.00000	9.00000	0.00000	0.00000	0.000	0.000
9	131	frame	9.00000	9.00000	0.00000	0.00000	0.000	0.250
10	11	guide_parallel	11.30000	11.29998	0.00000	0.01004	0.000	0.250
11	11	guide_parallel	18.50000	18.49991	0.00000	0.04146	0.000	0.250
12	11	guide_parallel	20.22000	20.21989	0.00000	0.04896	0.000	0.250
13	131	frame	20.22000	20.21989	0.00000	0.04896	0.000	0.000
14	11	guide_parallel	31.00000	30.99989	0.00000	0.04896	0.000	0.000
15	31	Disc Chopper	31.00000	30.99989	0.00000	0.04896	0.000	0.000

X3D-Player:
'Default: InstantReality'

Option: 'Generate Series'

Defining variable parameters

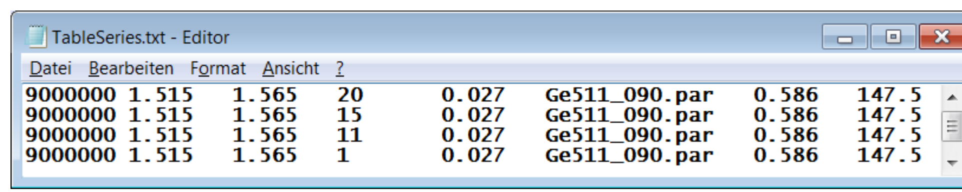




Excel or other Table calculator

num traj.	lmbd$_{min}$ [Å]	lmbd$_{max}$ [Å]	coll imator		monochr		
			no	d_{blade}	file	norm.fact.	radius
9000000	1.515	1.565	20	0.027	Ge511_090.par	0.586	147.5
9000000	1.515	1.565	15	0.027	Ge511_090.par	0.586	147.5
9000000	1.515	1.565	11	0.027	Ge511_090.par	0.586	147.5
9000000	1.515	1.565	1	0.027	Ge511_090.par	0.586	147.5

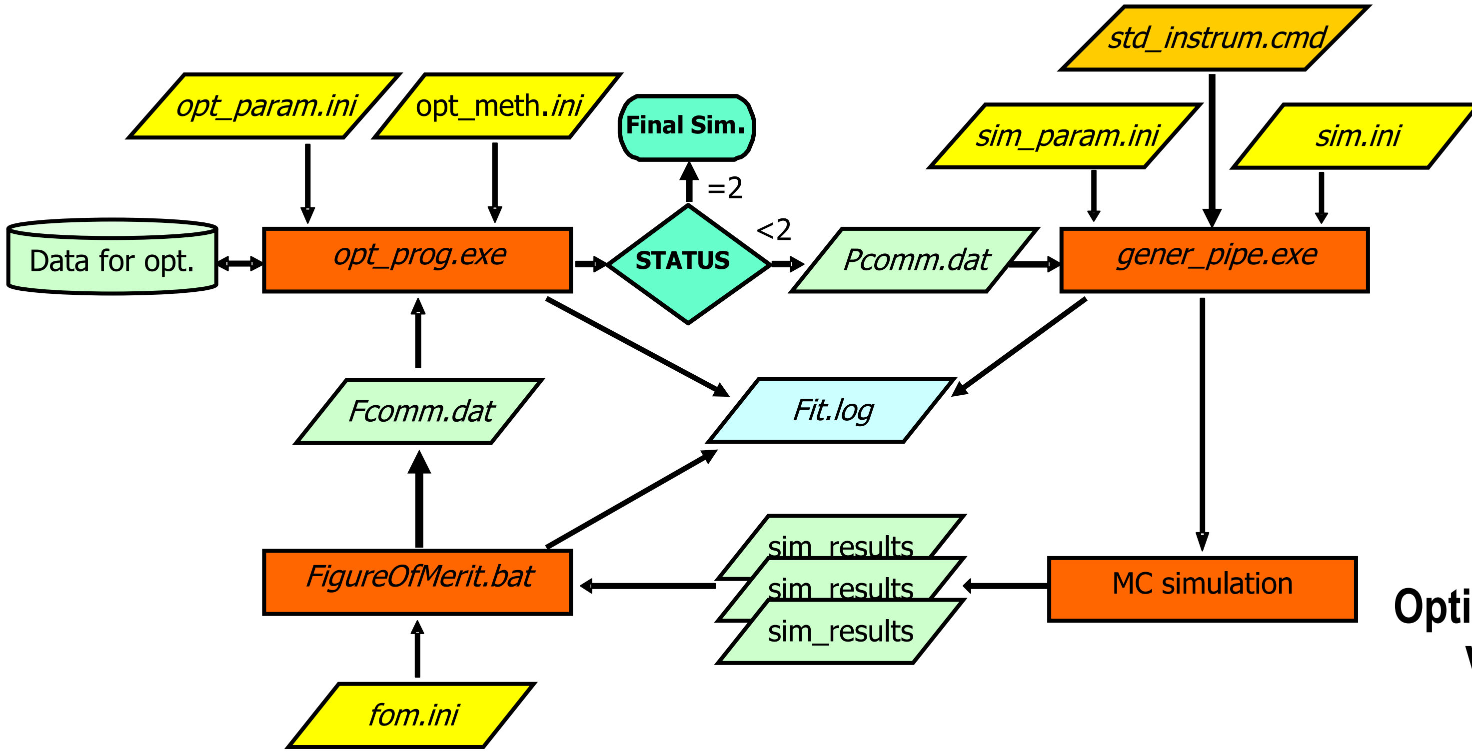
ASCII file


TableSeries.txt - Editor

Datei Bearbeiten Format Ansicht ?

```
9000000 1.515   1.565   20      0.027   Ge511_090.par   0.586   147.5
9000000 1.515   1.565   15      0.027   Ge511_090.par   0.586   147.5
9000000 1.515   1.565   11      0.027   Ge511_090.par   0.586   147.5
9000000 1.515   1.565   1       0.027   Ge511_090.par   0.586   147.5
```

Optimization



Optimization in VITESS

- MC simulation and numerical optimisation combined
  - Several Mio. trajectories need to be started in order to have 20'000 to 100'000 contributing to the figure of merit

Long Guide Systems – Gains

Gains relative to guide of constant cross-section

$$Gain = \frac{I_{sample,shape}}{I_{sample,const}}$$

total length [m]	max. div. [deg]	moderator	elliptic	parabolic	ballistic
				VITESS	
50	0.5	Thermal	1.91	1.97	1.67
50	0.5	Cold	0.96	1.04	1.04
50	2.0	Thermal	10.04	8.88	5.26
50	2.0	Cold	5.14	5.52	3.92
100	0.5	Thermal	2.52	2.62	2.24
100	0.5	Cold	1.07	1.08	1.11
100	2.0	Thermal	15.29	13.12	6.04
100	2.0	Cold	6.89	6.59	5.09
150	0.5	Thermal	3.01	3.24	2.79
150	0.5	Cold	1.10	1.10	1.14
150	2.0	Thermal	21.68	19.37	6.06
150	2.0	Cold	8.48	8.21	6.06
300	0.5	Thermal	3.84	4.45	3.34
300	0.5	Cold	1.25	1.28	1.29
300	2.0	Thermal	29.37	23.85	7.72
300	2.0	Cold	9.40	10.90	7.94

- Gains depend strongly on divergence and wavelength range and also on guide length

	low gain	high gain
divergence	low	high
wavelength	long	short
guide length	short	long

- Comparison of shapes
  - Elliptic guides are usually best
  - Parabolic – constant – parabolic guides yield nearly the same intensity
  - Ballistic guides have lower gains
  - Guides of constant cross-section can only compete for cold neutrons of low divergence

Principle: Monte Carlo Simulation of Instruments
Example: R2D2

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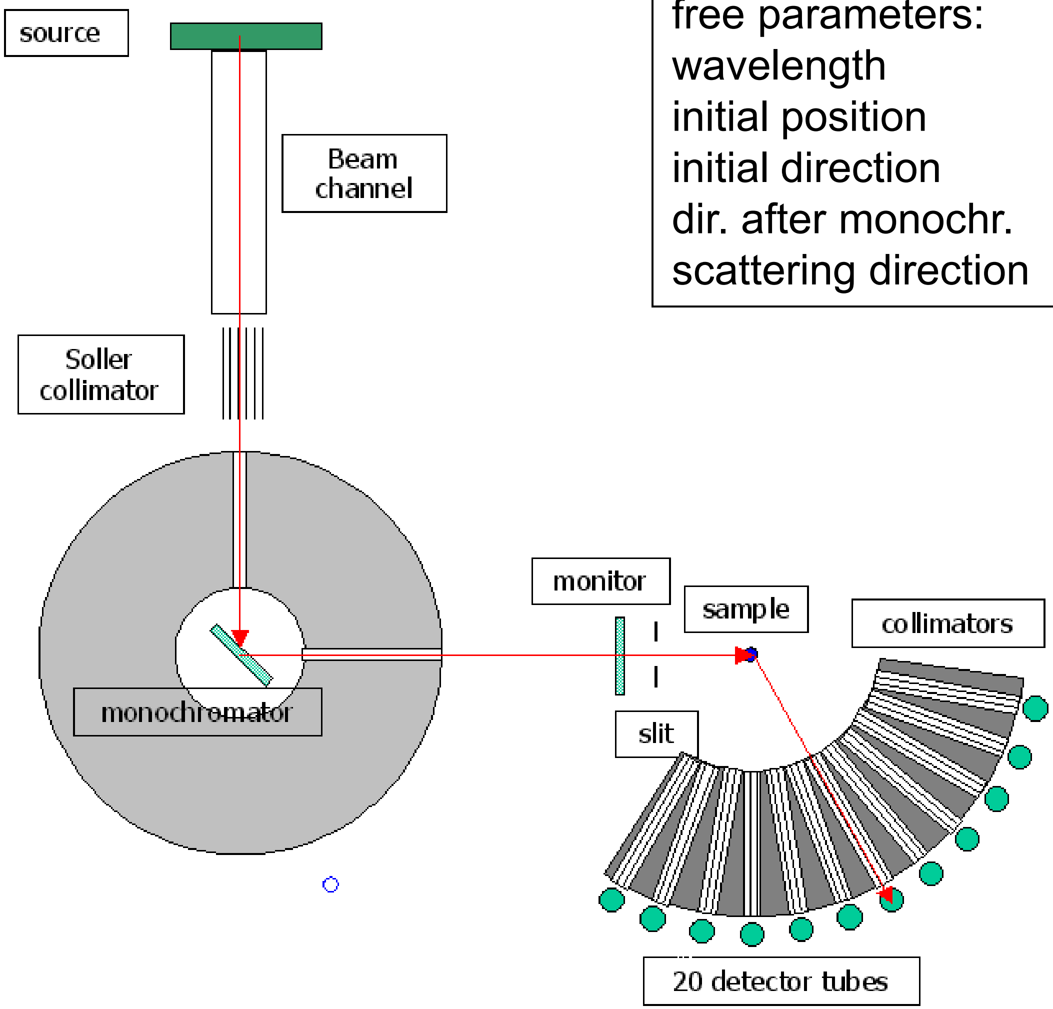

free parameters:	
wavelength	λ
initial position	x,y
initial direction	v_{hor}/v, v_{vert}/v
dir. after monochr.	θ_m, φ_m
scattering direction	θ_s, φ_s

Possible Requirements for Instruments

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- High intensity
  - Focusing of neutron beam
  - Large detector coverage

- High resolution
  - Well collimated beam
  - Narrow wavelength band (steady state instrument)
  - Short pulses and long instrument (time-of-flight instrument)

- Flexibility
  - change between high resolution and high intensity

- Whole measurement in one shot
  - Broad Q-range

- General
  - Effective neutron transport from source to sample
  - No direct view from source to sample
  - Low background (-> long instruments)

Why is designing Neutron Scattering Instruments important ?

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- Neutron sources have a low brilliance
  - “brightest neutron source emits as many neutrons as a candle emits photons”
  - Source brilliance cannot be increased any more by orders of magnitude

- Consequences
  - Neutrons have to be used efficiently
  - Instruments have to be as good as possible

Monte Carlo Simulations – a Design Tool for Instruments

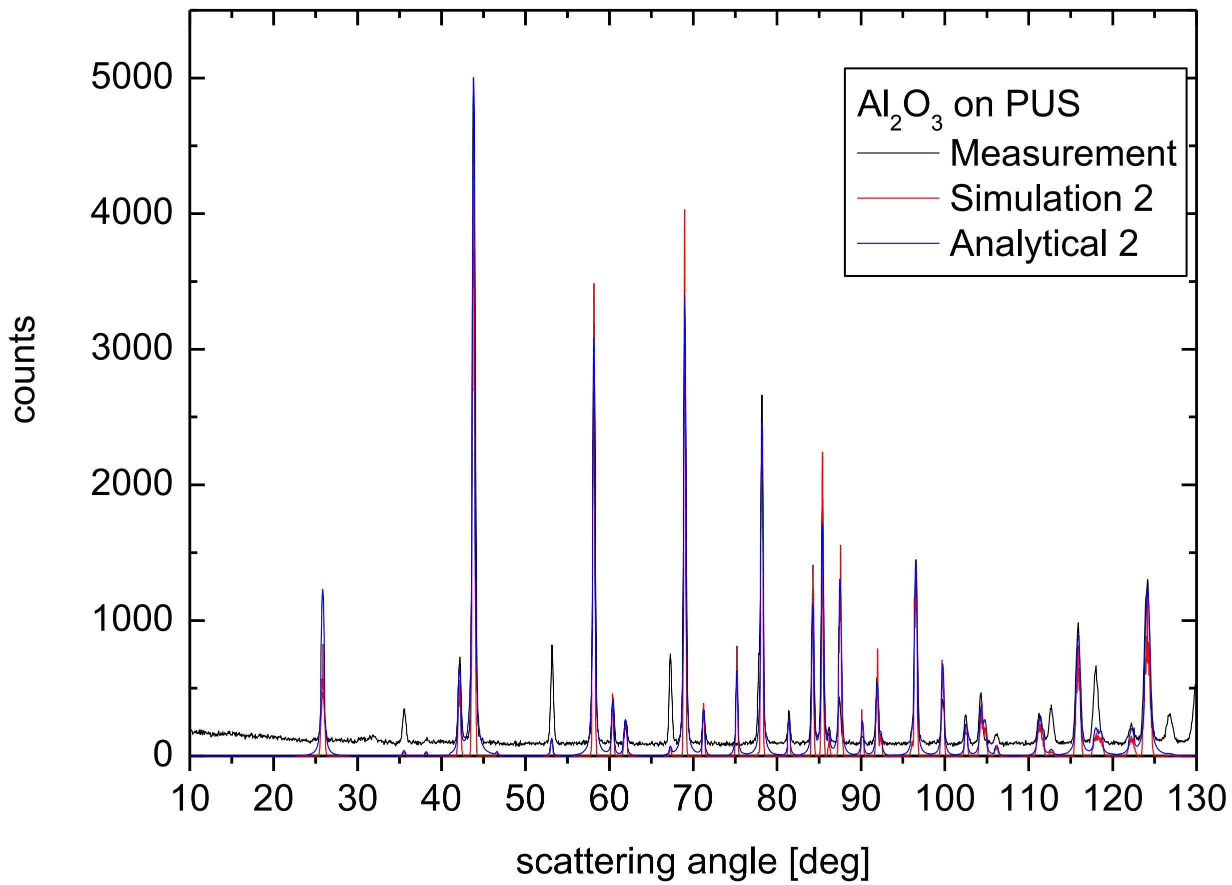
- Origin: Manhattan project, Los Alamos

- Used in a wide range of applications
  - physics
  - finance and business
  - telecommunication
  - ......

- Several programs exist for neutron instrumentation (McStas, VITESS, Restrax, NISP, IDEAS, …)

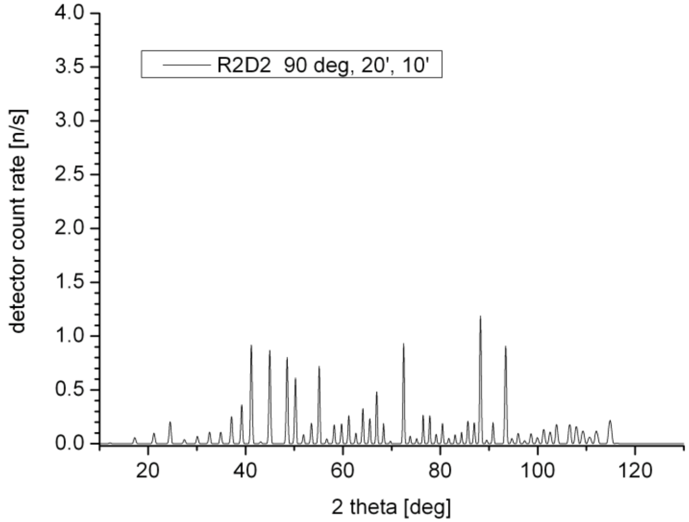
- Basic Idea: Random choice of parameters instead of scanning through parameter space
  - In the beginning, use of roulette numbers as random numbers
    (Therefore the name Monte Carlo simulations)
  - Nowadays, special routines to create series of ‘independent’ numbers

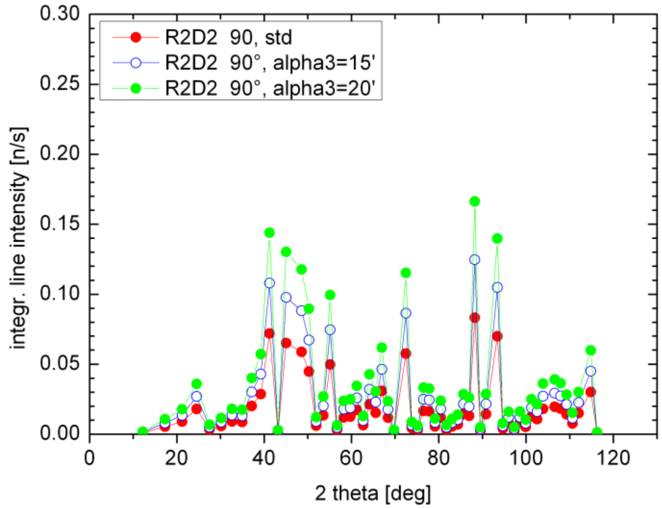
Example: Al_2O_3 on PUS

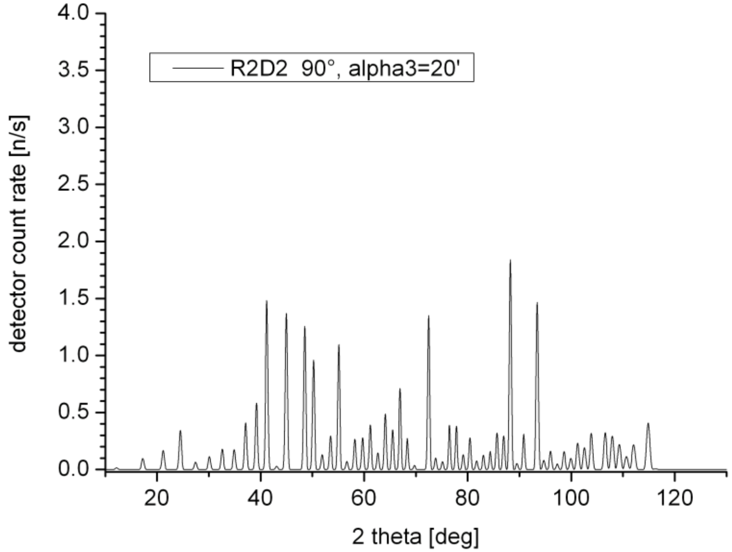


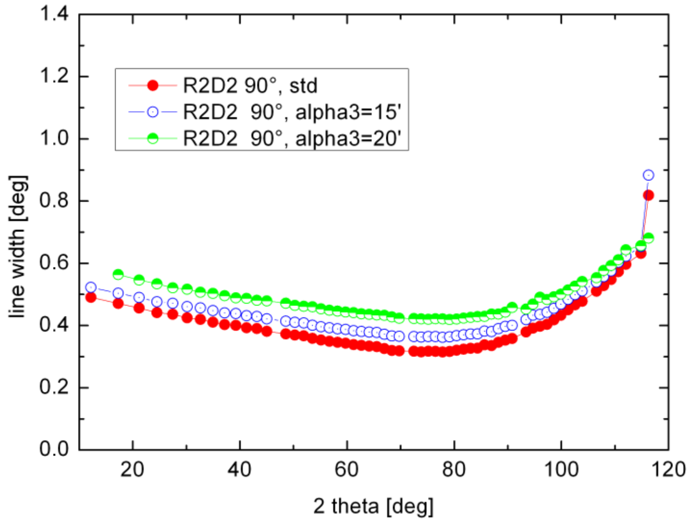
- Good agreement between simulation and analytical calculations, but not with measurement

Example: Improvement of R2D2 using NAC sample



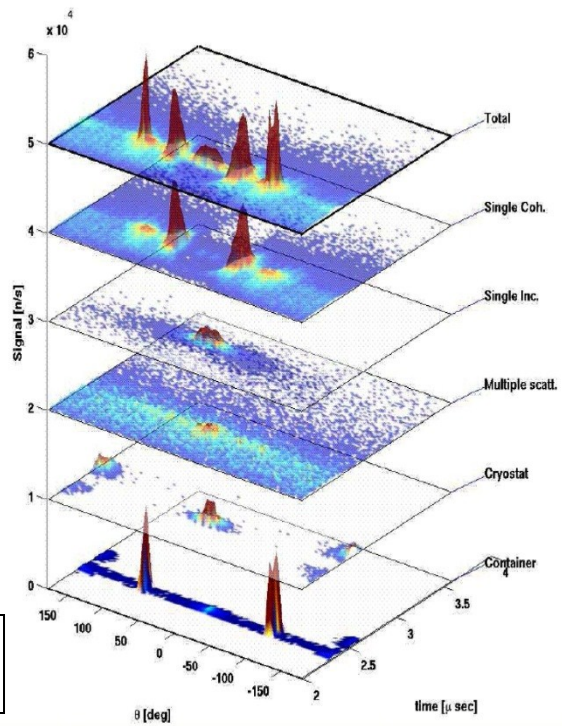






Why Monte Carlo Simulations of Neutron Scattering Instruments

- Instrument optimization
  - New ideas can be tested first in a simulation
  - Different option can be compared
  - Numerical optimization is possible
- Virtual experiments
  - If some information about the sample is available, it can be checked what time and which settings are needed for the real experiment
- Instrument and data analysis
  - Simulations provide a large amount of information on the properties of the neutrons (e.g. on correlations in phase space and spin space)
  - They allow comparing true and measured sample properties
- Teaching



E. Farhi, M. Johnson, V. Hugouvieux and W. Kob, ILL Annual Report (2006) 87.

Parallelisation