K7 – 2013 Q2 Work Package Report

DOCUMENT REVISION HISTORY

Revision	Reason for revision	Date
1	New Document	

List of Authors	List of Reviewers	List of Approvers
Oliver Kirstein (ESS) interim Klaus Lieutenant (HZB)		MXApprover

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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 activities in this quarter were the release of VITESS version 3.1 (D.K.7.2.4) and the completion of the brilliance comparison (D.K.7.1.6).

VITESS version 3.1 was released on 26.06.2013 after being thoroughly on all platforms. It contains all features foreseen for this version plus most of the improvements of the detector module, which was planned for version 3.2.

The comparison of brilliances (D.K.7.1.6) has been completed by checking and correcting the SNS moderator characteristics. All moderators at ESS, ILL, ISIS and SNS are now correctly described and McStas and VITESS output are in agreement.

Organization of the training course (D.K.7.3.3) has begun; it will take place 18 – 20 Sep 2013.

D.K.7.1.6 Brilliance comparison of different neutron sources

The comparison of brilliances in McStas and VITESS was continued: It has become clear that the characteristics of the methane moderator at TS1 and the 'groove' moderator at TS2 are based on wrong MCNPX results. A correction in VITESS (or McStas) is not possible. K. Andersen plans to inform ISIS.

As the last facility the SNS moderators were compared: VITESS used an extrapolation from the ESS characteristics released by F. Mezei end of 2000 to the SNS conditions – this description is in fact based on MCNPX simulations of the SNS source. (This approach has now been implemented in McStas as well.)
McStas used special components written by SNS employees based on later MCNPX calculations. A comparison showed rather good agreement for the cold source, but much higher flux of the thermal source in the VITESS description (see Fig. 1). As the McStas data are based on later MCNPX simulations, they are regarded as more reliable. So the performance of the thermal source was overestimated in VITESS. As the ratio of peak flux and time averaged flux was different, a simple scaling was not sufficient. Instead the McStas curve obtained by the Gallmeier component was fitted varying several parameters of the function used in the Mezei description. The resulting moderator characteristics are shown in Figure 2.

There is one McStas component describing one J-PARC beam-line. Due to lack of knowledge of the source characteristics and the code, it was transferred to VTIESS.

The corrections and the new simulation results of the SNS (and J-PARC) source are described in a document called *SourceBrightness_SNS_J-PARC* that is published as ESS document.
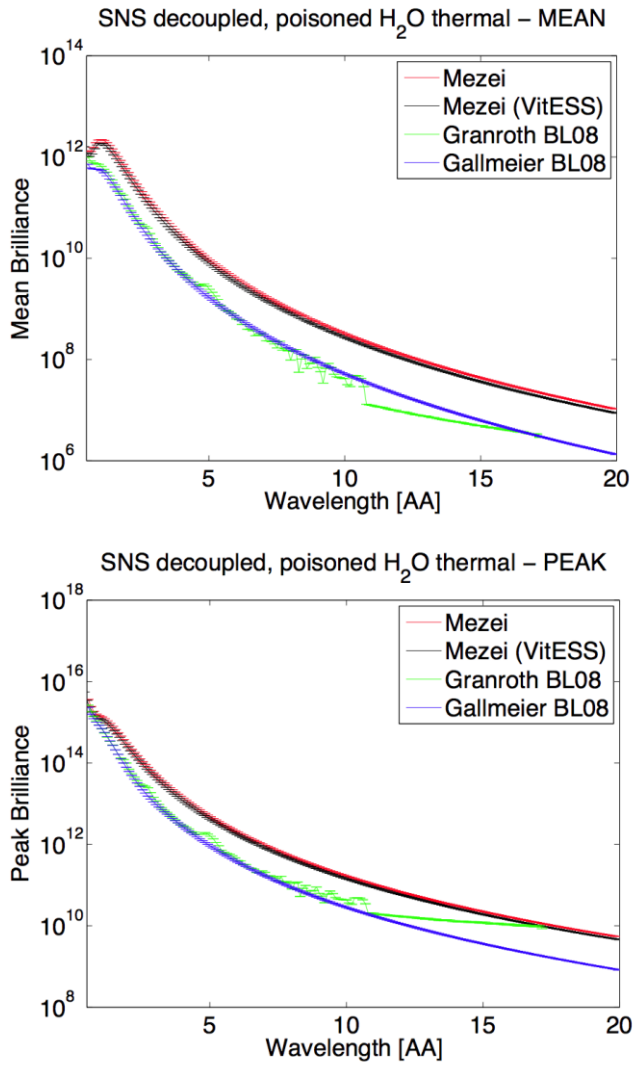
Fig. 1: Comparison of the performance of the SNS beam-line 08 in VITESS and 3 different McStas descriptions
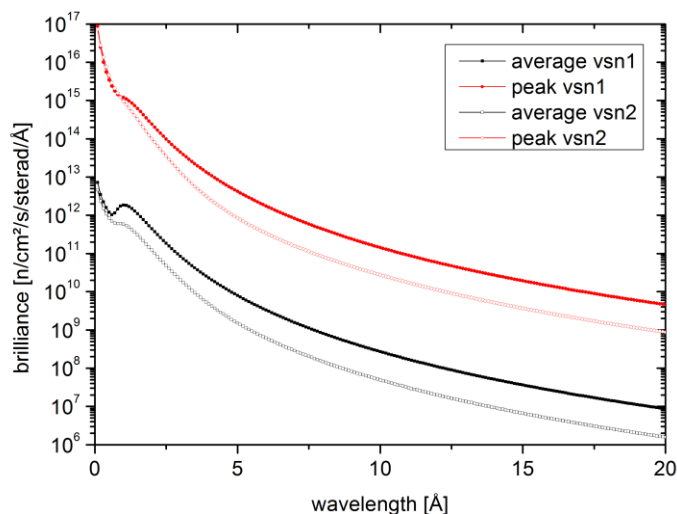
*Fig. 2: Average and peak flux of the SNS thermal source in the old description from 2001
(vsn 1) and the new description following the description by Gallmeier (vsn 2)*

D.K.7.2.4 and D.K.7.2.5 VITESS versions 3.1 and 3.2

Version 3.1 has been released on 26.06.2013 after intensive tests. The main new features

- the optimization
- a new way of parallelization

were already described in the previous report. But this version also includes

- the completion of the visualization.
- improvements of the detector module, (which were foreseen for version 3.2). Details will be given in the next report.
- a **filter** module that removes neutrons with certain properties (e.g. divergence above a certain limit) from the simulation
- the **writeout** module can also write trajectories in McStas format; the ASCII files containing these trajectories (in VITESS or McStas format) can now be read by a new module **read_in**
- (new) moderator characteristics of the
    - 'Chinese Spallation Neutron Source'
    - ISIS
    - ESS version 2013
    - SNS (see above)
    - HZB
    - ILL
- improved monitors
- the module *sample_reflectom* handles offspecular scattering now
- improvement in the GUI

- o the GUI silently stores the state of the active session at reasonable times
- o you may give the actual module a specific name.
- o The actual module is emphasized in the module list.
- a new tool to generate bi-spectral extraction systems consisting of many mirrors

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	100	new
D.K.7.1.7	95	new
D.K.7.2.1	100	
D.K.7.2.2	100	
D.K.7.2.3	100	
D.K.7.2.4	100	
D.K.7.2.5	30	
D.K.7.3.1	100	
D.K.7.3.2	100	
D.K.7.3.3	20	
D.K.7.3.4	0	
D.K.7.3.5	95	
M.K.7.2.1	100	

<u>Status of work unit</u>

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 3rd quarter 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 is written. The brilliance comparison is finished.

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 are nearly finished and will be completed in the third 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 were delayed by some months, because priority was given to the study of general questions of instrumentation for the ESS and the instrument simulations for the German work-packages.. Now progress is much faster; version 3.0 was released in November 2012, version 3.1 in June 2013 and 3.2 is foreseen for November 2013. Work for this version has already begun.

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 and for general features like visualization.

The organisation of the training course for VITESS 3 has begun. It will take place 18 – 20 Sep 2013 and will be a joint course for McStas and VITESS.
The handbook will be written in summer and autumn 2013; the concept is developed and the tasks are distributed. The help files are improved continuously and nearly finished.

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	0.8	1.0
D. Nekrassov	HZB	0.8	1.5
C. Zendler	HZB	0.8	1.5

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	1.5	0.0
Fluid capital	HZB	10.2	12.6

2.1.4   Risks

(Update when needed)

2.1.5   Collaborations/Partners

(Update when needed)

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)