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K7 – 2012 Q4 Work Package Report

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DOCUMENT REVISION HISTORY

Revision	Reason for revision	Date
1	New Document	

List of Authors	List of Reviewers	List of Approvers
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GENERAL INTRODUCTION

Work Package report for the period 1st October to 31st December 2012.

The ESS WP coordinator fills in section 1.

- Sub-section 1.1 should be filled in before distribution to WP leaders
- The other subsections in section 1 should be filled in after section 2

Section 2 is filled in by the WP leader(s).

- Exception: subsection 2.1.1 (same for subsequent WU's) should be filled in by ESS secretariat before distribution to WP leaders
- Sub-sections 2.1.4-2.1.8 (same for subsequent WU's) only need to be filled in when a change occurs

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LIST OF ABBREVIATIONS

Abbreviation	Definition
HZB	Helmholtz-Zentrum Berlin
VITESS	The Monte Carlo simulation package developed at HZB (Virtual Instrumentation Tool for the ESS)
ILL	Institut Laue-Langevin
JINR	Joint Institute for Nuclear Research
RWTH	Rheinisch-Westfälische Technische Hochschule

1. GENERAL WORK PACKAGE STATUS

1.1 Work package overview

- Simulation Code Development, Helpdesk, Work Package K7 (SD015DE)
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  The work will provide support for simulation tasks with VITESS and McStas in cooperation with the ESS Data Management Centre (University of Copenhagen). Further development of VITESS incl. instrument visualization, numerical optimization, multi-processor capability, extension of user interface functionality, source code development for new components and general overhaul of existing components are indispensible for allowing thorough simulation capabilities for ESS instruments.

1.2 Summary of main achievements

<< A summary of the work performed. This could include a table showing a column with the deliverables and milestones and a %age of work complete, followed by one or two sentences with more detail. >>

1.3 Focus for next quarter

<< A summary of the key milestones and work to be performed in the next quarter. >>

1.4 Issues

<< A summary for any issues identified in this quarter and what they require. >>

1.5 Top risks identified

<< A summary of the key risks identified. >>

2. WORK UNITS

2.1 Work unit 1: Simulation Code Development, Help Desk

2.1.1 Deliverables & Milestones

Deliverables:		
D.K.7.1.1	Performance characteristics of the instruments as a function of pulse length and frequency	01/2011
D.K.7.1.2	Comparison of different neutron guide geometries	03/2011
D.K.7.1.3	Simulation of “day-1 instruments”	11/2012
D.K.7.1.4	Influence of waviness on guide performance	01/2012
D.K.7.1.5	Performance of extraction systems	12/2011
D.K.7.1.6	New: Brilliance comparison of different neutron sources	12/2012
D.K.7.1.7	New: Influence of gravity on guide performance	10/2012
D.K.7.2.1	User meeting	02/2011
D.K.7.2.2	VITESS 2.10 release (multi-processor capability, help for all existing modules, new modules: elliptical mirror, diffraction lenses)	05/2011
D.K.7.2.3	VITESS 2.11 release (Macintosh version, new level of user interface, new modules 'imaging sample' and 'monitor2D)	12/2011
D.K.7.2.4	VITESS 3.1 release (instrument visualisation, numerical optimization, improved module 'reflectometry sample')	06/2012
D.K.7.2.5	VITESS 3.2 release (New program structure, new detector and monochromator module)	11/2013
D.K.7.3.1	Email list for VITESS users	11/2011
D.K.7.3.2	Support for Macintosh users	11/2011
D.K.7.3.3	Training course for VITESS 3	05/2012
D.K.7.3.4	VITESS manual (print version)	11/2012
D.K.7.3.5	Complete documentation for VITESS (html documentation)	11/2013

Milestones:		
M.K.7.2.1	VITESS 3.0 (beta test version of VITESS 3.1)	04/2012

2.1.2 Achievements for the period (2-5 pages)

The main activity in this quarter was the development of the VITESS package: version 3.0 (M.K.7.2.1) was released and the work on version 3.1 (D.K.7.2.4) organized and continued.

The work on bi-spectral extraction systems (D.K.7.1.5) is nearly finished; one paper is published now (C. Zendler et al. NIM A 704 (2013) 68-75.), another one sent for publication.

The simulations of the gravity effect on guide performance (D.K.7.1.7) are completed. A publication is in preparation.

The system to communicate with users (D.K.7.3.1) has been completed now by installing a second mailing list, a Facebook account and a Wikipedia article. They are linked with each other and the VITESS home page.

D.K.7.1.5 Bi-spectral extraction systems

Bi-spectral extraction systems were studied in combination with feeder systems (see previous report). The resulting paper is now published:
C. Zendler, K. Lieutenant, D. Nekrassov, L. D. Cussen, M. Strobl, *Bi-spectral beam extraction in combination with a focusing feeder*, Nucl. Instr. Meth. Phys. Res. A 704 (2013) 68-75.

In addition, there was a collaboration with the simulation group in Copenhagen on bi-spectral extraction systems for elliptic guides. H. Jacobsen performed optimizations for different wavelength ranges, different accepted divergences and different guide lengths using McStas. Results were cross-checked by C. Zendler and K. Lieutenant using VITESS. Finally agreement between the packages could be reached.
The final design showed good performance – 75% to 95% efficiency - for neutrons above 1 Å and usually a symmetric and often a smooth divergence distribution. A paper about this study was written and sent to NIMA for publication.

It remains to improve the performance of a compact bi-spectral extraction system, which consists of many mirrors of 25 to 50 cm length.

D.K.7.1.7 Gravity effect on guide performance

The simulations of the gravity effects on the performance of elliptic guides were performed by D. Nekrassov and have been finished by now. The result is that the vertical divergence distribution is disturbed by gravity, especially for long wavelengths, small (virtual) sources and large source-to-guide distances. It has also been found that smooth and symmetric distributions in space and divergence can be obtained by using (virtual) sources significantly larger than the guide entrance (see Fig. 1). A publication of this study is in preparation.

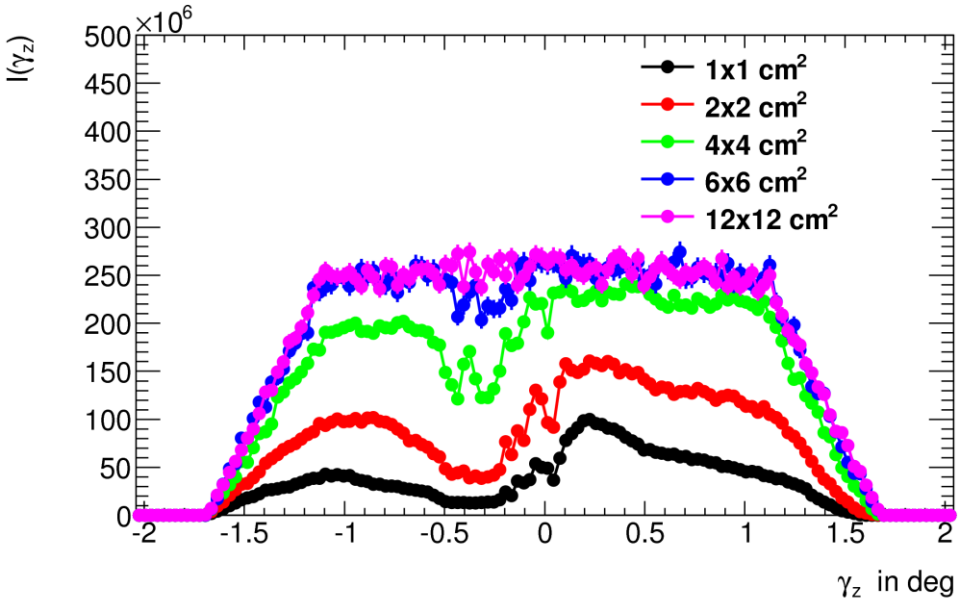

Fig. 1: Simulations of the vertical divergence distribution at a 1x1 cm² sample of a neutron beam transported by a 148 m long elliptical guide from a (virtual) source of different sizes. Neutron flux was assumed to be constant in the wavelength range 1 to 12 Å. The distances source – guide and guide – sample were both 1 m; guide entrance and exit width and height are 4.9 cm.

D.K.7.2.4 and M.K.7.2.1 VITESS 3

VITESS 3.0 has been released on 14 Nov 2012. The visualization features were improved before the release (cf. Fig. 2).

The contents of version 3.1 were fixed, the tasks were distributed among the members of the developer team and a decision taken that code development should be finished in March 2013. Apart from the features foreseen for version 3.1, it will also contain a new detector module, which was originally planned to be released in version 3.2.

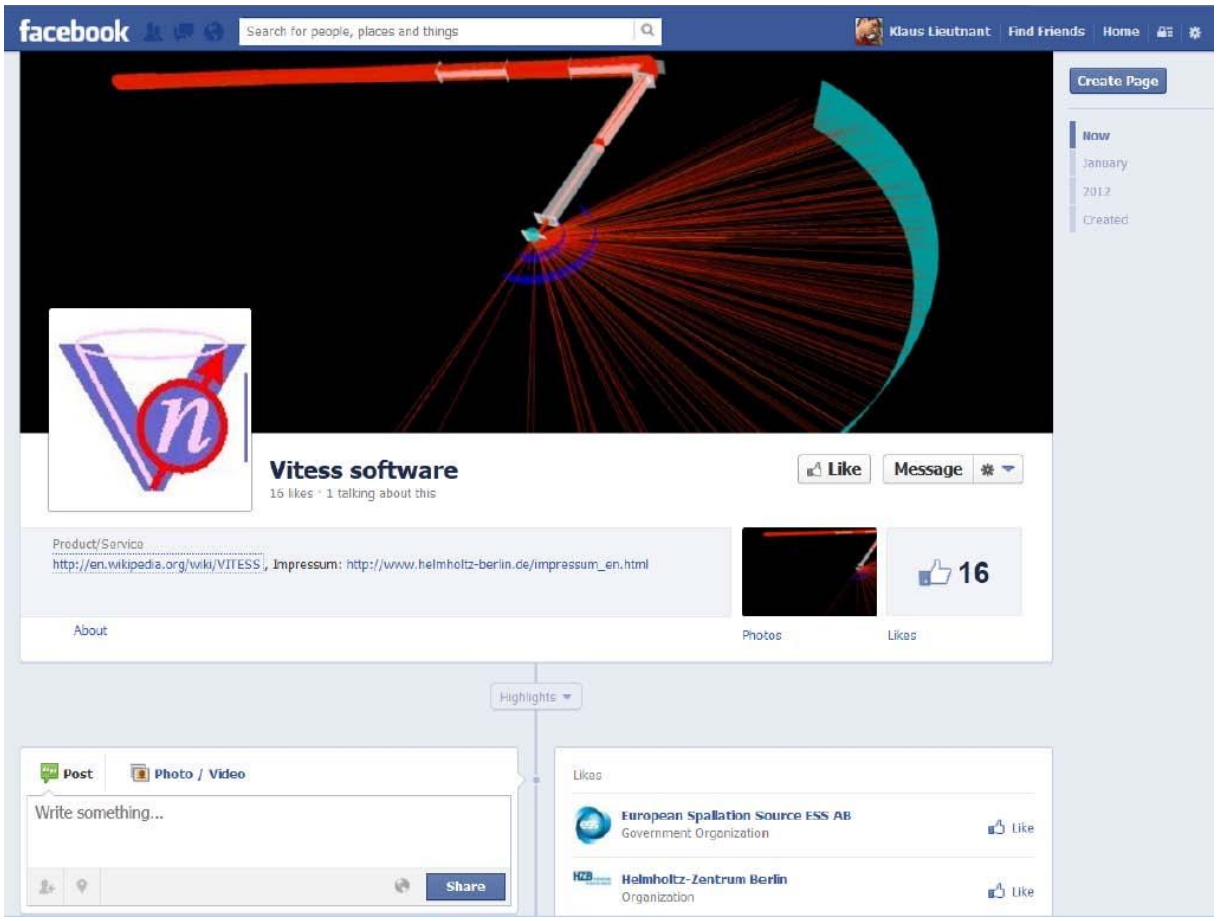

Fig. 3: VITESS Facebook account containing the visualization of the IFE-Diffractometer ODIN from VITESS 3.0

D.K.7.3.1 Email list for VITESS users

There are now two VITESS email lists:

- One is for users (vitess@helmholtz-berlin.de). It is an open list; emails are sent to the central developer team in Berlin (M. Fromme, K. Lieutenant, D. Nekrassov and C. Zendler)
- Another one is for communication among the developers. It is a non-public LISTSERV-List; members are those 4 persons in Berlin who get the user emails (s. above) and the collaboration partners A. Houben, S. Manoshin, T. Zuo, S. Zhang (cf. sub-section 2.1.5).

Information about the package is available on the homepage (http://www.helmholtz-berlin.de/vitess/), via Facebook (http://www.facebook.com/VitessTeam; see Fig. 1) and Wikipedia (http://en.wikipedia.org/wiki/VITESS). They are linked with each other.

The Wikipedia page contains a short description of the package. The homepage contains more information: parts of the documentation, version history, announcments etc. A section 'known problems' will be added soon. The program can be downloaded from there.
The Facebook account is meant to keep users updated about developments and changes. New releases are also announced through the neutron mailing list.

D.K.7.3.5 Documentation

The documentation of the simulation package is continuously improved.

Deliverables and milestones achieved

Deliverable/Milestone	% Completion	Comments
D.K.7.1.1	100	
D.K.7.1.2	95	
D.K.7.1.3	90	
D.K.7.1.4	50	added
D.K.7.1.5	95	added
D.K.7.1.6	60	new
D.K.7.1.7	80	new
D.K.7.2.1	100	
D.K.7.2.2	100	
D.K.7.2.3	100	
D.K.7.2.4	80	
D.K.7.2.5	0	
D.K.7.3.1	100	
D.K.7.3.2	100	
D.K.7.3.3	0	
D.K.7.3.4	0	
D.K.7.3.5	85	
M.K.7.2.1	100	

Status of work unit

7.1 Collaboration with the Data Management Center in Copenhagen

The first task (source time structure) is finished, the second task (guide performance) was regarded as finished, but had come back; it will be finished in the first half of 2013. The influence of waviness has been found to be of minor importance, a completion of this work (including publication) will be done at the end of the project time.

The studies of bi-spectral extraction systems are nearly finished; the only thing left to do is to improve the compact extraction system. Simulations of the influence of gravity are completed; a publication will be written in early 2013. The brilliance comparison will be continued in 2013.

The simulations of the Day-1-Instruments are performed by the individual groups; so we are only responsible for the Liquids Reflectometer, the Imaging Instrument and the Extreme Environment Instrument. These simulations will be completed in the first quarter of 2013.

7.2 Development of VITESS

Version 2.10 and 2.11 were released roughly according to schedule. The releases of versions 3.0 and 3.1 are delayed by some months, because priority was given to new requests from the ESS, the study of general guide properties and the instrument simulations, i.e. the postdocs who are partly working on the VITESS work unit (K7) and on instruments (German work units I3, I6 and I1) have spent most of their time on instrument simulations until September 2012. Now progress is much faster; version 3.0 was released in November 2012, and version 3.1 is foreseen for spring 2013.

7.3 Helpdesk function

The main tasks are fulfilled:

- The Macintosh version is running and Macintosh users get support.
- Users can address to the developer team for support via mailing list and get information through VITESS homepage, Facebook and Wikipedia. Developers have their own mailing list.
- There are help files for all existing modules now.

A training course for VITESS 3 will be held before the release of version 3.1. The handbook will be realized after this release. The help files are improved continuously.

Generally the project is on schedule.

2.1.3 Costs / Resources

Resources:													
	Staff					Expenditure					Investment		
Task	FZJ	HZG	HZB	TUM		FZJ	HZG	HZB	TUM		FZJ	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

Manpower committed in the reporting period

<< This should detail who is working on the work unit and how much, so the total manpower can be calculated and compared with the project plan. This allows manpower problems to be identified early. It should be presented in the form of a short table: >>

Name	Participating lab	Manpower allocated for reporting period (in man-months)	Manpower used in reporting period (in man-months)
K. Lieutenant	HZB	1.5	1.8
D. Nekrassov	HZB	1.0	0.5
C. Zendler	HZB	1.0	1.0
L. Cussen	HZB	0.0	0.5

Capital expenditure committed in reporting period

<< This should detail capital spent in the period and where it was spent with regard to the initial project plan. This allows over- and under-spend to be identified. >>

Item	Participating lab	Capital allocated for reporting period (in k€)	Capital used in reporting period (in k€)
Investments	HZB	0.0	0.0
Fluid capital	HZB	4.4	2.3

2.1.4 Risks

(Update when needed)

2.1.5 Collaborations/Partners

(Update when needed)

Michael Fromme, HZB, Berlin	GUI and releases
Sergey Manoshin, JINR, Dubna	Programming of individual modules
Andreas Houben, RWTH, Aachen	Programming of individual modules
Nikolaos Tsapatsaris, ESS, Lund	Testing
Taisen Zuo, CSNS, Beijing	Programming of code to describe CSNS source
Shengkai Zhang, CSNS, Beijing	Programming of a web application

Their work is not accounted as costs for the project.

2.1.6 Other

(Update when needed)

2.1.7 Planned achievements for the next period

(Update when needed)

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2.1.8 Main issues foreseen in the next reporting period

(Update when needed)