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K7 – 2013 Q1 Work Package Report

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DOCUMENT REVISION HISTORY

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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 indispensable 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 VITESS version 3.1 (D.K.7.2.4). Most changes are included: parallelization, numerical optimization, extension of visualization, new and improved modules (e.g. detector, reflectometer sample, monitors, i/o of trajectories), and improvements in GUI and moderator characteristics. Testing has started; the release is planned for May 2013.

A publication about the effect of gravity on a neutron beam transported in elliptic guides (D.K.7.1.7) has been written. The results will be presented on NOP&D in July.

The comparison of brilliances (D.K.7.1.6) has been continued. Most ISIS moderators are now correctly described and McStas and VITESS output are in agreement. Two moderators still need to be checked.

D.K.7.1.6 Brilliance comparison of different neutron sources

The comparison of the brilliance of the ISIS sources in McStas and VITESS was continued. The reason for the discrepancies could be identified: the normalization to frequencies and proton current. Now both packages use correct normalization to the frequencies and the proton current used today. Now there is good agreement for most of the sources, both for the peak brilliance and the average brilliance. A document called *Minutes_SourceBrightnessMeeting-3* containing a description of the corrections and the new simulation results has been written and sent to Ken Andersen.

For two moderators – methane at TS1 and 'groove' at TS2 – it still has to be clarified if the description in the packages is correct. This and a comparison of the SNS source will be done in the next quarter.

D.K.7.1.7 Gravity effect on guide performance

The work on this subject is nearly finished. The results will be presented on the NOP&D workshop in Ismaning and published in the proceedings of this conference. A publication is already written.

As expected, the effect of gravity on a beam transported by an elliptical guide is only small for short wavelengths. But for long wavelengths it is very pronounced (see Fig. 1). But also for long wavelengths it can be avoided by choosing a proper ratio of source size to guide entrance size, i.e. having a size of the source at least something like 50% larger than the guide entrance size (see Fig. 1) – independent of the distance between guide and source.

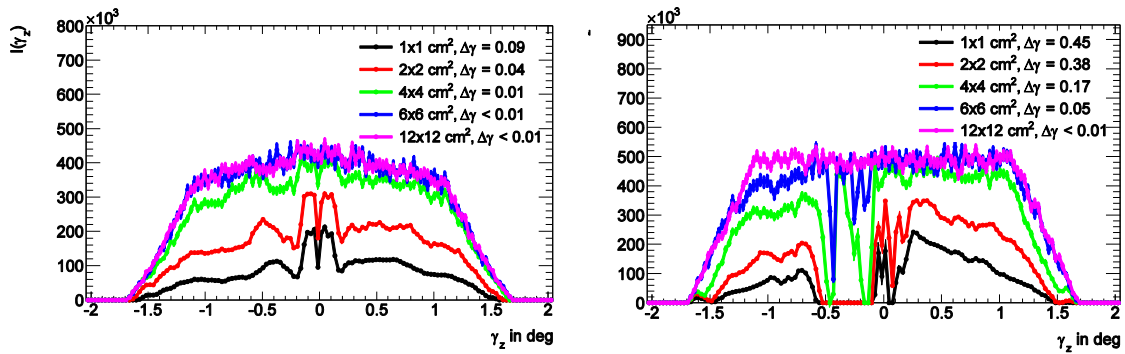


Fig. 1: Vertical divergence distribution at sample position for 1 m distance from source to guide and from guide to sample, a guide entrance and exit of 4.9 cm.

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

Most of the work for version 3.1 is finished, testing has started. The main new features in version 3.1 will be the optimization and a new way of parallelization and the extension of the visualization. It also includes some of the improvements of the detector module, which were foreseen for version 3.2, new (filter, reading of events) and improved modules (reflectometer sample, monitors, writing of events), improved GUI, new tool (to generate extraction systems) and new or improved moderator characteristics.

Optimization and Parallelization will be discussed here, the rest in the next report:

Figure 2 shows the principle of the optimization. In contrast to preliminary version, the optimization routine is the main program now and the simulation is called as a subroutine. Two gradient methods and a Metropolis algorithm can be used in this first version, others will follow.

The handling is quite easy; it is described in detail in a pdf file. In many cases, it can be used by just editing three ASCII control files: *opt_param.ini*, *sim_param.ini* and *fom.ini*. Advanced users might additionally change the control file for the algorithm in use.

The figure of merit can varied in a wide range from transmission to intensity times wavelength to the power of n by varying *fom.ini*. This should cover most applications; for more advanced figures-of-merit, the user can write a program of his own.

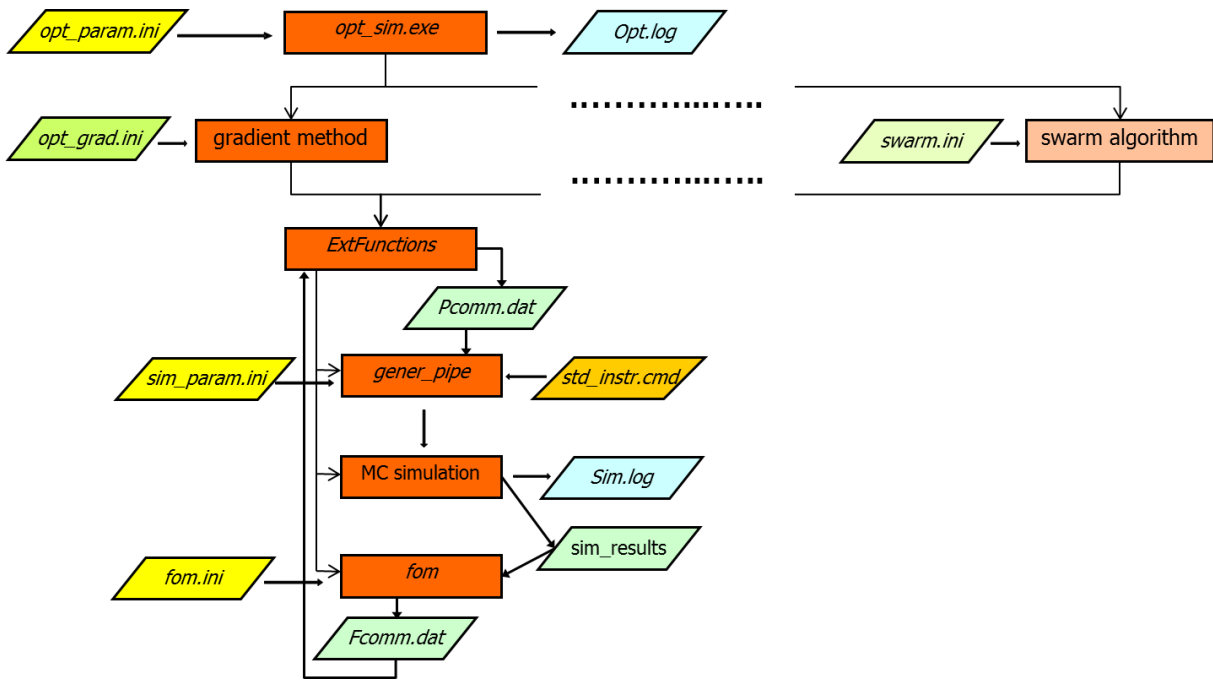


Fig. 2: Scheme of the algorithm for numerical optimization in VITESS

Figure 3 shows the principle of the new parallelization strategy: the whole simulation is split into several individual jobs that are sent to different computers on the cluster. The individual output files are then combined to give one output file for the whole simulation.

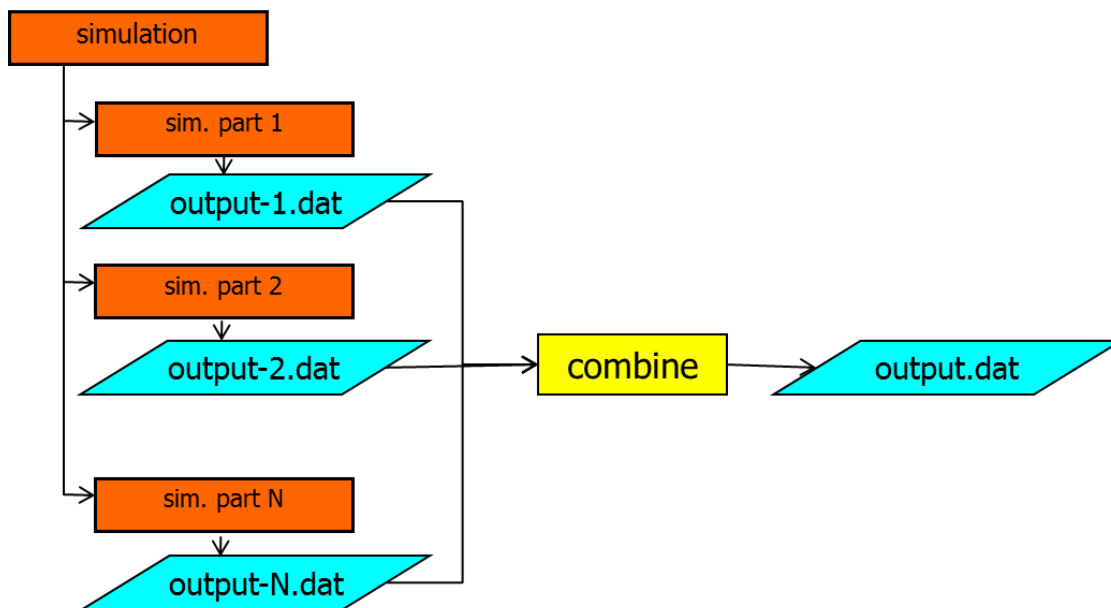


Fig. 3: Scheme of the parallelization in VITESS

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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	75	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	90	
D.K.7.2.5	20	
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	90	
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 is written. The brilliance comparison will hopefully be finished in the second quarter of 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 second 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 will be released in May 2013 and 3.2 in November 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 and for general features like visualization.

A training course for VITESS 3 is now foreseen for September 2013; it is planned as joint course for McStas and VITESS. Organization will start in May.

The handbook will be in summer 2013; the concept is developed and the tasks are distributed. The help files are improved continuously.

Generally the project is on schedule.

2.1.3 Costs / Resources

Resources:														
Task	Staff					Expenditure					Investment			
	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	0.6
D. Nekrassov	HZB	0.8	0.7
C. Zender	HZB	0.8	0.7

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	1.9

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)