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VITESS 3
New features

Joint Vitess and McStas workshop

D. Nekrassov, C. Zendler,
K. Lieutenant, M. Fromme

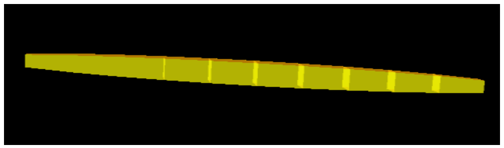
VITESS

Outline

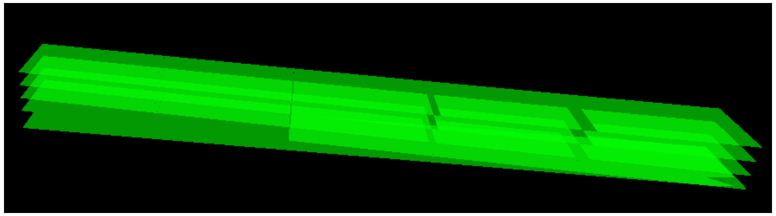
- New features in version 3
  - Visualization
  - Numerical optimization
  - Improved detector module
  - Sample properties
  - Cluster parallelization (talk by Michael Fromme in the afternoon)
  - Further new features

Visualization of the instrument

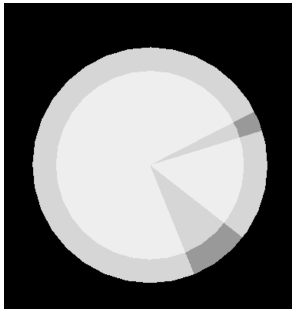
- Before Vitess 3.0, information about instrument layout in stored in an ascii file (instrument.inf) ->Now graphical visualisation available
- Each component is represented by a geometrical shape



guide

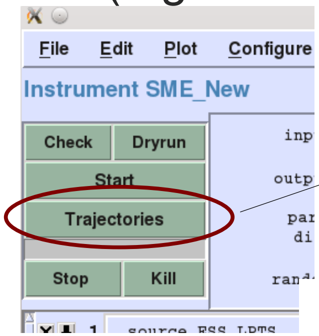


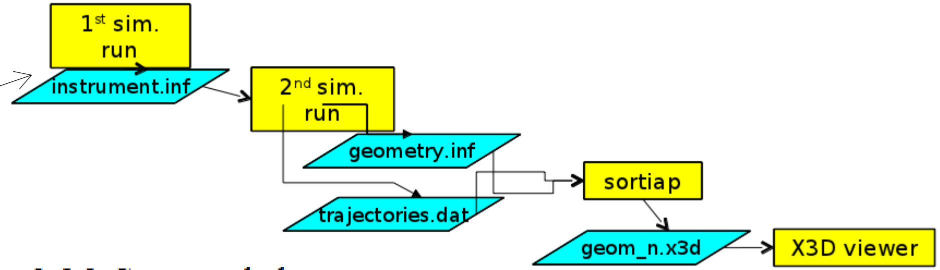
supermirror ensemble



chopper

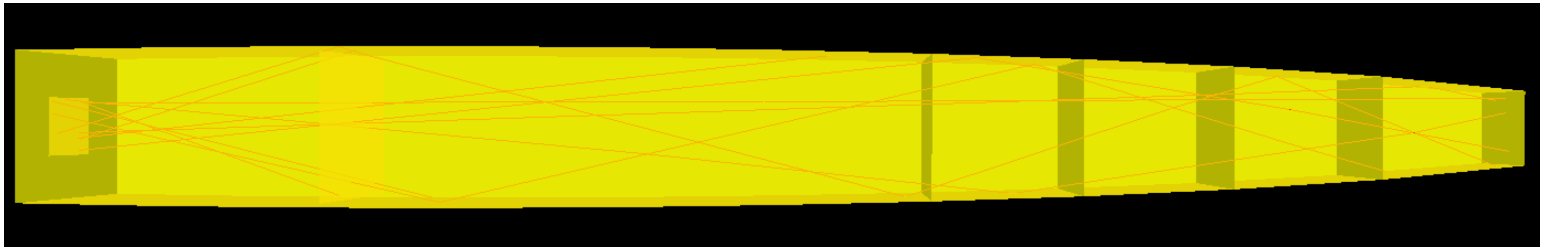
- Geometrical information and position in global coordinate system are stored in common ascii file (geometry.inf)
- Dedicated routine convert to .x3d file
- X3D viewer (e.g. Instantreality player) needs to be installed on the user's system



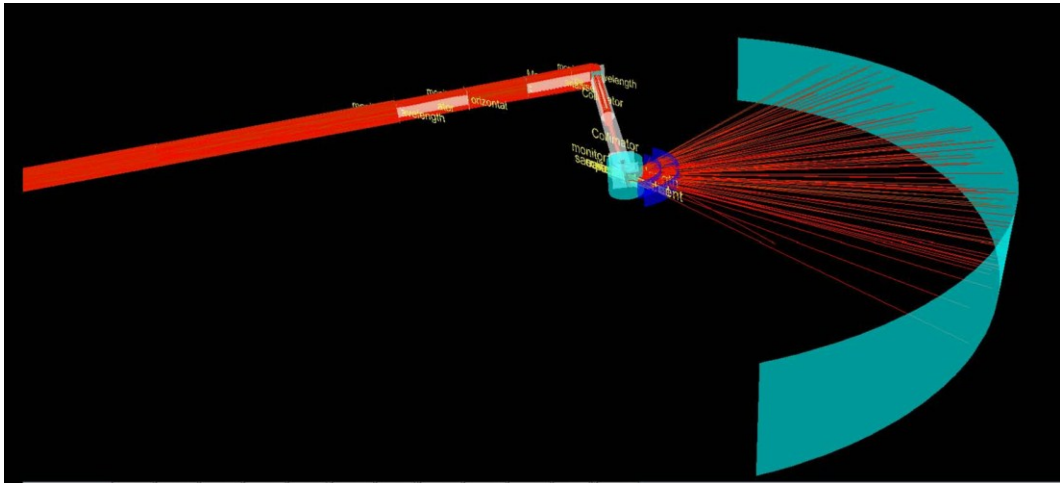


Visualization of neutron trajectories

- Each component writes the location of interaction points as well



trajectories in
elliptic guide



diffractometer ODIN
at IFE

- Visualization of a subset of trajectories possible by tracing
- Possibility of extension to background simulations

Components with visualization in VITESS 3.0

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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

comp1 — **trajectories and component**

comp2 — **not yet implemented**

All Monitors work by default settings

First version of optimization (since 3.1)

- Framework for numerical optimization of instrument parameters provided with Version 3.1

Example: Optimization of guide trumpet

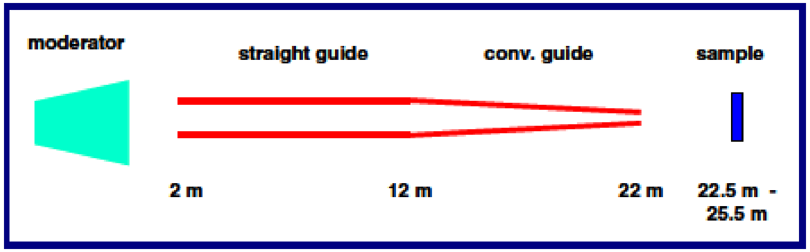

Table 3. Properties of a converging guide with elliptic shape obtained in runs with different initial values using the least-square fitting method and the Metropolis algorithm.

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).

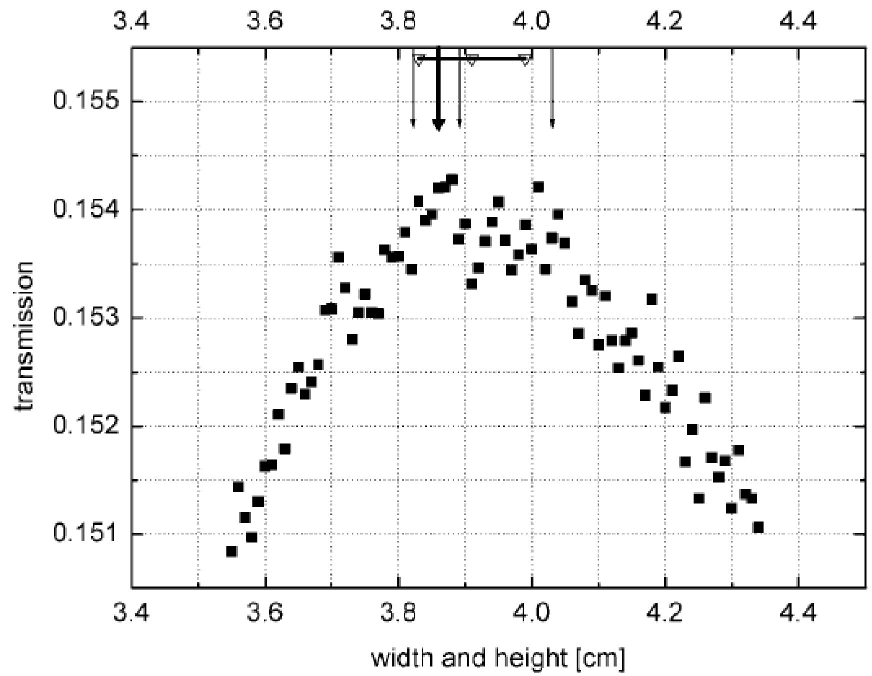

Figure 3. Transmission as a function of exit width (full squares). The arrows mark the sizes found in optimization runs using least-square fits (thin arrows) and Metropolis algorithm (thick arrow). The indicated range shows average value and standard deviation (for the size) of the random walk within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

First version of optimization (since 3.1)

- Framework for numerical optimization of instrument parameters provided with Version 3.1
- Binaries to read in optimization options, start a VITESS pipe, read required monitor output, calculate new simulation parameters, ...
- Three algorithms implemented: two **gradient methods** (opt_grad, opt_grad_mc) and **metropolis**; more to come in 3.2 (e.g. swarm)
- Optimization parameters:
  - default (and well tested) is direct mapping

    Parameter of instrument components = OptimizationParameter
  - Simple mathematical relations accepted, or write your own function
- Delivered figures of merit: Sum or average of a 1D monitor, noise can be included separately
- Detailed description in vitess/Concepts/Optimization.pdf
- **please try it and give feedback!**

New Optimization Concept for VITESS 3.1

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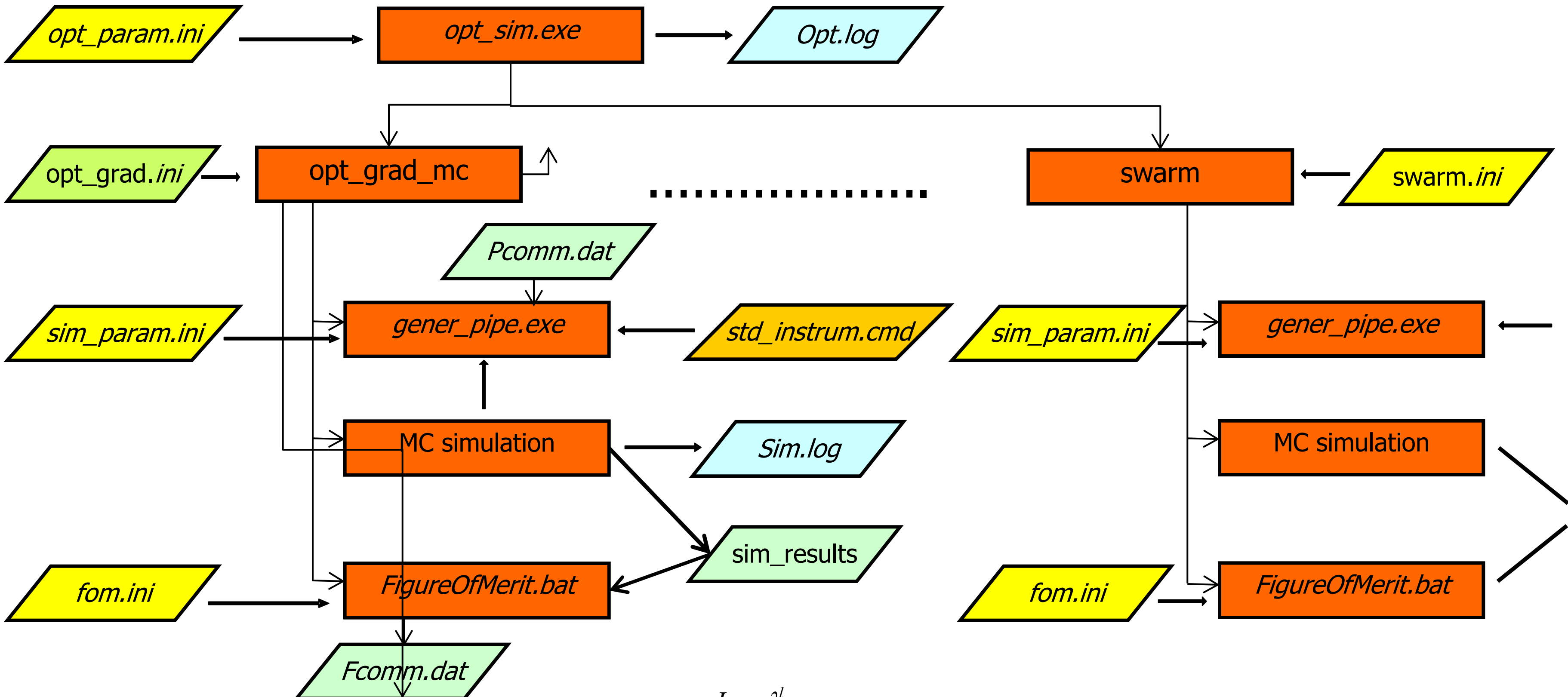
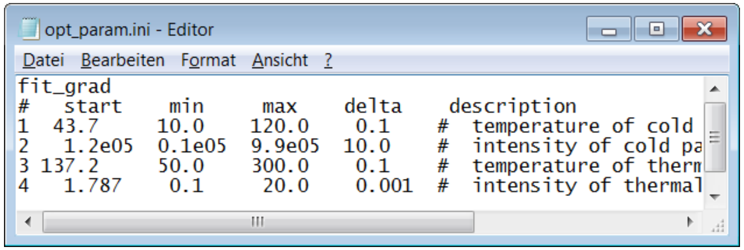




opt_param.ini - Editor

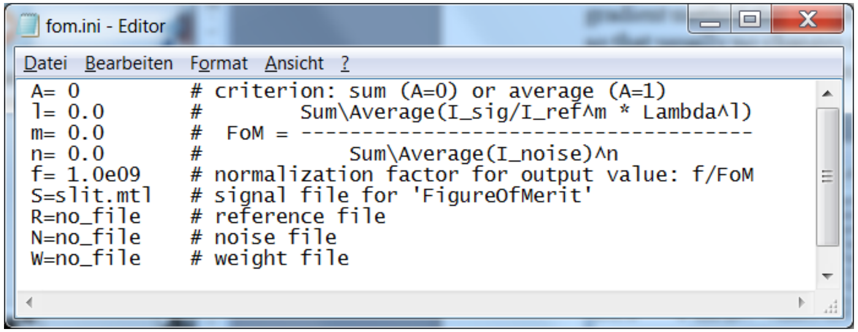
Datei Bearbeiten Format Ansicht ?

```
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
```

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

or

$$FoM = \frac{\sum_i \frac{w_i I_{sign,i} \lambda_i^l}{I_{ref,i}^m}}{\sum_i I_{noise,i}^n}$$



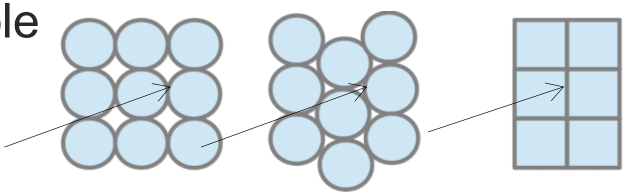
fom.ini - Editor

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
```

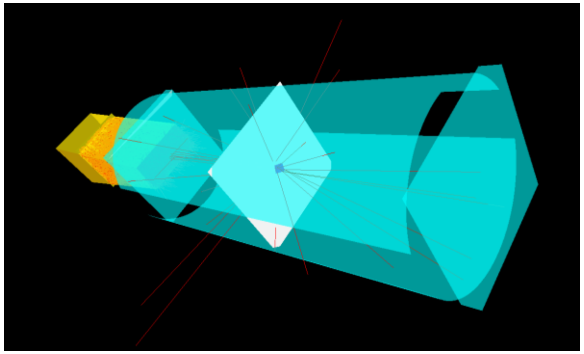
Improved detector module (since 3.1)

- 3D volume detector instead of 2D flat area
- tube geometry possible



area between tubes and tube walls treated as vacuum

- improved detection probability: choice between
  - common materials: He_3, BF_3 gas, solid ^{10}B, ^{6}Li
  - input file giving efficiency(wavelength); independent of pathlength
  - constant mean detection efficiency



- more flexible detector geometry
  - cylinder shape with axis along x, y or z axis
  - array of several detector modules
  - pixel in cyl. det. with const. phi angle
- Event mode output file:

neutron list with (pixel) position, detection time, *weight and colour*

New guide module: Guide_ideal

- Conventional guide module splits a guide in segments
- Calculations can take very long, in large number of segments
- Segmentation influences on the performance of elliptic guides
- New module to treat elliptic shapes analytically
  - No segmentation required
  - Collision points calculated analytically: Intersection of a parabola (gravity!) with an elliptic function → quartic equation, problems with computer precision do occur!
  - Calculations significantly speeded up
  - Elliptic parameters can differ for horizontal and vertical planes
- To do in (distant future): Parabolic shape, coating as function of length, incorporated beamstop

New in VITESS 3: Sample properties

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Simulation of realistic samples

- Variety of samples provided with the VITESS package:
    - Diffraction
    - Single crystal
    - SANS
    - Reflectometry
    - Elastic/inelastic (lookup)
    - Generic elastic sample (cell structure) → J. Appl. Cryst. (2012). 45, 603-607!
- Some include incoherent background
    - New in version 3: Incoherent and offspecular scattering from a reflectometer sample
- Try your own look-ups
- Try your own data analysis
- Monte-Carlo simulations programs (Vitess, McStas, ...) include realistic samples: Virtual experiments important!

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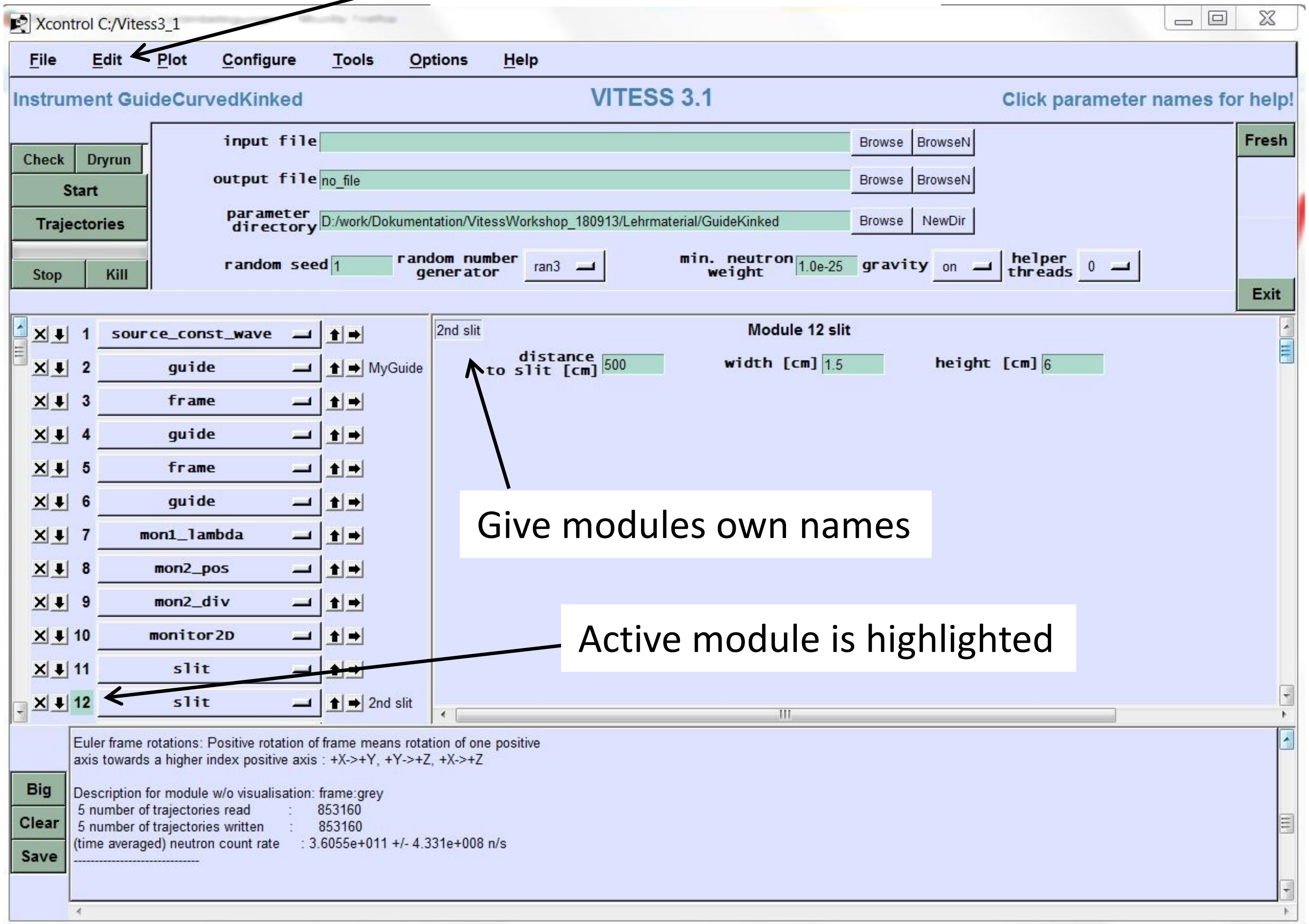
Further improvements

- read_in module: read trajectories files, compatible with McStas!
- new reflectivity model (H. Jacobsen) in `Generate Mirror Files` tool (3.0)
- new tool for sm_ensemble file generation: `Generate Extraction System`
- new reflectivity and attenuation model in `sm_ensemble`, can choose mirror substrate (silicon, sapphire) (3.1)
- new monitors: `brilliance`, generic `monitor 1D`, `monitor 2D` (3.0)
- new `filter` module with up to 3 filter parameters (3.1)
- Updated sources
  - HZB, ESS updated, FRM2 added in 3.0
  - ISIS, HMI, ILL, ESS updated; choice between mod. versions for SNS, ESS; CSNS added (Chinese Spallation Neutron Source) in 3.1
- re-import pipes into GUI (3.0)
- `guide` and `sm_ensemble` count reflections
- *Please note: slightly different use of “color”: 0 is default, -1 is all*

Further improvements

Undo! (Recover instrument)



Give modules own names

Active module is highlighted

Summary

VITESS version 3

- VITESS is a user-friendly simulation package easy to get started with
- major improvements in the last two versions 3.0 and 3.1
  - Visualization of instruments and trajectories
  - Numerical optimization
  - Parallelization for computer clusters
  - Many new or significantly improved modules/tools

THANK YOU FOR YOUR ATTENTION

VITESS HZB TEAM

Daniil Nekrassov, Carolin Zendler, Michael Fromme, Klaus Lieutenant

Contributing

Andreas Houben (FZJ), Sergei Manoshin (JINR), Alexander Joffe(JCNS), Mirko Boin (HZB), Jennifer Schulz (HZB)

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

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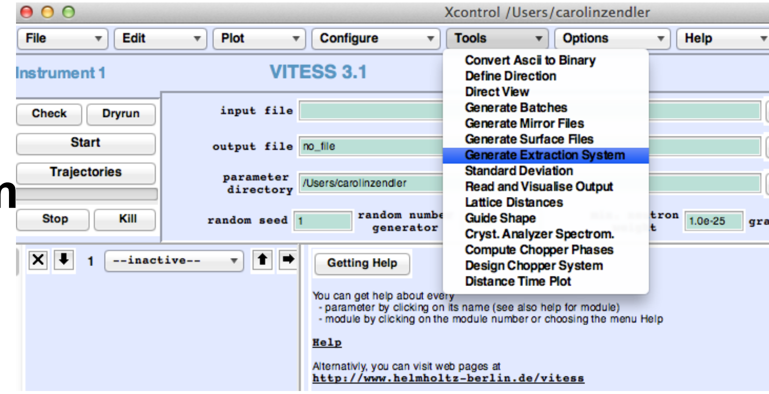
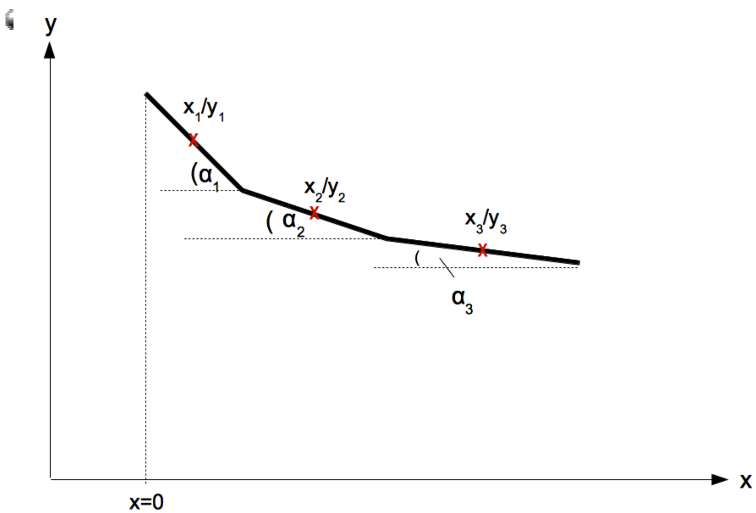
backup slides

New tool: Generate extraction system



- generates input file for `sm_ensemble` m



- written with bi-spectral extraction mirror system in mind, but can be used for any mirror system

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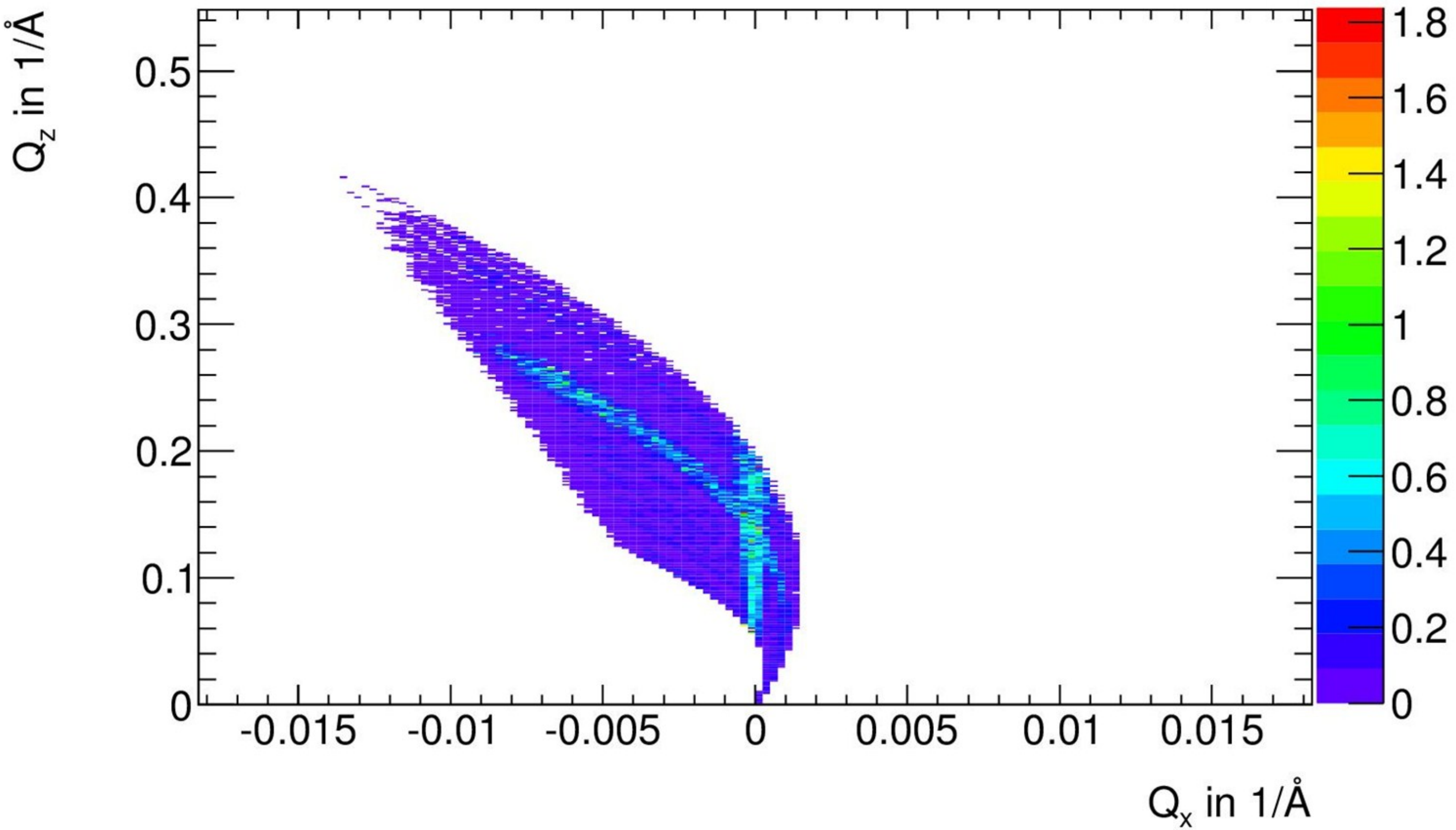
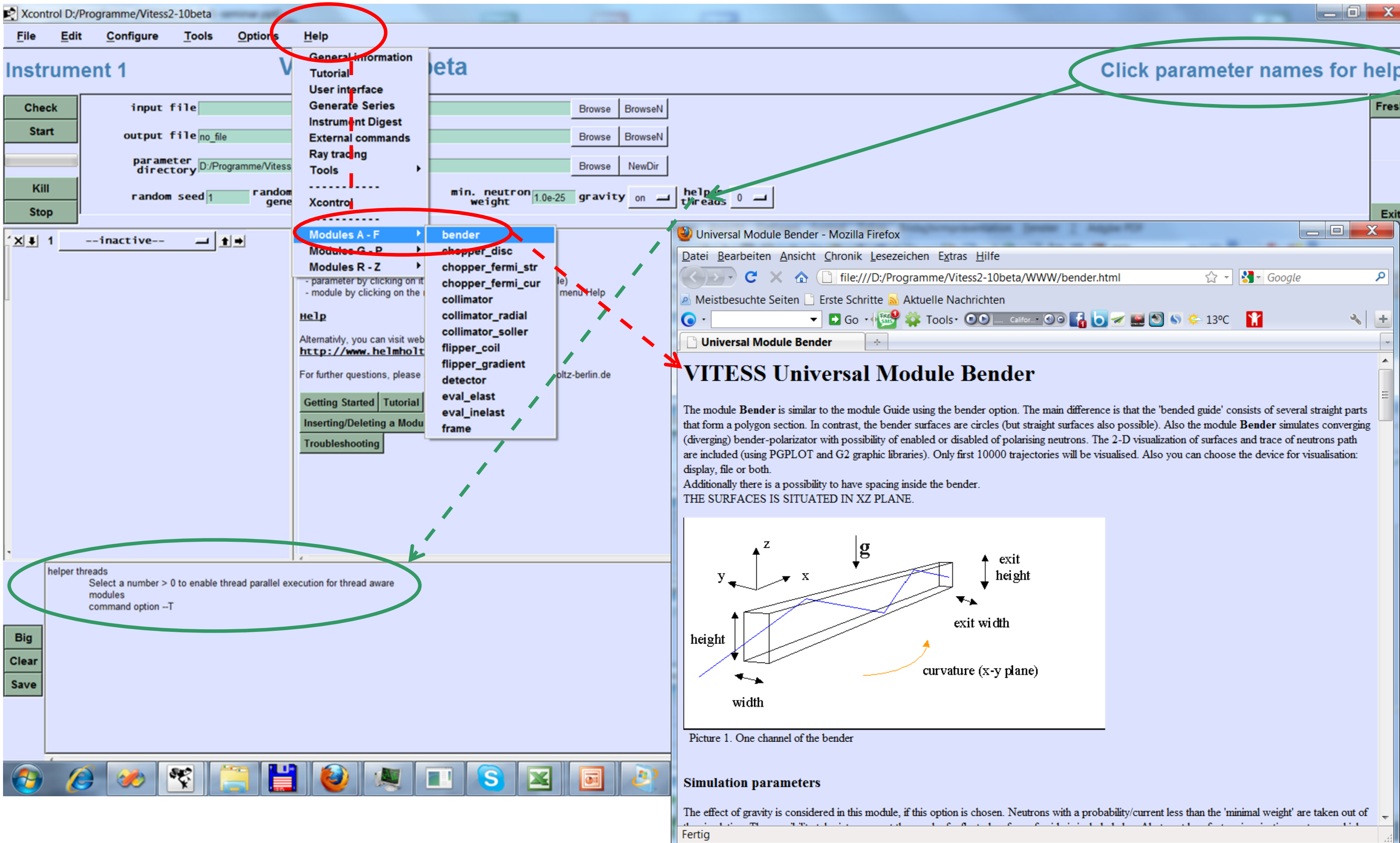
Simulation of realistic samples

- Simulation of offspecular scattering from a reflectivity module

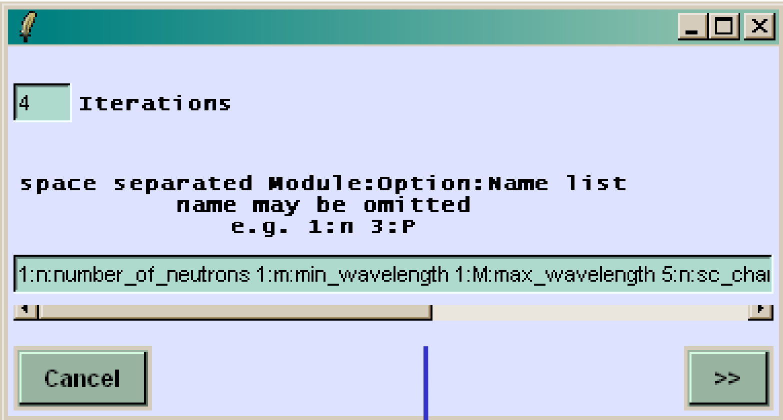


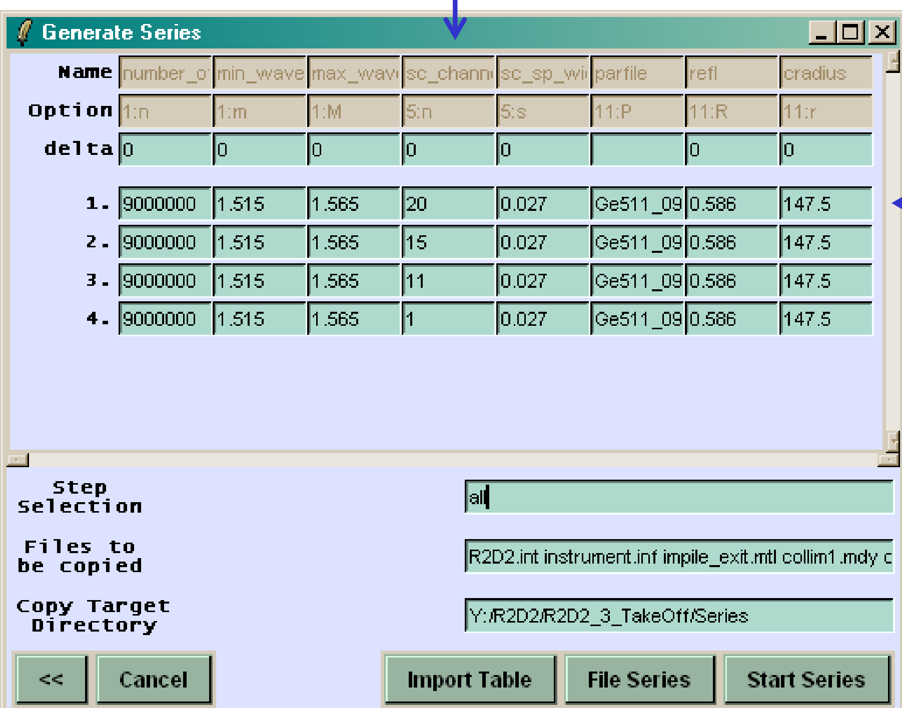
Help System


Xcontrol D:/Programme/Vitess2-10beta
File
Edit
Configure
Tools
Options
Help
Instrument 1
Click parameter names for help!
Check
Start
Kill
Stop
input file
output file
parameter directory
random seed
Browse
BrowseN
NewDir
min. neutron weight
gravity
helper threads
General information
Tutorial
User interface
Generate Series
Instrument Digest
External commands
Ray tracing
Tools
Xcontrol
Modules A - F
Modules G - P
Modules R - Z
bender
chopper_disc
chopper_fermi_str
chopper_fermi_cur
collimator
collimator_radial
collimator_soller
flipper_coil
flipper_gradient
detector
eval_elast
eval_inelast
frame
Getting Started
Tutorial
Troubleshooting
helper threads
Select a number > 0 to enable thread parallel execution for thread aware modules
command option --T
Big
Clear
Save
Fresh
Exit
Universal Module Bender - Mozilla Firefox
file:///D:/Programme/Vitess2-10beta/WWW/bender.html
VITESS Universal Module Bender
The module Bender is similar to the module Guide using the bender option. The main difference is that the 'bended guide' consists of several straight parts that form a polygon section. In contrast, the bender surfaces are circles (but straight surfaces also possible). Also the module Bender simulates converging (diverging) bender-polarizator with possibility of enabled or disabled of polarising neutrons. The 2-D visualization of surfaces and trace of neutrons path are included (using PGPLOT and G2 graphic libraries). Only first 10000 trajectories will be visualised. Also you can choose the device for visualisation: display, file or both.
Additionally there is a possibility to have spacing inside the bender.
THE SURFACES IS SITUATED IN XZ PLANE.
z
y
x
g
exit height
exit width
height
curvature (x-y plane)
width
Picture 1. One channel of the bender
Simulation parameters
The effect of gravity is considered in this module, if this option is chosen. Neutrons with a probability/current less than the 'minimal weight' are taken out of
Fertig

Option: 'Generate Series'

Defining variable parameters

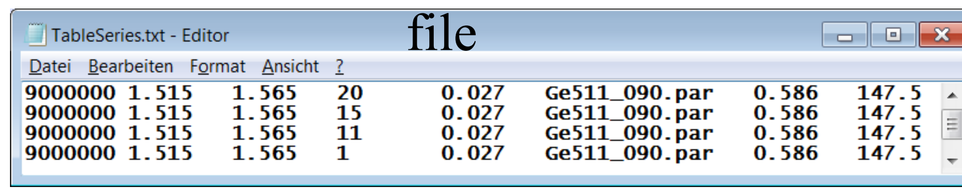




Excel or other Table calculator

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



Visualization of Instruments and Trajectories

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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
```

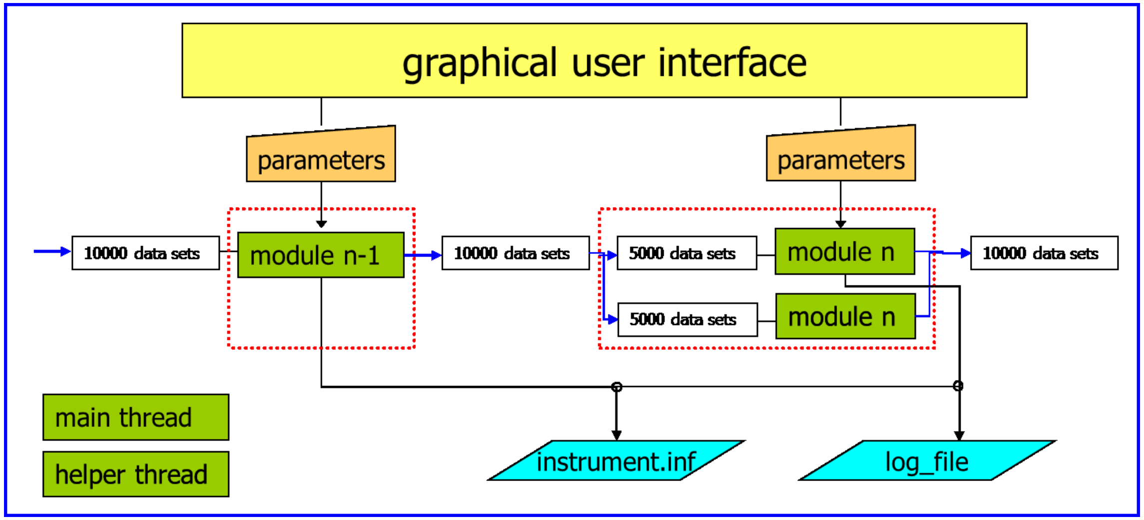
- Each Module adds lines to the geometry file that describe the component geometry
- Each event of a neutron creates a line in the trajectories file
  - Entering, passing or exiting a component
  - Reflection, scattering or absorption

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
```

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