Work package number [9]	WP8	Lead beneficiary [10]	13 - DTU
Work package title	Instrumentation – e-tools		
Start month	1	End month	48

Objectives

The ground-breaking developments of E-science have strongly influenced the way the neutron community sees not only data treatment and interpretation but also the interplay between science and instrumentation. Simulation tools help to plan and optimise neutron sources of the present and future (neutronics), design complete instruments and simulate experiments. This instrumentation task embraces several, distinct e-science related activities to provide an integrated approach to neutron instrumentation by incorporating neutronics and thus enable optimisation of instruments from the source to the sample and the detector, including the background signal (i.e. noise). The goal is to combine the world-leading, European expertise in this field and enable the elaboration of qualitatively new approaches and new developments leading to innovation. The work comprises three tasks:
(1) E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing
(2) Innovative Shielding Concepts and Materials, and
(3) Compact Instrumentation for Larmor Labelling applications at the ESS.

Description of work and role of partners

WP8 - Instrumentation – e-tools [Months: 1-48]
DTU, ESS, STFC, PSI, TUM, TU Delft, NPI, ESS-B, MTA EK
Task 8.1. E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing.
Coordinator: DTU, Partners: PSI, NPI, ESS-B, MTA EK, Observers: ISIS, ILL, UCPH, ESS, SNS (US)
This task will develop and assess new e-science tools for very accurate simulation of neutron beam-lines. The activity brings together experts from both (a) neutronics, e.g. MCNP used for simulating production and transport of neutrons from the target through moderators and reflectors and (b) Monte Carlo ray-tracing, e.g. McStas and RESTRAX, which simulate the transport of neutrons along guides and their interaction with other optical elements and samples. The combination of these two types of code will give a unique tool for optimising instruments and experiments from the source to the sample, including shielding and thus background optimisation. This will increase the realism of neutron simulation to a completely new level, since also unwanted spurious scattering signals are modelled, thereby addressing the signal-to-background ratio of instruments for the first time. Based on existing prototypes, the collaboration aims to deliver an easier-to-use and benchmarked solution, as well as establish networking and knowledge sharing between the partners and facilities.
The efforts will be based on existing know-how within neutronics (ISIS, PSI, DTU, ESS-B) and Monte Carlo ray-tracing (DTU, ILL, NPI, UCPH). Main target areas of development, where prototypes exist, are:
• The DTU-PSI initiated MCNP-McStas interface
• The NPI code RESTRAX/SIMRES has very efficient instrument optimization for instrument design
• The ISIS initiated CombLayer, which allows automation and optimization of neutronics simulation
• Further, experience in a similar simulation strategy (using Vitess and MCNP) exists at MTA EK, however this is not implemented in actual code.
A central collaboration strategy will be ensured by a series of workshops and online meetings. The first of these workshops will be "Requirements/Development for a reverse Monte Carlo variance reduction method applied to neutron beamline transport systems" – aimed at discussing how variance reduction schemes as implemented in CombLayer and RESTRAX can benefit other codes. Further, the collaboration aims to share code and know-how wherever possible, e.g. component models between RESTRAX and McStas. The developed software will be benchmarked both between codes with similar features (e.g. McStas and RESTRAX), but importantly also experimentally at existing experimental facilities (ISIS, PSI). In addition, the collaboration will evaluate the signal-to-background ratio for two selected ESS instrument designs.
Manpower will be concentrated at DTU, the main development hub of the McStas simulation code, in the form of a Post-Doc who will work both with the McStas team, the consortium behind the existing MCNP-McStas coupling prototype, RESTRAX and CombLayer as well as the rest of the consortium partners to provide the deliverables. Task 8.1 will share know-how and information with Task 8.2 that addresses other issues related to the instrument performance and background, ESS-Bilbao being involved in both tasks will ensure their coherence.
The software developed in Task 8.1 will be made available to for e-Learning in WP3 as early as possible. We will also liaise closely with WP7 “Sample Environment" because of the common emphasis on signal-and-background, with a

view to complete integration of software components. In addition, the newly integrated e-tools will be highly beneficial for WP9 in accurately estimating the signal-to-background threshold for detector performance.

Overview of responsibilities:
• DTU: Central code development, MCNP-McStas, McStas, simulations (12 PM)
• PSI: Simulations, experimental campaign (w. Task 2, 6 PM)
• NPI: RESTRAX, McStas, simulations (6 PM)
• ESS-B: simulations, connection with Task 2 (6 PM)
• MTA EK: Application of Vitess+MCNP for comparison (6 PM)
• ISIS: Observer, CombLayer, workshop(s)
• ILL: Observer, optimised scattering kernels, McStas, iFit
• UCPH: Observer, McStas
• ESS: Observer, future end-user of developed software
• SNS: Observer, future end-user of developed software

Task 8.2. Innovative Shielding Concepts and Materials.
Coordinator: PSI, Partners: ESS, ISIS, ESS-B, TUM, MTA EK, DTU Observer: SNS
The task will enhance our understanding of high-energy neutron background, and optimise biological shielding through the development of new materials. The activity combines detailed, fast neutron background measurements at PSI and ISIS, which will be carried out using procedures common in the high-energy physics community and confronted with simulations. This work will lead to better neutron instrument design with lower fast neutron background. The development of new shielding materials will also reduce the costs of neutron instruments since, nowadays, shielding constitutes an important fraction of an instrument budget. The new concepts will be tested at PSI on the BOA beamline, and at ISIS on the ChipIR beamline, before being more widely deployed.
Task 8.2 will use and augment e-tools developed in Task 8.1. ESS-Bilbao is involved in both tasks and will ensure coherence.
Overview of responsibilities:
• PSI: Measurements, simulations & prototypes (9 PM)
• ESS: Measurements, simulations & prototypes (9 PM)
• ISIS: Measurements & simulations (3 PM)
• ESS-Bilbao: Simulations for concrete compositions & laminate shielding design (supporting PSI activities, 6 PM)
• TUM: Measurements; 2-3 measurement series at FRM-2 (3 PM)
• MTA EK: Measurements; 2-3 measurement series at Budapest reactor (6 PM)
• DTU: Simulations for laminate shielding design (supporting ESS-Lund activities, 9 PM)
• SNS: Observer, future end-user of developed shielding concepts

Task 8.3. Compact Instrumentation for Larmor Labelling applications at the ESS.
Coordinator: TUD, Partners: ISIS, MTA EK, ESS, Observer: DTU
Larmor labelling is widely used to increase the resolution of neutron scattering both in energy (e.g. neutron spin echo spectroscopy) and momentum transfer (Spin Echo SANS, Larmor diffraction). Since these techniques are well-suited to poorly monochromatized and collimated neutron beams they potentially offer high resolution without sacrificing too much flux. However, most existing instruments are long, due to homogeneity requirements for the precession areas, and this in fact collimates the beam and significantly reduces the effective neutron count rate. This task therefore aims to investigate the implementation of new magnetic field configurations, e.g. triangular coils, which should lead to compact Spin Echo SANS and Larmor diffraction instruments and therefore high brilliance combined with high performance. New instrument designs for both monochromatic and wide-band (time-of-flight) operation will result. This development will be of particular relevance to the ESS, where the proposed flat (pancake) moderator design will result in high intensity, small cross-section neutron beams that are well-adapted to small samples and compact instruments.
Manpower will be concentrated at TU Delft in the form of a Post-Doc. Based on the well-known Spin-Echo competences in Delft, the Post-Doc will work with partners from the existing ISIS and MTA EK facilities, the future ESS facility and an observer from the McStas instrument simulation project to produce the deliverables. An essential component of this feasibility study is the input from tasks 8.1 and 8.2 on instrument signal-to-background: high-performance neutron optics and efficient non-magnetic shielding is a critical requirement for any Larmor-based instrument.
Overview of responsibilities:
• TUD: Spin-Echo expertise, simulations, experiments using existing hardware (12 PM)
• ISIS: Know-how from experiments at existing facility
• MTA EK: Know-how from experiments at existing facility, Spin-Echo expertise
• ESS: Specification of future requirements for ESS
• DTU: Observer, simulation “back-office”

Participation per Partner

Partner number and short name	WP8 effort
2 - ESS	9.00
3 - STFC	3.00
4 - PSI	15.00
5 - TUM	3.00
8 - TU Delft	12.00
13 - DTU	21.00
14 - NPI	6.00
15 - ESS-B	12.00
16 - MTA EK	6.00
Total	87.00

List of deliverables

Deliverable Number [14]	Deliverable Title	Lead beneficiary	Type [15]	Dissemination level [16]	Due Date (in months) [17]
D8.1	Evaluation of detectors for fast neutron and gamma spectroscopy	4 - PSI	Report	Public	9
D8.2	Improved code interface	13 - DTU	Other	Public	12
D8.3	Computational tests (multiple platforms)	15 - ESS-B	Report	Public	18
D8.4	Experimental test A - “BOA@PSI”& Experimental test B - “ChipIR@ISIS”	4 - PSI	Report	Public	18
D8.5	Simulating laminate shielding concepts	15 - ESS-B	Report	Public	18
D8.6	Evaluation of material compositions & Developing special heavy concretes for fast neutron shielding	4 - PSI	Report	Public	24

List of deliverables

Deliverable Number [14]	Deliverable Title	Lead beneficiary	Type [15]	Dissemination level [16]	Due Date (in months) [17]
D8.7	Analytical calculation of magnetic field configurations for compact Larmor schemes for ESS instruments/ Evaluation of implications on the design of both inelastic and static neutron scattering generic instrumentation	8 - TU Delft	Report	Public	24
D8.8	Port of selected scattering kernel code from McStas to RESTRAX	13 - DTU	Other	Public	24
D8.9	Improved description of materials for high-energy neutron transport codes	1 - ILL	Websites, patents filling, etc.	Public	24
D8.10	Several background measurement series at different facilities in Europe	4 - PSI	Report	Public	24
D8.11	Improved user interface	13 - DTU	Other	Public	36
D8.12	Software documentation and report on combined RESTRAX + McStas simulations	14 - NPI	Report	Public	36
D8.13	Optimization study of a selected instrument using CombLayer and McStas-MCNPX	13 - DTU	Report	Public	36
D8.14	Investigation of effective shielding concepts for high energy particles	4 - PSI	Report	Public	36
D8.15	Recommendations for ESS instruments	8 - TU Delft	Report	Public	36

List of deliverables

Deliverable Number [14]	Deliverable Title	Lead beneficiary	Type [15]	Dissemination level [16]	Due Date (in months) [17]
D8.16	Activation studies, radiation resistance	16 - MTA EK	Report	Public	36
D8.17	Investigation of different test samples	3 - STFC	Report	Public	42
D8.18	Comparative Vitess+MCNP simulations	16 - MTA EK	Report	Public	46
D8.19	Validation of the measurements by Monte Carlo Simulations	15 - ESS-B	Report	Public	48
D8.20	Final release of all software	13 - DTU	Other	Public	48

Description of deliverables

Task 8.1: E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing 8.2 Improved code interface, pre-release (M12) 8.3 Computational tests (multiple platforms) (M18) 8.4 Experimental test A - “BOA@PSI”& Experimental test B - “ChipIR@ISIS”, with T8.2 (M18) 8.8 Port of selected scattering kernel code from McStas to RESTRAX (M24) 8.9 Improved description of materials for high-energy neutron transport codes (H2O, D2, H2) (M24) 8.11 Improved user interface, investigate possibilities for inclusion of RESTRAX and/or Geant4 (M36) 8.12 Software documentation and report on combined RESTRAX + McStas simulations (M36) 8.13 Optimization study of a selected, either existing or close-to-completed instrument (e.g. at ISIS or PSI) using CombLayer and McStas-MCNPX (M36) 8.18 Comparative Vitess+MCNP simulations (M46) Task 8.2: Innovative Shielding Concepts and Materials 8.1 Evaluation of detectors for fast neutron and gamma spectroscopy – mainly for background measurements (M9) 8.5 Simulating laminate shielding concepts (M18) 8.6 Evaluation of material compositions & Developing special heavy concretes for fast neutron shielding (draft in M12, final version M24) (M24) 8.10 Several background measurement series at different facilities in Europe (PSI, ISIS, TUM) scattering generic instrumentation (M24) 8.14 Investigation of effective shielding concepts for high energy particles (M36) 8.17 Investigation of different test samples at ISIS and/or PSI and/or FRM II and/or BRR (M42) 8.19 Validation of the measurements by Monte Carlo Simulations (min. two different MC codes), collaboration with T8.1 (M48) 8.20 Final release of all software (M48) 8.16 Activation studies, radiation resistance (M36) Task 8.3: Compact Instrumentation for Larmor Labelling applications at the ESS 8.7 Analytical calculation of magnetic field configurations for compact Larmor schemes for ESS instruments/ Evaluation of implications on the design of both inelastic and static neutron scattering generic instrumentation (draft in M12, final version M24) (M24) 8.15 Recommendations for ESS instruments, possibly also with the help of simulations (M36)

D8.1 : Evaluation of detectors for fast neutron and gamma spectroscopy [9]

Evaluation of detectors for fast neutron and gamma spectroscopy – mainly for background measurements (M9)

D8.2 : Improved code interface [12]

Improved code interface, pre-release (M12)

D8.3 : Computational tests (multiple platforms) [18]

Computational tests (multiple platforms) (M18)

D8.4 : Experimental test A - “BOA@PSI”& Experimental test B - “ChipIR@ISIS” [18]

Experimental test A - “BOA@PSI”& Experimental test B - “ChipIR@ISIS”, with T8.2 (M18)

D8.5 : Simulating laminate shielding concepts [18]

Simulating laminate shielding concepts (M18)

D8.6 : Evaluation of material compositions & Developing special heavy concretes for fast neutron shielding [24]

Evaluation of material compositions & Developing special heavy concretes for fast neutron shielding (draft in M12, final version M24) (M24)

D8.7 : Analytical calculation of magnetic field configurations for compact Larmor schemes for ESS instruments/ Evaluation of implications on the design of both inelastic and static neutron scattering generic instrumentation [24]

Analytical calculation of magnetic field configurations for compact Larmor schemes for ESS instruments/ Evaluation of implications on the design of both inelastic and static neutron scattering generic instrumentation (draft in M12, final version M24) (M24)

D8.8 : Port of selected scattering kernel code from McStas to RESTRAX [24]

Port of selected scattering kernel code from McStas to RESTRAX (M24)

D8.9 : Improved description of materials for high-energy neutron transport codes [24]

Improved description of materials for high-energy neutron transport codes (H2O, D2, H2) (M24)

D8.10 : Several background measurement series at different facilities in Europe [24]

Several background measurement series at different facilities in Europe (PSI, ISIS, TUM) scattering generic instrumentation (M24)

D8.11 : Improved user interface [36]

Improved user interface, investigate possibilities for inclusion of RESTRAX and/or Geant4 (M36)

D8.12 : Software documentation and report on combined RESTRAX + McStas simulations [36]

Software documentation and report on combined RESTRAX + McStas simulations (M36)

D8.13 : Optimization study of a selected instrument using CombLayer and McStas-MCNPX [36]

Optimization study of a selected, either existing or close-to-completed instrument (e.g. at ISIS or PSI) using CombLayer and McStas-MCNPX (M36)

D8.14 : Investigation of effective shielding concepts for high energy particles [36]

Investigation of effective shielding concepts for high energy particles (M36)

D8.15 : Recommendations for ESS instruments [36]

Recommendations for ESS instruments, possibly also with the help of simulations (M36)

D8.16 : Activation studies, radiation resistance [36]

Activation studies, radiation resistance (M36)

D8.17 : Investigation of different test samples [42]

Investigation of different test samples at ISIS and/or PSI and/or FRM II and/or BRR (M42)

D8.18 : Comparative Vitess+MCNP simulations [46]

Comparative Vitess+MCNP simulations (M46)

D8.19 : Validation of the measurements by Monte Carlo Simulations [48]

Validation of the measurements by Monte Carlo Simulations (min. two different MC codes), collaboration with T8.1 (M48)

D8.20 : Final release of all software [48]

Final release of all software (M48)

Schedule of relevant Milestones

Milestone number [18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
MS2	Workshop: "Requirements/ Development for a reverse Monte Carlo	13 - DTU	9	The workshop is aimed at discussing how variance reduction schemes as implemented

Schedule of relevant Milestones

Milestone number [18]	Milestone title	Lead beneficiary	Due Date (in months)	Means of verification
	variance reduction method applied to neutron beamline transport systems"			in CombLayer and RESTRAX can benefit other codes.
MS3	Prerelease, advanced guide for McStas-MCNPX	13 - DTU	12	Software prototype released to community, relating to Task 8.1, D8.3.
MS4	Completion of validation campaign	13 - DTU	24	Reports on experimental and computational tests, relating to T8.1+2, D8.4, D8.5.
MS5	Workshop on Larmor concepts for ESS	13 - DTU	36	Months 36 to 48
MS6	Workshop on use of the developed integrated e-Tools for instrument simulation	13 - DTU	46	Related to T8.1.