Final Report

German Work package K7
"Simulation Code Development, Help Desk"

ESS-ID: SD015DE

Summary

The work package K7 - Simulationscode-Entwicklung, Helpdesk – comprised the further development of the Monte Carlo simulation package VITESS for the simulation of neutron scattering experiments, its use to study general questions related to ESS instrumentation in collaboration with the ESS Data Management and Software Center (DMSC) in Copenhagen and support for users.

The package contains now a visualization of instrument and trajectories, the possibility for numerical optimization of instrument parameters and options for parallelization of the simulation for multi-core PCs and for computer clusters. Among other improvements, modules to simulate lenses and true elliptical guides have been written, and the monochromator and the detector module have been improved significantly. The graphical user interface and the treatment of events are more user-friendly now.

For the ESS project, the performance of different guide geometries were compared, different options for extraction systems and guides without direct line of sight developed and optimized, and the effect of gravity and waviness investigated. The work was executed in collaboration with the DMSC. Most of the results have been published already.

Apart from direct support for some users, user support was realized by completing and improving the documentation, updating the internet site, setting up a Facebook account and a new email list.

Content

1 General Aspects

Tasks of the Work Package and Degree of Completion

Table 1 contains the original tasks of this project and four additional tasks that were added according to wishes from ESS and shows their degree of completion on 31. Oct 2013.

Table 2 is a list of the original deliverables and milestones of the work package with the planned release dates according to the changed schedule from autumn 2011. It also shows the resources for this project.

All but three tasks have been completed to 100%. The release of VITESS 3.2 (D.K.7.2.5) will take place in January 2014. The manual (D.K.7.3.4) will be finished until end of February 2014. The study of the influence of waviness (D.K.7.1.4) yielded the main result that there is little negative effect of waviness on neutron transport in guides for magnitudes of waviness that are state of the art today (see chapter 2.4). The surprising effect of increased transmission for high waviness and long wavelengths would be interesting to study, but is probably due to a simplified description of waviness in the code and of no practical interest.

Table 1: Deliverables and milestones of the German work package K7 and the degree of completion at the end of the project time

Deliverable	Completion	Comment	Schedule	Description
D.K.7.1.1	100%		01.01.2011	Instrument performance as a function of pulse length and repetition rate
D.K.7.1.2	100%		01.03.2011	Comparison of the performance of different neutron guide geometries
D.K.7.1.3	100%		01.11.2012	Simulation of Day-1-Instruments
D.K.7.1.4	75%	added	01.01.2012	Influence of waviness on guide performance
D.K.7.1.5	100%	added	01.12.2011	Performance of extraction systems
D.K.7.1.6	100%	added	01.09.2012	Brilliance comparison of different neutron sources
D.K.7.1.7	100%	added	01.07.2012	Influence of gravity on guide performance
D.K.7.2.1	100%		01.02.2011	User meeting
D.K.7.2.2	100%		01.05.2011	Release of VITESS 2.10 (Multi-processor capability, Help for all existing modules, new modules: elliptical mirror, refraction lense)
D.K.7.2.3	100%		15.12.2011	Release of VITESS 2.11 (Macintosh version, new level of user interface, new modules 'imaging sample' and 'monitor2D')
D.K.7.2.4	100%		01.06.2012	Release of VITESS 3.1 (instrument visualisation, numerical optimization, improved module 'reflectometry sample')
D.K.7.2.5	80%		01.11.2013	Release of VITESS 3.2 (New program structure, new detector and monochromator module)
D.K.7.3.1	100%		01.11.2011	Email list for VITESS users
D.K.7.3.2	100%		01.11.2011	Support for Macintosh users
D.K.7.3.3	100%		01.05.2012	Training course on VITESS 3
D.K.7.3.4	20%		01.11.2012	VITESS manual (print version)
D.K.7.3.5	100%		01.11.2013	Complete Documentation of the VITESS package (html-documentation)
Milestone				
M.K.7.2.1	100%		01.04.2012	VITESS 3.0 (beta-Test-Version of VITESS 3.1)

Staff and Contributors

Klaus Lieutenant and Michael Fromme have permanent positions at HZB and have been working on the VITESS package for several years before. Klaus Lieutenant is employed for instrument simulations and responsible for K7 and spent (at least) half of his time on this work-package (18 months). Michael Fromme was not officially included in the ESS project, but contributed significantly (parallelisation, visualization, releases …) to the VITESS development as part of his regular work in the IT department.

Daniil Nekrassov and Carolin Zendler were employed in May / June 2011 at HZB for 3 years to work on the ESS Design Update Programme. They have been working a third of their time on this work-package (giving another 24 months). The remaining time they were working on different German instrument simulation work-packages (I3, I5, I6).

Leo Cussen was employed for 1 year at HZB to work on the work-packages I8 (ESS Extreme Environment Instrument, ESSEX) and I7 (Alternative Methods), but collaborated strongly with the VITESS group, especially on task 1.2 (guide geometries), because a guide design to fulfil the needs of the ESSEX was difficult to find.

Sergey Manoshin is employed at the Frank Laboratory of JINR. He made his PhD in Berlin about VITESS related subjects and has written new modules and used the package ever since. He contributed with two new modules.

Mirko Boin is employed at HZB working on residual stress analysis. Originally, he wrote a new sample component for McStas; he converted it to a VITESS module then.

Andreas Houben is employed at RWTH Aachen. He wrote and upgraded a few VITESS modules while designing the JCNS instrument PoxTex and continues improving and maintaining his modules.

Publications

There are altogether 14 publication related to this work-package, 7 of them - [1] To [7], see chapter 5 – deal directly with the tasks of this work-package and thus reflect its main activities. Four of these are published already, two are sent for publication and one is in preparation. Two of them [1, 6] are about the development of the program (task K7.2), the others deal with simulation results (task K7.1): neutron transport in guides and extraction systems.

4 publications resulted from collaboration with the group of Kim Lefmann from Niels Bohr Institute (NBI) of the University of Copenhagen. In all cases, this group did the major part of the work; members of the K7-team were only involved in supporting or advising the activities [8], [10], cross-checking the results [11] or performing a smaller fraction of the work [9] (see chapters 2.1, 2.2 and 2.5 for details). They are all published already.

3 publications treat topics that came up in other German work-packages while designing these instruments: the question of wavelength frame chopper arrangement [12] in I3 (Liquids Reflectometer THOR) , homogeneous divergence profile of a guide without direct line of sight [13] in I8 (ESSEX) and I6 (Imaging Instrument ODIN) , and bi-spectral extraction in compact form [14] in I5 (Bi-spectral powder diffractometer PowHow). The studies were executed in collaboration with these work-packages. One is published already; the other two are in preparation.

Results of the instrument design work will be published in separate papers [15 – 18].

Table 2: Resources, deliverables and milestones of the German work package K7 after rescheduling in autumn 2011

Work package no.:	K7	Start date:			01.11.2010		
Coordination:	Lieutenant, HZB						
Participating institutions:	JÜLICH	HZG	HZB	TUM	DESY	KIT	FZD
Person months per institution:	0	0	42	0	0	0	0

Work description:	
K.7.1	Consulting for and support of simulation tasks with VITESS and McStas in cooperation with the ESS Data Management Centre (University of Copenhagen)
K.7.2	Further development of VITESS (instrument visualization, numerical optimization, multi-processor capability, extension of user interface functionality, source code development for new components and general overhaul of existing components: monochromator, detector, diffraction lenses, …)
K.7.3	Help desk function, completion of documentation, improvement of communication with and among VITESS users, Macintosh support

Deliverables:		
D.K.7.1.1	Performance characteristics of the instruments as a function of pulse length and frequency	x+2
D.K.7.1.2	Comparison of different neutron guide geometries	x+4
D.K.7.1.3	Simulation of "day-1 instruments"	x+24
D.K.7.2.1	User meeting	x+3
D.K.7.2.2	VITESS 2.10 release (multi-processor capability, help for all existing modules, new modules: elliptical mirror, diffraction lenses)	x+6
D.K.7.2.3	VITESS 2.11 release (instrument visualization, new monochromator module)	x+12
D.K.7.2.4	VITESS 3.1 release (new user interface, new program architecture)	x+24
D.K.7.2.5	VITESS 3.2 release (numerical optimization, new detector module)	x+36
D.K.7.3.1	Email list for VITESS users	x+12
D.K.7.3.2	Support for Macintosh users	x+12
D.K.7.3.3	Training course for VITESS 3	x+18
D.K.7.3.4	VITESS manual (print version)	x+24
D.K.7.3.5	Complete documentation for VITESS (html documentation)	x+36

Milestones:		
M.K.7.2.1	VITESS 3.0 (beta test version of VITESS 3.1)	x+18

Resources:													
	Staff					Expenditure					Investment		
Task	JÜLICH	HZG	HZB	TUM		JÜLICH	HZG	HZB	TUM		JÜLICH	HZG	HZB	TUM
K.7.1	0	0	9	0		0	0	25	0		0	0	0	0
K.7.2	0	0	24	0		0	0	20	0		0	0	14	0
K.7.3	0	0	9	0		0	0	5	0		0	0	6	0

2 Simulation Tasks

2.1 Performance characteristics of the instruments as a function of pulse length and frequency

A systematic study of the influence of repetition rate and pulse length on the performance on the whole instrument suite of the ESS [19] was undertaken by the group of Kim Lefmann from NBI in Copenhagen. It was nearly finished when the German project started. Klaus Lieutenant, who had been adviser to some of the simulation activities – of a reflectometer and a thermal diffractometer - already before the German project started, continued this collaboration.

For each instrument, the figure of merit relative to the old baseline (16.67 Hz, 2 ms) was determined for 20 combinations of frequency and pulse length by optimizing each set-up. Averaging over all 16 instruments yielded the main result that the ratio of period and pulse length determines the performance, but not the absolute values. This result helped fixing the final values (14 Hz, 2.587 ms).

A general publication about this study was written [10]. The results of some of the instrument simulations were published in a separate papers, one of them is about the diffractometer simulations [8].

2.2 Comparison of different neutron guide geometries

In a collaborative study between the Niels Bohr Institute (NBI) , University of Copenhagen and the Helmholtz-Zentrum Berlin (HZB), 4 different kinds of guides were optimized for highest flux on 1 cm^2 source using 4 different lengths (50, 100, 150 and 300 m), 2 different maximal divergences (± 0.5° and ±2.0°) and 2 different wavelength ranges (average wavelength 1.5 and 5.0 Å) [9].

Table 3: Gain factors by advanced guide shapes relative to a guide of constant cross-section for different guide length, divergences and wavelength ranges, obtained by combination of Monte Carlo simulation and numerical optimization of the guide parameters [9]

total length [m]	max. div. [deg]	moderator	elliptic	parabolic ballistic	linear ballistic
50	0.5	thermal	1.91	1.97	1.86
50	0.5	cold	0.96	1.04	1.04
50	2.0	thermal	10.04	8.88	5.28
50	2.0	cold	5.14	5.52	3.92
100	0.5	thermal	2.52	2.62	2.31
100	0.5	cold	1.07	1.08	1.11
100	2.0	thermal	15.29	13.12	6.65
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	7.64
150	2.0	cold	8.48	8.21	6.06
300	0.5	thermal	3.84	4.45	3.60
300	0.5	cold	1.25	1.28	1.29
300	2.0	thermal	29.37	23.85	9.94
300	2.0	cold	9.40	10.90	7.94

K. Klenø from NBI optimized elliptical guides, guides of constant cross-section and a ballistic guide with parabolic diverging and converging section using McStas [20 – 22]. K. Lieutenant from HZB a ballistic guide with linear converging and diverging section using VITESS [23,24]. Horizontal and vertical shape was identical in all cases; each ballistic section was restricted to 30% of the total length. Final results were cross-checked using the other package.

Table 3 shows the final results, the gain factors of advanced guides shapes compared to a guide of constant cross-section. Gains of nearly 30 can be achieved for high divergence, short wavelength and long instruments. In the opposite case – long wavelength, low divergence and short instruments – there is not much gain by using advanced guide shapes. The most interesting result was that the ballistic guide with parabolic sections is competitive to the elliptic guide, showing the best performance for thermal neutrons of low divergence. The linear ballistic guide is best for cold neutrons of low divergence (see Table 3).

To understand elliptic guides better and to be able to design them for specific beam properties, the team of the K7 work-package studied what happens inside the guide [2]. The main finding was that the common view of neutrons being reflected only once per dimension [25] is only true for a minority (of some percent) of the neutrons for realistic source sizes in the cm^2 range, though elliptical guides reduce the number of reflections significantly (see Fig. 1a). This is a consequence of the coma aberration [26]. Neutrons with one reflection per dimension cause the 4 peaks in the center of the divergence distribution, the multiply reflected neutrons the 8 spots around (see Fig. 1b).

It also showed that a one bounce transport requires precise guide shaping, especially in the beginning. As a consequence, the idea of getting an identical phase space after a double ellipse only holds for small sources and very well aligned guides. This subject will be treated in a separate paper [7].
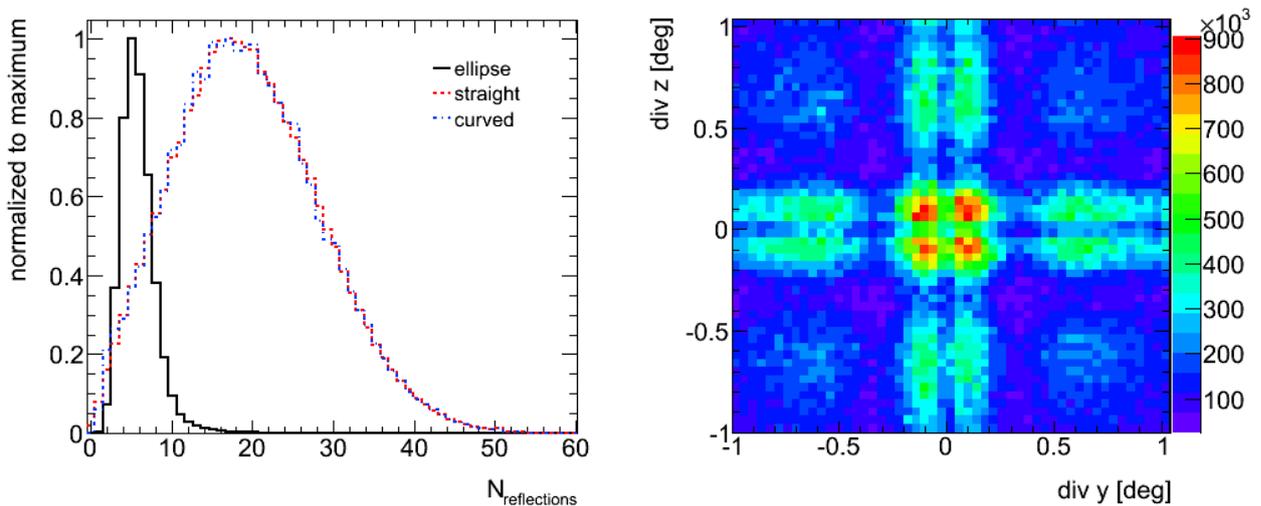
Figure 1: Distribution of the number of reflections of neutrons passing through a 150 m long neutron guide of different shapes (counted in VITESS simulations) (a) and a typical divergence distribution of an elliptic guide at sample (b)

While elliptic guides still have the best performance for some cases (see Table 3), they have the drawbacks that they don't avoid direct line of sight from source to sample and that their cross-section is so large in the central part that including a chopper is difficult.

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Additionally the divergence distribution is not ideal for short wavelength (see Fig. 1a). So the K7 team carried out another study trying to find guide shapes without direct line of sight, containing a narrow section in the central part and yielding high brilliance transfer as well as smooth and symmetric divergence distribution. This study was initiated by trying to fulfill the requirements for the ESS EXtreme Environment Instrument (ESSEX).

After several months of work, we succeeded in designing such guides. The shapes found consist of elliptical sections in the beginning and the end and linear sections and a kink in the center. The results will be published shortly [4, 7, 13].
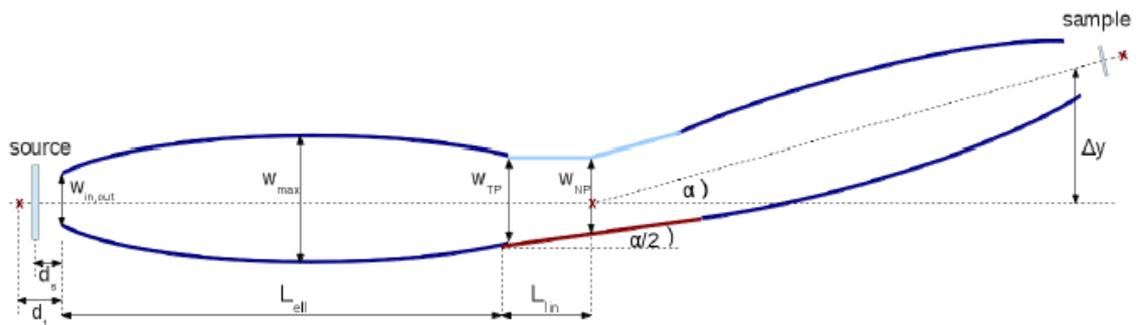
Figure 2: Principle shape of guides to obtain a high brilliance transfer and a homogeneous divergence distribution, while avoiding direct of sight and having a narrow region (for chopper positioning)

2.3 Simulation of "day-1 instruments"

All HZB Workpackages which were tasked to develop instrument concepts were heavily supported by the VITESS group at HZB. In collaboration with these groups, we carried out complete simulations for the ESS EXtreme Environment Instrument (ESSEX, German work package I-8), The HOrizontal Reflectometer for the ESS (THOR, German work package I-3), the bi-spectral powder diffractometer (PowHow, German work package I-5) and the beamline of the imaging instrument (ODIN, German work package I-6).

2.4 Influence of waviness on guide performance (added)

The surface of neutron guides cannot be produced perfectly flat; it has a short range roughness and a long range waviness. Both are treated in the same way in a simulation. The influence of waviness on the flux at sample was studied for guides of constant cross-sections and elliptical guides using VITESS at HZB and McStas at NBI. For values of waviness below 0.01° FWHM, which is state of the art today, only a minor loss for wavelengths above 1 Å can be found, for 0.5 Å it is about 10 to 20% (see Figure 3). Short wavelength neutrons seem to be more strongly effect by waviness in elliptic guides than in constant guides, for long wavelengths it is the other way round.

Even a gain was found for long wavelength neutrons in elliptic guides of very high waviness (see figure 3). Similar results were obtained by the NBI group using McStas. A systematic study of this phenomenon was planned, but not realized within the frame of

this project. Anyway, the effect is most probably only due to a simplified description of waviness in the simulation packages, as found by the NBI group for McStas already.
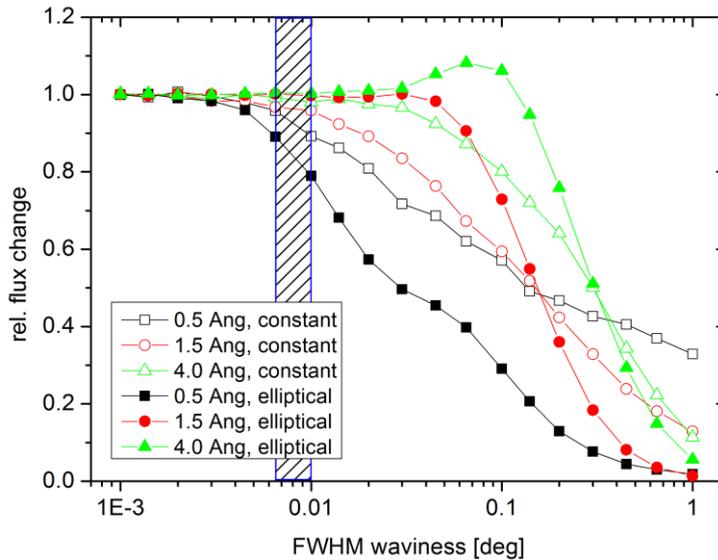
Figure 3: VITESS simulations of the influence of waviness on transmission for guides of constant cross-section and elliptical guides. The shaded area indicates the range of guide waviness that can be achieved nowadays.

2.5 Performance of extraction systems (added)

F. Mezei's had the idea to get the maximum of the thermal and the cold brilliance by using a mirror in front of the thermal moderator to switch from one spectrum to the other in the region of identical brilliance and suggested it for ESS [27]. Further mirrors might be added to improve the performance of the system. This principle is called bi-spectral extraction.

Simulations showed that this works well for guides of constant cross-section; and the principle could even be shown to work in practice at HZB (unpublished result). But as the mirror is typically several meters in length, the question arose how to combine it with elliptical guides and feeders, which often extend as close to the source as practically feasible, i.e. 2 m for the ESS, usually about 1.5 m for reactor sources.

The performance of an extraction system has to be evaluated behind the guide that it feeds, i.e. usually at the sample position. One straightforward solution is to calculate the ratio of flux at the sample with bi-spectral extraction system to the maximum of flux at sample from cold and thermal source, both installed at the central beamline position. This ratio will be called efficiency here. Identical flux as the (more brilliant of the two) single moderator set-ups would mean efficiency 1. This is the optimal case, because a bi-spectral extraction system does not add the fluxes of both moderators, but switches from one to the other.

The group from NBI in Copenhagen followed the approach to combine extraction system and elliptical guide by having guide segments and the mirror at the same distance range

from source, i.e. setting the extraction system into the guide (entrance). They simulated the system using McStas and optimized it numerically for highest flux at the sample to find the ideal mirror position and achieved a very good efficiency of 90% over the whole wavelength range. We cross-checked the results by simulating the same system with VITESS and confirmed the result [11].

We had the idea to 'cut' the mirror into several pieces (of about 1 m length) and stack the pieces in such a way that neutrons from the thermal moderator (without divergence) are transmitted through exactly one mirror (see Fig. 4b). As a consequence, neutrons from the cold moderator being reflected to zero divergence are reflected exactly once. This concept was tested in combination with a feeder and found to work better than 1 mirror (see Fig. 4c). By varying the system, an efficiency above 76% for most of the wavelength range could be reached (red curve in Fig. 4d). The ideal system seems to have mirrors of about 1 m length consisting of several straight, slightly inclined pieces forming a focusing mirror.

(a)

(b)

(c)

(d)
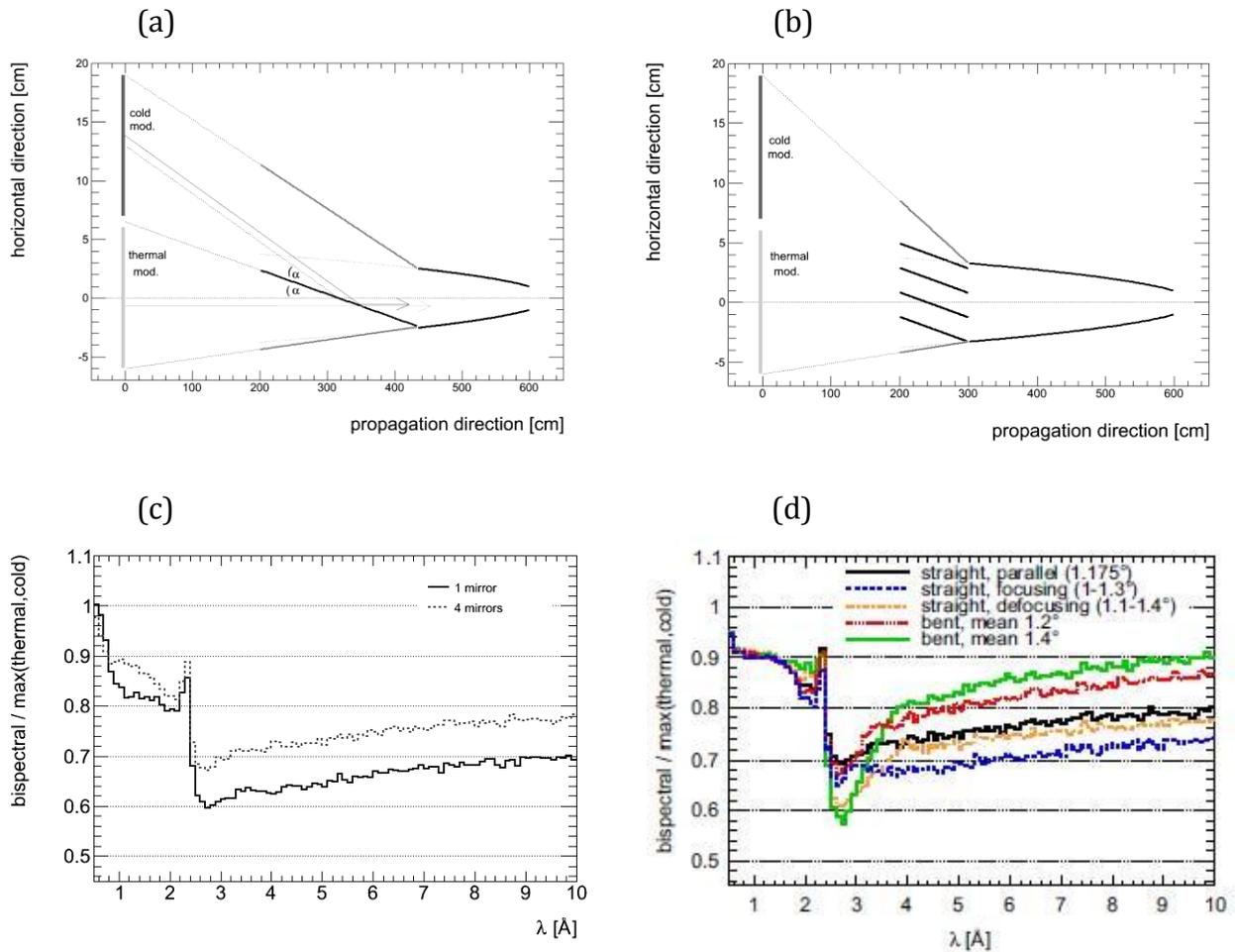
Figure 4: Set-up with 4 m long mirror (a) and 1 long mirrors (b) and the comparison of their efficiency (c). By variation of the 1 m solution the efficiency could be increased to more than 75 % in nearly the whole wavelength range (d).

The results have been published [3]. The system can also be used for other purposes, e.g. in combination with an elliptic guide. Following this idea, we have also examined even

shorter systems of 25 cm length or less. Their performance is slightly worse, but they have practical advantages. The study will be finished and published soon [14].

2.6 Brilliance comparison of different neutron sources (added)

The peak and average brilliance of several sources - ESS, SNS, ILL, FRM-2 and ISIS - were calculated as a function of wavelength and compared between the simulation packages McStas and VITESS in a collaboration between HZB and DTU. After some corrections, the outputs of both packages were identical.
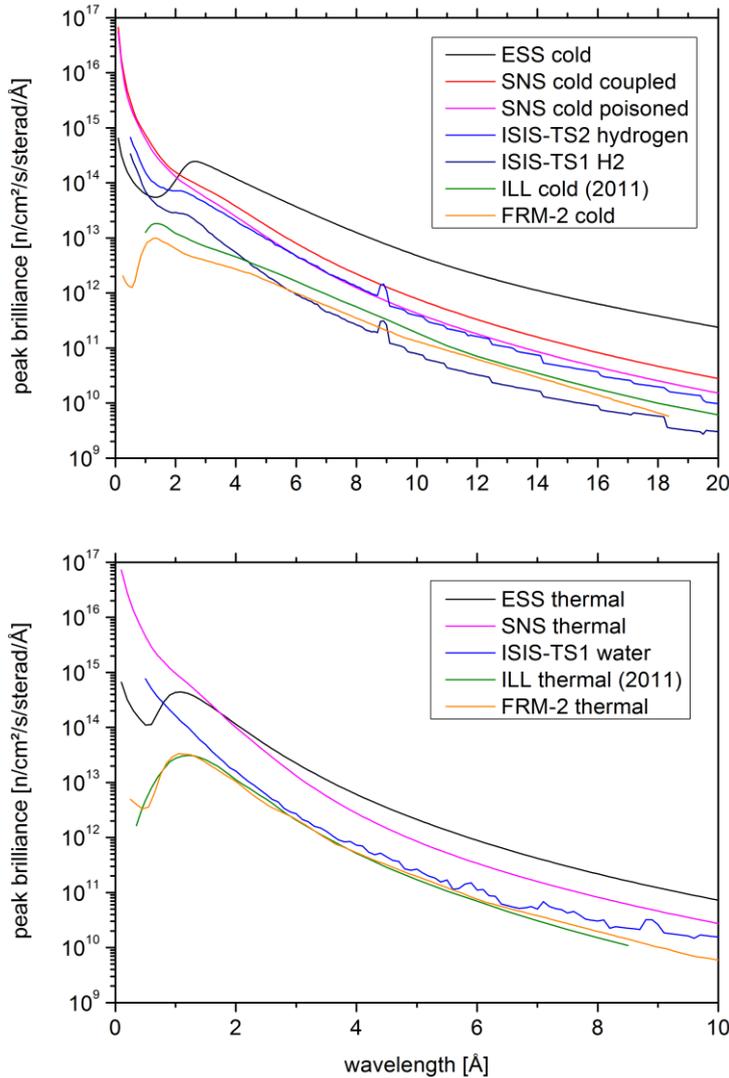
Figure 5: Peak brilliance of different neutron sources, cold moderators (upper figure) and thermal moderators (lower figure).

The characteristics of the ISIS sources were adapted to the actual proton current of 160 µA (TS1) and 40 µA (TS2). For ILL, there exist two descriptions in VITESS now: one reflecting the brilliances given in the Yellow Book (named 'YellowBook') [28], and one based on recent measurements and simulations (named '2011') [29]. Here the brilliance of the cold source is higher and that of the thermal source is lower than in the Yellow Book. All SNS characteristics in VITESS were originally extrapolations from the ESS

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characteristics published by F. Mezei end of 2000 [30]. In contrast to the cold moderators, the performance of the thermal moderator seems to be overestimated there. Therefore we have included a second version for the thermal (decoupled poisoned) moderator using the same analytical functions as in the first version, but fitting it to the curve found by Gallmeier based on later MCNPX simulations, as it was released in McStas.

There exist now four versions of ESS source characteristics: the original data released by F. Mezei (named 2001_Mezei), the data describing the brilliance of the improved cold moderator ('2012_Zanini') [31] by an empirical correction function, the new functions and parameters for cold and thermal moderator ('2013_ Schoenfeldt') [32] and the height dependent brilliances to describe also the pancake moderator ('2013_VarHeight').

Figure 5 shows the comparison for the cold and thermal moderators after all corrections using the 'Schoenfeldt version' from summer 2013 for the ESS, the corrected ISIS and SNS characteristics and the 2011 version for ILL. These final results seem all in good agreement now.

2.7 *Influence of gravity on guide performance (added)*

Initiated by a question by W. Schweika we examined the influence of gravity on beam properties in long guides. The first result was that the influence in elliptical guides is stronger than in guides of constant cross-section. The second result was that the effect is visible only for small (virtual) sources.

So we started a systematic analysis varying the size of the (virtual) source illuminating the guide and varying the guide entrance and exit size, both for different wavelength ranges. The result be can summarized in the rule of thumb that the effect becomes significant, if the source is smaller than the guide entrance (see Figure 6). Otherwise the guide is fed with the full phase space resulting in a phase space without gaps at the sample position. This study is submitted for publication [5].
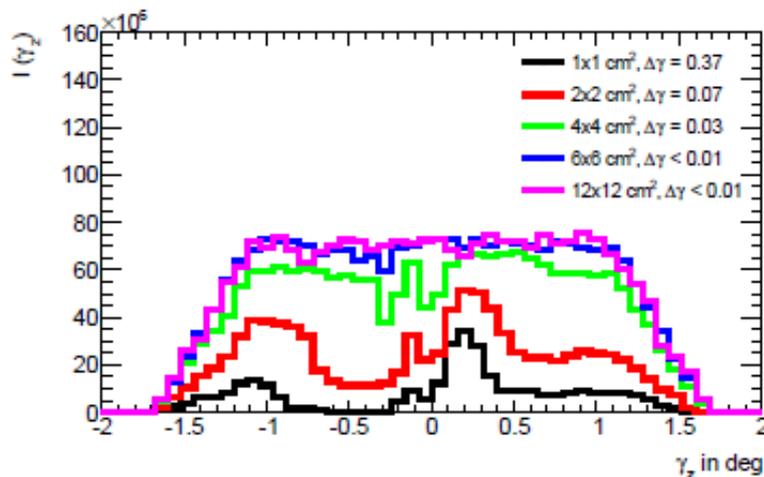
Figure 6: Vertical divergence distribution at a 1x1 cm^2 sample for a guide entrance of 4.9x 4.9 cm^2 and a wavelength of 6 Å. Δγ is a measure for the asymmetry of the distribution.

3 Development of VITESS

VITESS is a Monte Carlo simulation package to simulate (experiments on) neutron scattering instruments. It works with executables, which are delivered with the package, running in a pipe controlled by input parameters (cf. Fig. 10). These input parameters are given by a graphical user interface. This allows simulations without writing any script or code, which makes it easy to use.

It can be used to simulate any kind of neutron scattering instrument. Nevertheless, development was necessary to enable visualization and numerical optimization of the instrument, parallel execution of the simulation and the usage of Macintosh computers. Moreover, documentation and a few modules, especially monochromator and detector, needed improvement.

3.1 User Meeting

A meeting of the complete developer team with experienced VITESS users was held 27 – 28 June 2011 to find out about needs and wishes of users.

 The developer team presented new features in version 2.10 and plans for future version. The users presented their way of using the program and wishes for improvements. The developers also discussed about guidelines for programming. At the end of the meeting, there was agreement about a roadmap for the upcoming versions.

3.2 Releases

Table 4 gives an overview of the versions released during the project time. Altering the original plan, version 3.0 was released as a full, tested version, not only as a beta-version (on the way to VITESS 3.1) as foreseen in the task list.

Table 4: Release dates and main improvements of the VITESS versions released since the beginning of the project

version	release date	main new or improved modules	main new features
2.10	11.07.2011	elliptical mirror refraction lense	multi-core capability
2.11	16.12.2011	2D monitor imaging sample	Macintosh version python and perl scripts
3.0	14.11.2012	elliptical guide, brilliance monitor improved reflectometer sample	visualization
3.1	26.06.2013	new detector 'read_in', filter	optimization cluster capability
3.2	December 2013	new monochromator	extension of optimization and cluster usage

Versions 2.10, 2.11 and 3.2 were roughly released according to schedule, while version 3.1 was significantly delayed. This was partly because of the release of 3.0, but mainly because preference was given to instrument and component simulations and because the inclusion of the visualization was a major undertaking. It also included the new detector module that was foreseen for version 3.2 only.

3.3 Improvements in VITESS versions 2.10 to 3.2

Version 3.2 contains all new features that were foreseen within this work-package K7. Some of the new features have been incorporated in steps, for instance visualization was first included for the most important modules (version 3.0); the others were added in versions 3.1 and 3.2. Therefore it seems reasonable not to discuss the individual versions, but only compare the VITESS 3.2, which is the result of the activities in this work-package, with version 2.9 that existed when the project started. Two papers were written about the progress from version 2.9 to 3.2 [1, 6].

Apart from the new features described in the following chapters it should be noted that we started to write parts of the code in C++ instead of C.

3.3.1 Visualization

The most important new feature is the visualization, which users have been missing for years. The plan was to visualize the instrument as well as trajectories of neutrons through the instrument, both using 3D graphics.

The VITESS concept of independent executables, running simultaneously and working in their own local coordinate systems made this task difficult, because there is a-priori no knowledge about the instrument as a whole, especially no knowledge about the position of the actual component in global co-ordinate system.
Therefore it needs two runs: In a first run (with a very low number of trajectories), each module reads the position of the previous component and writes its own position (into the file instrument.inf). This file is then used by each module in the main run to calculate positions of the neutrons or parts of the component in the global co-ordinate system (see Fig. 7).
The modules write this information into two files – geometry.inf and trajectories.dat - in formats defined by the VITESS team. After the run, a special program – sortiap - converts this information into commands for 2- or 3-dimensional visualization .The X3D format is used for 3-dimensinal visualization. The recommended viewer is 'InstantPlayer' (freely available from http://www.instantreality.org/, ©Fraunhofer Gesellschaft). Fig. 8 shows an example of instrument and trajectory visualization using this 3D viewer.
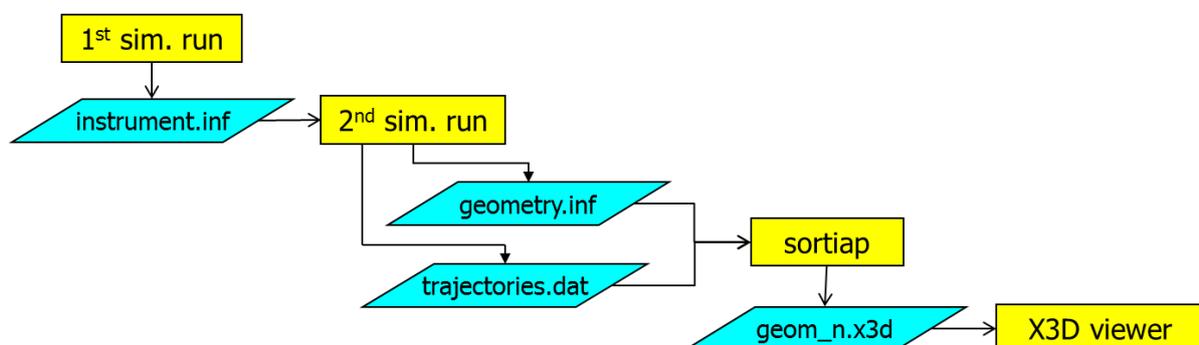
Figure 7: Realization of instrument and trajectory visualization in VITESS

All points of neutron absorption, reflection, entering or exiting a component are written to the trajectory file, together with an ID for the type of event. Additionally information about the loss in intensity is saved for later use to estimate radiation background.

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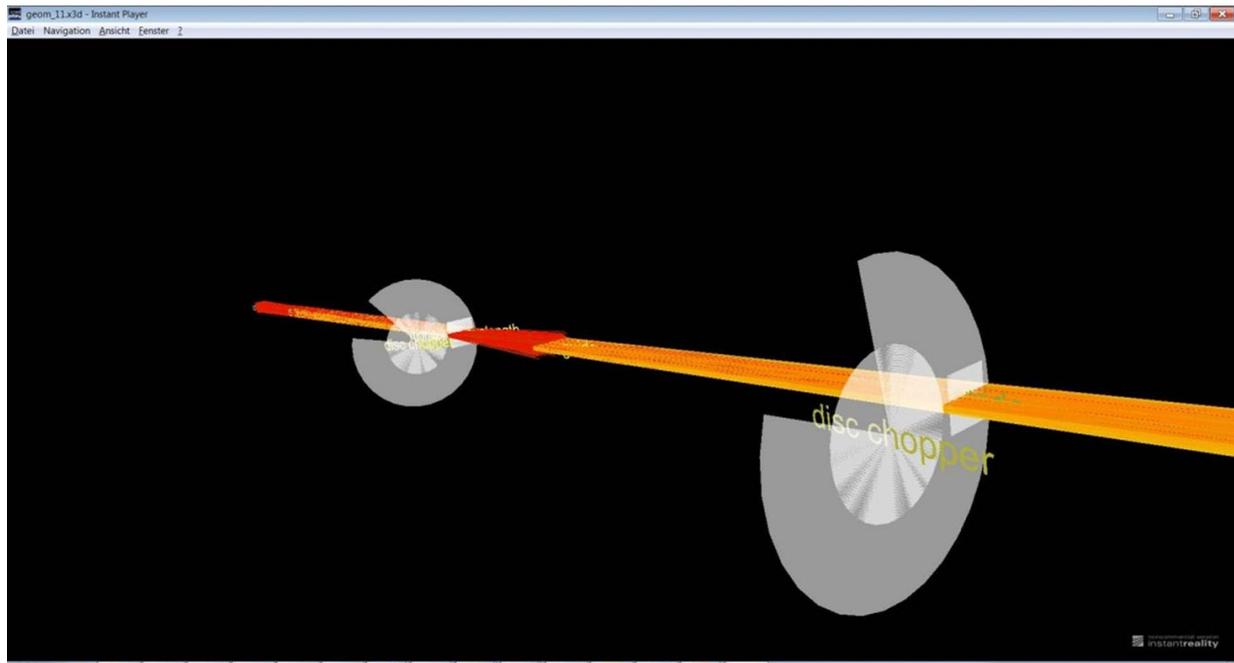
Figure 8: Example of instrument and trajectory visualization in VITESS using the X3D viewer *InstantPlayer*. (First part of the reflectometer THOR proposed for the ESS)

3.3.2 Optimization

There is growing interest in combining MC simulations (of neutron scattering instruments) with numerical optimization. Though there has been a framework for numerical optimization with VITESS simulations for nearly a decade [33], it has been used only rarely because its usage was complicated. This first approach offered a gradient method and a Metropolis algorithm [34]. A second approach by P. Bentley used a swarm and a genetic algorithm. Its usage was not significantly easier. Both tools have not been part of the usual VITESS release.

We have now changed the concept: a general optimization framework is now the main program; this chooses an optimization routine, which calls the simulation in 3 steps (cf. Fig. 9):
- Build the pipe command(s) from the standard instrument and the actual status of the parameters to be optimized
- Run the simulation(s)
- Determine the figure of merit from output files of the simulation

These 3 steps together replace the function call in a normal fit. We would like to stress that the user can define freely the figure of merit. A function that probably covers 90% of the cases in neutrons scattering (transmission, flux, flux*λ^n, …) is already delivered, but it is not difficult for the user to include any function.

In VITESS 3.2, there are two gradient methods, the Metropolis algorithm and a swarm algorithm. The first gradient method is based on a fitting routine by D. Braess [35]; the second has been developed by K. Lieutenant over the last 3 years by adapting this

algorithm to the specifics of the statistical nature of MC simulations. The swarm algorithm has been written by C. Zendler based on the original program by P. Bentley.
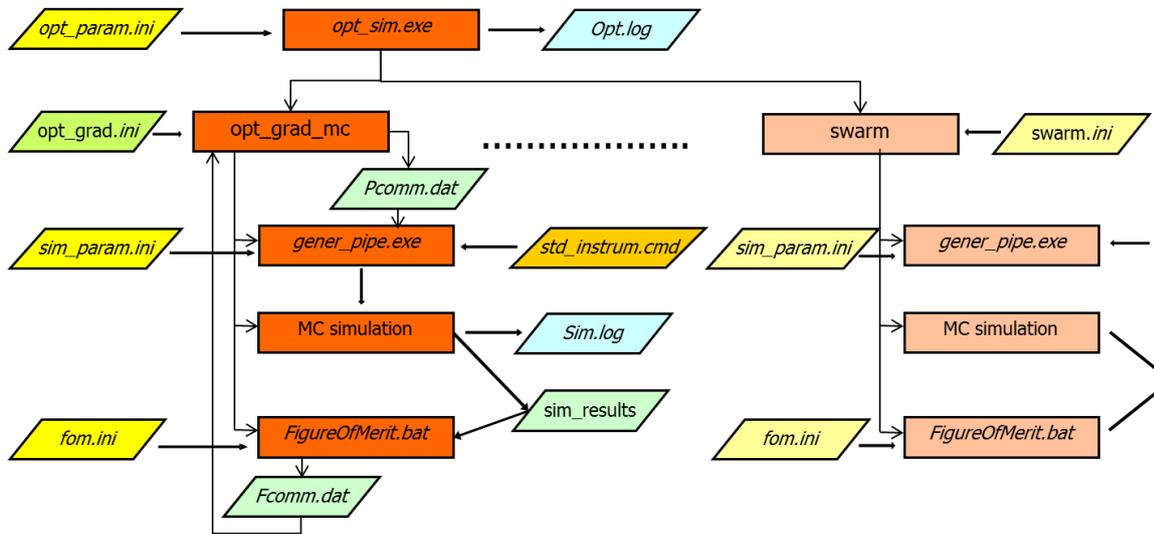
Figure 9: Concept for optimization in VITESS

Including new optimization routines is not too difficult (for the developers), so we like to include a genetic algorithm in the near future. A choice of optimization algorithms is necessary, because the advanced algorithms like the swarm algorithm are stable in finding the optimum, but need many simulations. So using a gradient in simple cases is probably much quicker, while it might not find the global optimum in case of a complicated parameter space.

If there is a one to one relation between optimization parameters and simulation parameters, the optimization can be started and controlled by simply editing ASCII control files. If several simulation parameters are changed by one optimization parameter or if a calculation from optimization to simulation parameter is necessary, this has to be programmed in a C-function.

3.3.3 Parallelization

With a growing number of computer clusters and an increasing number of cores in any PC, parallelization of programs becomes more and more important. We have included features for both, more efficient use of several cores in a PC and of computer clusters:

Helper Threads for PCs with Several Cores
In many cases, the VITESS concept of executables running in a pipe directly enables the use of several processors. As an example, the first core treats the neutrons at the source and passes the results to the second core, which treats them in the guide; the third treats them at chopper and so on (cf. Fig. 10). But this becomes ineffective, if one of the modules consumes most of the computation time, e.g. a guide consisting of many pieces. For this case the concept of helper threads was included by M. Fromme: the main thread creates N helper threads, divides the incoming number of events into N+1 parts, which are executed in parallel and combined by the main thread afterwards again to be delivered to the next module (see Fig. 10).

It was realized for the four modules: guide, supermirror-polariser, supermirror-ensemble and Fermi-chopper, which were suspected to consume most of the computation time (in some cases); the bender module is a candidate for a future extension of this concept. The code had to be changed for this 'parallel version'. Performance tests using a guide of many pieces showed a reduction of execution time to 40% on a PC with 4 cores.
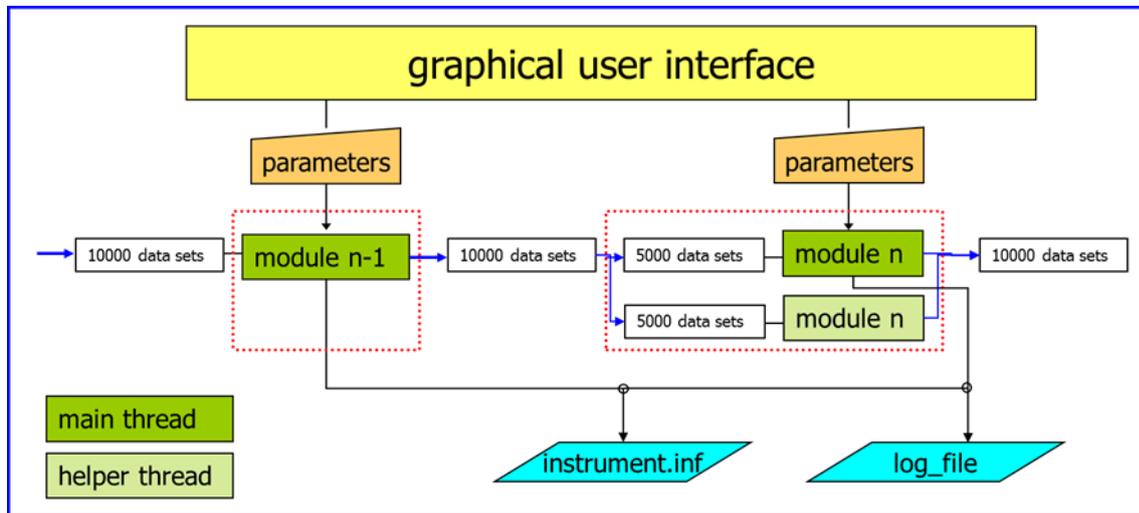
Figure 10: Concept of parallelization for multi-core PCs in VITESS using helper threads

Split of the Simulation for Clusters

For a computer cluster that might have hundreds of cores this is not an adequate solution any more. Instead the straightforward solution is to split the whole simulation into subtasks, e.g. let each of the 100 cores of a cluster calculate 10 Million trajectories and combine the results in the end to perform a simulation of 1 Billion trajectories.
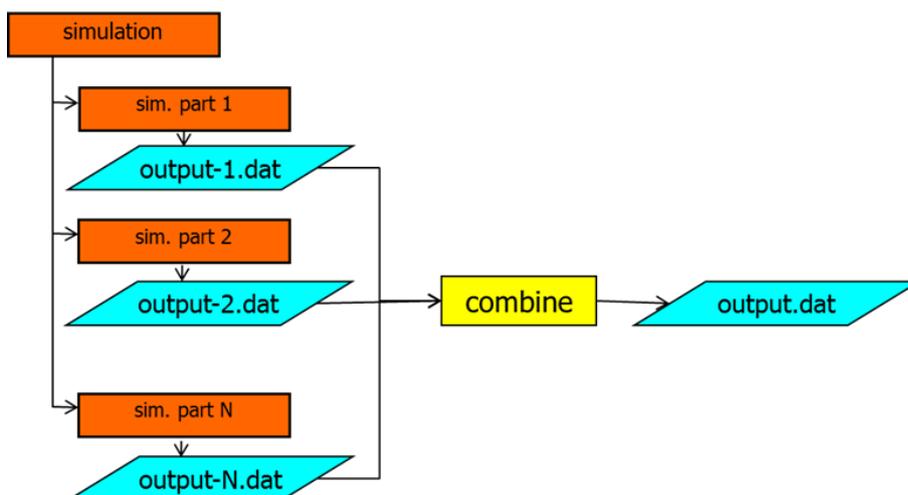
Figure 11: Concept of *gridrun*, the parallelization for computer clusters in VITESS by splitting the simulation and combining the results

The special VITESS concept of executables running in a pipe does not allow simply using the standard tool 'Message Passing Interface' (MPI). Another difficulty is that every core must have access to the input files. Therefore, M. Fromme implemented a VITESS-specific solution – for Unix/Linux clusters only. The version is designed for the HZB cluster and will need minor changes for other clusters; but it was already successfully adapted to the ESS cluster without problems.

Apart from very long runs for some kinds of instruments (like e.g. SANS) and scans of parameters resulting in many simulations, clusters will often be used for instrument optimization, which requires many simulations. Therefore, a special option has been realized to run the optimization on clusters. Here the individual simulation is not split, but all variations of the actual parameter set are executed simultaneously. The algorithms have been adapted to use that efficiently.

3.3.4 New Modules

New Monochromator/Analyzer

The monochromator module that has been part of VITESS for many years had the disadvantage that normalization was necessary for each setting. Though the procedure was described in the help text, many users had problems to pursue that and asked for improvement. The new module avoids this problem by doing the normalization itself. It also has the new features that it can be used in an array of monochromators and in transmission mode.

It was written by D. Nekrassov and was first released in VITESS 3.2.

Lense

The module *lense* simulates neutrons passing through a lense or a system of N identical lenses of spherical or parabolic shape. It also includes a diaphragm after the lense. Material, radii and thickness are input parameters. It was written by S. Manoshin and was first released in VITESS 2.10.

Ideal Guide

The normal guide module simulates a guide consisting of (any number of) linear pieces. Any shape is possible, but it is always an approximation by linear parts. So a good representation of an elliptic shape needs many short pieces, especially at the edges. This increases computation time significantly. Therefore a new module with a truly elliptical shape was written: *guide_ideal*. The shape can also be constant or linear to be able to treat guides that are elliptic in only 1 dimension. It calculates the points of reflection by solving a forth order equation and reduces the simulation time significantly (compared to guide consisting of many short pieces). It was written by D. Nekrassov and was first released in VITESS 3.0. Further shapes are foreseen for future VITESS versions.

Elliptical Mirror

The module *mirror_elliptical* simulates a truly elliptically shaped mirror. It treats spin-up and spin-down neutrons separately.
It was written by S. Manoshin and was first released in VITESS 2.10.

Imaging sample

The module *sample_nxs* simulates transmission and scattering of a polycrystalline sample based on scattering and absorption neutron cross sections and the unit cell

definition. It can be used for virtual imaging experiments including Bragg edge transmission experiments. But it can also be used as a powder sample.
It was written by M. Boin, originally for McStas and then adapted to VITESS. It was first released in version 2.11.

Brilliance Monitor
After the decision of the 'ESS guide task force' to use the brilliance transfer from source to sample to judge the quality of a guide system, a corresponding module in VITESS became necessary . The module *mon_brilliance* calculates peak and time averaged brilliance within a given range of space, divergence, wavelength and time as a function of one of these parameters. If only time averaged brilliance is of interest, the time can be left out.
It was written by K. Lieutenant and was first released in VITESS 3.0.

Trajectory input
The module *read_in* is the counterpart of the module writeout, which writes all parameters of all trajectories to an output file. read_in can read up to 3 of these files using normalization factors for each, thus allowing continuation of a simulation, combining different paths in the first part of the instrument or combining simulations of the same instrument.
Additionally, read_in and writeout can also treat events in McStas format to enable switching from one package to the other. MCNPX format is foreseen for the future.
It was written by K. Lieutenant and was first released in VITESS 3.1. In earlier versions, splitting the instrument was possible by using binary trajectory files.

1D- and 2D Monitor
The modules *monitor1D* and *monitor2D* monitor intensity as a function of any parameter (*monitor1D*) or any combination of 2 parameters (*monitor2D*). Thus, *monitor2D* renders new modules unnecessary if new parameter combinationsare needed.
They were written by D. Nekrassov and released in VITESS 3.0 and VITESS 2.11 resp. These were the first modules that are written in C++ to a large extent.

Beam-stop
There is a dedicated module *beamstop* to simulate a beam-stop now, for which the module *spacewindow* had to be used before.
It was written by K. Lieutenant and was first released in VITESS 2.10.

Filter
The module *filter* removes trajectories with parameters outside a certain range from the simulation. The idea was to remove this feature from the monitor modules to make this action more obvious.
It was written by D. Nekrassov and was first released in VITESS 3.1.

SANS Evaluation
The module *eval_sans* is a variation of the module *eval_elast*; it allows normalizing the output so that S->1 is obtained for Q->0.
It was written by K. Lieutenant and was first released in VITESS 2.11.

Top table (green = hardware modules):

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

Legend: **new** / upgraded / improved / unchanged

Bottom table (yellow = other modules):

Category					
Monitor 1	**monitor1D**	time	wavelength	y-/z-pos	div-y/-z	**brilliance**
Monitor 2	**monitor2D**	y-pos z-pos	div-y div-z	k-y k-z	r div-r	y z div-y div-z
		TOF λ	λ div-y/-z			
MonPol 1	time	wavelength	y-/z-pos	div-y / div-z		
MonPol 2	y-pos z-pos					
Evaluate	elast	elast2	inelast	**sans**	capt_flux	
Geometry	frame					**new**
Trajector.	**read_in**	writeout	spin_reset			upgraded
Other	**filter**	visualize				improved
						unchanged

Figure 12: Overview of modules in VITESS 3.2 compared to the situation before the beginning of the ESS work package K7. (Modules representing hardware in green, others in yellow.)

3.3.5 Upgrades

Detector

The module *detector* has been significantly improved; it has the following new features now:

- Detectors can be combined in an array
- The resolution can be chosen independently of the bin size
- Detector tubes can be treated - even in stacked form
- The efficiency can be read from file or be calculated from gas pressure, size and material

It was upgraded by C. Zendler and was first released in VITESS 3.1.

Reflectometer Sample

The module *sample_reflectom* can treat incoherent scattering and off-specular scattering now. For the latter one, data are taken from a look-up table containing reflectivity values as a function of initial and final wave-vector.

It was upgraded by D. Nekrassov and was first released in VITESS 3.2.

Further Improvements

- The evaluate modules take into account the real path lengths from sample to points of detection in time-of-flight mode (K.Lieutenant, A. Houben, 3.2).
- The source module can treat different versions of the moderator characteristics now (cf. chapter 2.6). It also contains the option to send out only neutrons that arrive in a specific space of time at a certain distance (K. Lieutenant, 3.1 and 3.2).
- The guide modules and the supermirror-ensemble can count reflections now and may be used by only giving the m-value to describe the coating based on the description by H. Jakobsen [11]. (D. Nekrassov, C. Zendler, K. Lieutenant, 3.0 to 3.2).
- A new tool *GenerateExtractionSystem* has been written to facilitate creating the input file for the module *sm_ensemble*, which describes an extraction system (C. Zendler, 3.1). - Tools in VITESS are used to check or generate input data, e.g. reflectivity files for guides.

3.3.6 Improvements in the (Graphical) User Interface

The main improvement in the user interface is that the instrument can now be exported as a python or a perl script in addition to a shell or tcl script, (which existed before). This script can be used as a basis to run a series of simulations and/or to calculate simulation parameters from physical parameters. The simulation can also be changed by editing the script file. The edited file can be re-imported to the gui file later on.

There are several minor changes in the graphical user interface, which make working much more convenient:

- Modules can be disabled and enabled again
- Each component can be given a name now
- Visualization of a single component is possible
- The instrument file is regularly saved and older versions can be recovered
- Monitor output files of identical runs with different random seeds can be merged
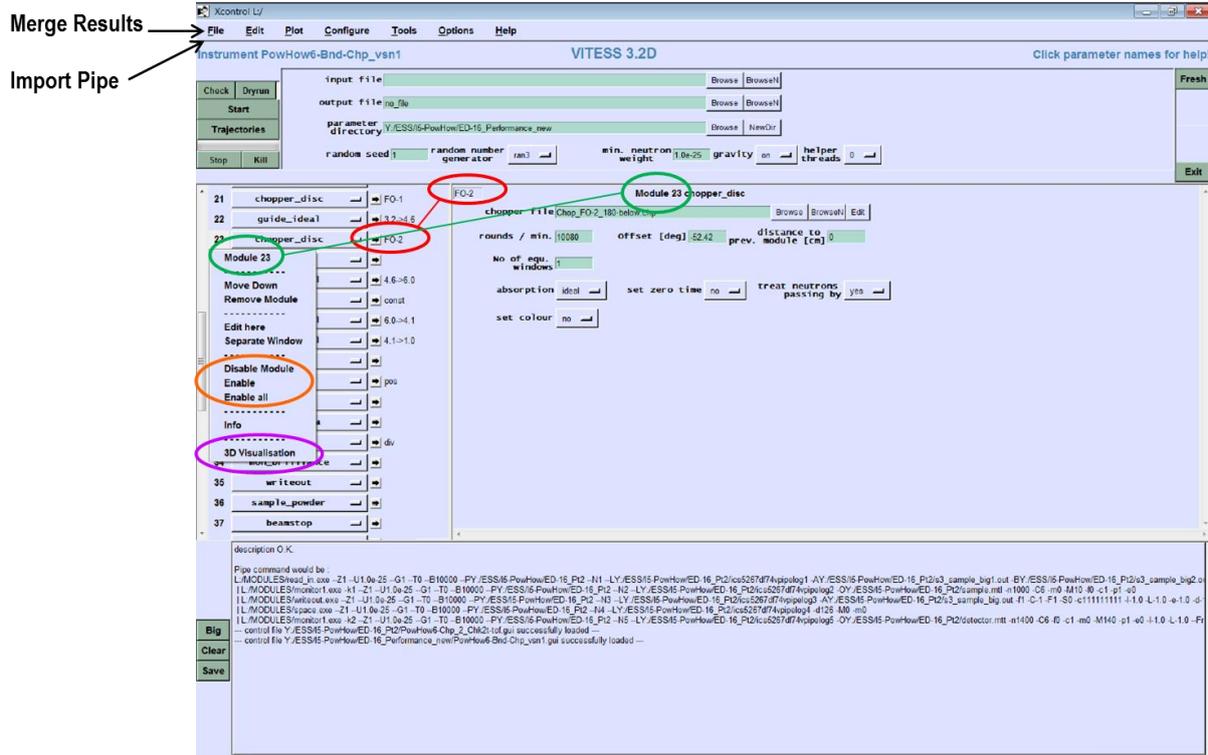
Figure 13: new features in the VITESS GUI in version 3.2: module names (red), disable (orange), component visualization (purple) and module number on the component window (green)

4 Help Desk Function

4.1 Email list for VITESS users

There are actually two VITESS mailing lists. One is vitess@helmholtz-berlin.de , which exists already for many years. It is announced on the VITESS website http://www.helmholtz-berlin.de/vitess and is meant for users to ask the developer team any question about the program. It is an unmoderated list. The recipients are the members of the central developing team at HZB, at the moment K. Lieutenant, M. Fromme, D. Nekrassov and C. Zendler.

The second, new email list – hzb-vitess-devel@listserv.dfn.de - is a moderated list meant for the communication among developers and users. Any user who is interested can be included in this list. He has to send an email to the central developer team for that.

The unmoderated list receives a lot of spams and is therefore not suited to have many recipients, but questions of general interest can be forwarded to the second list for discussion in a broader audience.

In addition to the mailing lists and the website, VITESS has now a Wikipedia site http://en.wikipedia.org/wiki/VITESS and a Facebook account https://www.facebook.com/VitessTeam. 22 users have become followers in the meantime and are thus kept updated about news related to the package: new versions, workshops etc. But of course main news are also announced via the neutron mailing list.

Figure 14: Facebook account of VITESS

4.2 Support for Macintosh users

Macintosh versions of VITESS are released from VITESS 2.11 on. User support is given by Carolin Zendler and Michael Fromme and will be continued in the future.

4.3 Training course for VITESS 3

A training course for VITESS was held in combination with a course for McStas 2 on 18 to 20 September 2013 in Berlin. 18 students took part in the course. It consisted of a general part on the first day, presentations of the new features on the second day, both as a combination of lectures and exercises – for VITESS and McStas. The third day was reserved to user presentations and discussion.

This gave precious feedback about needs and possible improvement for the package again. Some of the improvements (e.g. 'merge' and 'disable', see chapter 3.3.6) have already been realized in VITESS 3.2.

4.4 VITESS manual (print version)

A concept and a structure for the manual have been fixed. The content of the individual chapters will be completed in the near future.

4.5 Complete documentation for VITESS (html documentation)

The documentation of the VITESS concept, modules and tools has been completed and updated over the whole period of the project. For each module and each tool, there exists an html help file now reflecting the actual version of the program: it describes the module in general, partly supported by illustrating figures, explains the meaning of each parameter and gives typical values and a sensible range (see Fig. 15).
In addition, there are pdf files explaining the concept of VITESS, and how to use features like optimization or parallelization. A tutorial exists as well.
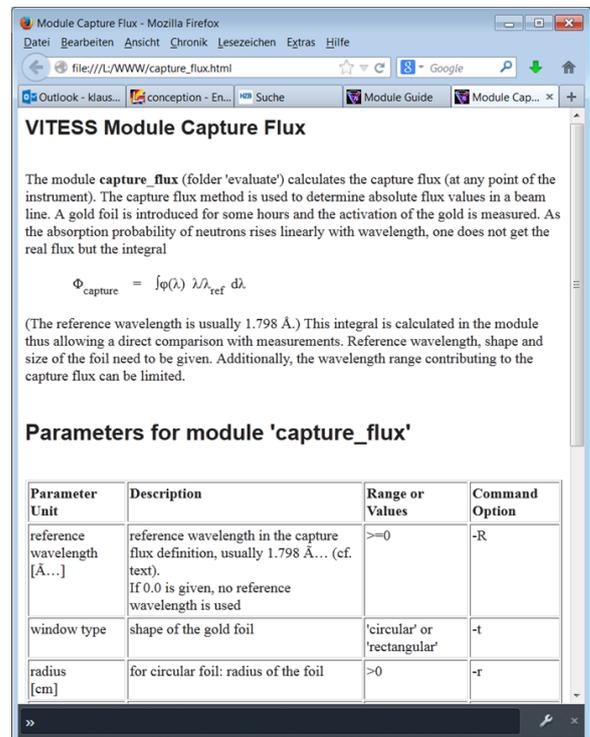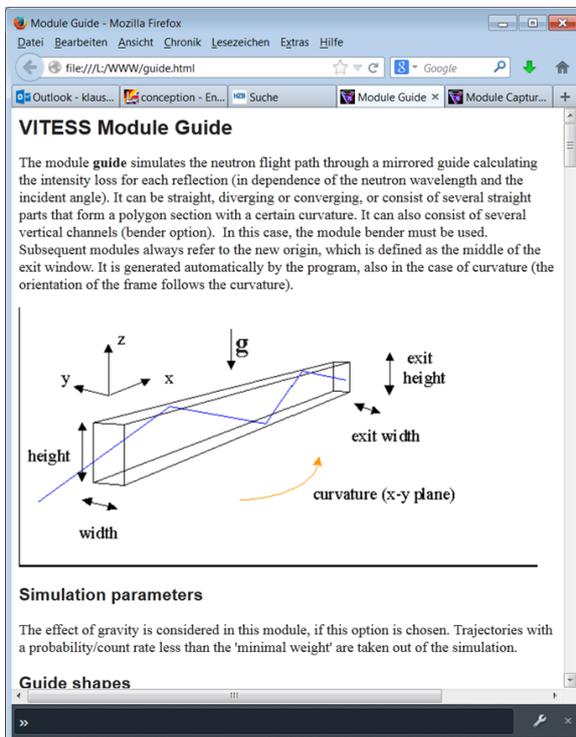
Figure 15: Two examples of a help files: for the modules *guide* and *capture_flux*

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6 Appendix

List of Abbreviations

HZB	Helmholtz-Zentrum Berlin
ILL	Institut Laue-Langevin
NBI	Niels Bohr Institute
JCNS	Jülich Centre for Neutron Science
JINR	Joint Institute for Nuclear Research
RWTH	Rheinisch-Westfälische Technische Hochschule
VITESS	Virtual Instrumentation Tool for the ESS
	(The Monte Carlo simulation package developed at HZB)
McStas	Monte Carlo Simulations of Triple Axis Spectrometers
	(The Monte Carlo simulation package developed in Denmark)
MPI	Message Passing Interface
THOR	The HOrizontal Reflectometer
ESSEX	ESS EXtreme environment instrument
ODIN	Optical and Diffraction Imaging with Neutrons