**Work package description for Networking activity or Joint research activity**

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| **Work package number 8a** |  | | **Start date or starting event:** | | | | |  | | | | |
| **Work package title** | **Instrumentation** and Detectors | | | | | | | | | | | |
| **Activity Type[[1]](#footnote-1)** | RTD (elements of COORD) | | | | | | | | | | | |
| **Participant number** |  |  | |  |  |  |  | |  |  |  |  |
| **Participant short name** | DTU | ESS | | ILL | PSI | UoC | STFC | | TUD | NPI | TUM | ESS-B |
| **Person-months per participant:** | 21 | 11 | | obs | 15 | obs | 5 | | 12 | 6 | 3 | 12 |

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| **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 optimize an experiment, to design a whole instrument and finally plan the neutron sources of the future such as the ESS. This instrumentation task embraces several e-science related activities that allow an integrated approach to neutron instrumentation by incorporating neutronics and thus being able to optimise instruments from the source to the sample and the detector. The goal is to combine the world leading European expertise in this field and by fully exploiting this human potential to 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.** |

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| **Description of work** (possibly broken down into tasks), and role of participants  **All partners: Common travel funds, workshop costs: 60 K€ at DTU**  **Task 1. E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing.**  The task is an activity to develop and assess new e-science tools for very accurate simulation on neutron beam-lines. The activity brings together experts from both (a) neutronics, e.g. MCNP[[2]](#footnote-2) used for simulating production and transport of neutrons from the target through moderator reflector and (b) Monte Carlo ray-tracing, e.g. McStas[[3]](#footnote-3), RESTRAX[[4]](#footnote-4) which simulate the transport of neutrons through guides and their interaction with instruments and samples. The combination of these two types of code shall 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 for the first time addressing the signal-to-noise ratio of neutron scattering instruments.  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 knowhow within neutronics (ISIS, PSI, DTU, ESS-BilBao) and Monte Carlo ray-tracing (DTU, ILL, NPI, UoC). Two main target areas of development are these, where prototypes exist:   * The DTU-PSI initiated MCNP-McStas interface * The NPI code RESTRAX/SIMRES has very efficient instrument optimization for instrument design * The ISIS initiated CombLayer[[5]](#footnote-5), which allows automation and optimization of neutronics simulation   A central collaboration strategy will be a series of workshops and online meetings. The suggested title for the first of these workshops is "*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 knowhow 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). Further, the collaboration will evaluate signal to noise for two selected ESS instrument designs.  The main manpower will be concentrated at DTU, where the aim is to recruit new workforce (e.g. a Post Doc). Being the main development hub of the McStas simulation code, the Post Doc 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 meet the central deliverables.  Task 1 will share knowhow and information with Task 2 that addresses other issues related to the instrument performance and background. A central point here is that ESS-Bilbao will be responsible of supportive simulation activities within both Task 1 and 2.  The developed software from Task 1 will be made available to the WP5 “Data” RTD and the WP3 e-Learning COORD as early as possible, for potential inclusion in the WP5-developed data-analysis pipelines and the WP3-developed e-Learning solution.  Overview of responsibilities:   * DTU: Central code development, MCNP-McStas, McStas, simulations * PSI: Simulations, experimental campaign (w. Task 2) * NPI: RESTRAX, McStas, simulations * ESS-Bilbao: simulations, connection with Task 2 * ISIS: Observer, CombLayer, workshop(s) * ILL: Observer, optimised scattering kernels, McStas, iFit * UoC: Observer, McStas * ESS: Observer, future end-user of developed software   **Needed resources:**  DTU: 12 PM Contact: Peter Kjær Willendrup (PI)  PSI: 6 PM Contact: Emmanouela Rantsiou  NPI: 6 PM Contact: Jan Saroun  ESS-Bilbao: 6 PM Contact: Jesus Pedro de Vicente  ISIS: Observer: Contact: Chris Frost, Stuart Ansell  ESS: Observer: Phil Bentley, Luca Zanini  ILL: Observer: Emmanuel Farhi  UoC: Observer: Kim Lefmann  **Task 2. Innovative Shielding Concepts and Materials.**  The task proposes to enhance our understanding on 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 which will be confronted with simulations. This work will lead to better neutron instrument design with lower fast neutron background. The development of new shielding materials shall also reduce the costs of neutron instruments, because nowadays shielding is an important fraction of the instrument budgets. The new concepts will be tested at PSI on the BOA beamline, and at ISIS on the ChipIR beamline, before deployment in the field.  Task 2 will share knowhow and information with Task 1 that addresses other issues related to the instrumental background and performance. A central point here is that ESS-Bilbao will be responsible of supportive simulation activities within both Task 1 and 2.  Overview of responsibilities:   * PSI: Measurements & simulations & prototypes * ESS-Lund: Measurements & simulations & prototypes * ISIS: Measurements & simulations * ESS-Bilbao: Simulations for concrete compositions & laminate shielding design (supporting PSI activities) * TUM: Measurements; 2-3 measurement series at FRM-2 * DTU: Simulations for laminate shielding design (supporting ESS-Lund activities)   !! Optionally include Swiss and Danish concrete-company expertise here at observer level !!  **Needed resources:**  PSI: 9 PM Contact: Uwe Filges (PI)  ESS: 9 PM Contact: Philip Bentley  DTU: 9 PM Contact: Esben Klinkby  ESS-Bilbao: 6 PM Contact: Fernando Sordo  ISIS: 3 PM Contact: Chris Frost, Goran Skoro  TUM: 3 PM Contact: Peter Böni.  **Task 3. Compact Instrumentation for Larmor Labelling applications at the ESS.**  **Partners: TUD, ISIS, ESS.**  Larmor labelling is nowadays widely used to increase the resolution of neutron scattering both in energy (neutron spin echo spectroscopy) and momentum transfer (Spin Echo SANS, Larmor diffraction). These techniques can reach very high resolutions even with poorly monochromatized and collimated neutron beams. However, most existing instruments are long, due to homogeneity requirements for the precession areas, and this in fact collimates the beam and consequently dramatically reduces the neutron brilliance and data acquisition rates. This task addresses this issue and aims to investigate the implementation of new magnetic field configurations, eg triangular coils, which may lead to compact Spin Echo SANS and Larmor diffraction instruments and will combine flexibility with high brilliance and high performance. The result will lead be a new instrument design for both monochromatic and TOF operation. This development will be of particular relevance to the ESS, where the proposed flat – pancake – moderator design will result in high intensity compact neutron beams best adapted to small samples and thus to compact instruments.  The main manpower will be concentrated at TU Delft, where the aim is to recruit new workforce (e.g. a Post Doc). Based on the well-known Spin-Echo competences in Delft, the Post Doc will work with partners from the existing ISIS facility, the future ESS facility and an observer from the McStas instrument simulation to meet the central deliverables.  Input from both Task 1 and 2 will be important in assessing the feasibility and performance of the developed solutions when used at ISIS as well as in the future at ESS.  Overview of responsibilities:   * TUD: Spin-Echo expertise, simulations, prototype, experiments * ISIS: Know-how from experiments at existing facility * ESS: Specification of future requirements for ESS * DTU: Observer, simulation “back-office”   !! Optionally include Dutch and Danish instrument development companies at observer level !!  **Needed resources:**  TUD: 12 PM Contact: Jeroen Plomp (PI)  ISIS: 2 PM Contact: Robert Dalgliesh  ESS: 2 PM Contact: Ken Andersen  DTU: Observer: Erik Knudsen |

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| **Deliverables** (brief description and month of delivery)  **Task 1: E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing**  Subtask 1: Facilitate Parallelism for McStas coupling subroutines – month 3  Subtask 2: Eliminate the need for user interaction with codes at each file exchange event( i.e. Fix the problematic issue with wrong N number transfered from mcstas to mcnp) – month 6  Subtask 3: Development of a well-thought, clever improved code interface – prerelease month 12  Figure out which list of software can be accomodated by such an interface (including tools for x-ray community). Figure out the needs/requests of each one of them, so that it is clear what needs to be included in the interface (the goal here is that a future version could accomodate the communication/file exchange between a more genral 'suite' of existing and widely used codes within the x-ray and neutron community)  what are the options/language/etc. Decide on look/functionalities/etc  Subtask 4: Computational Tests performed on a couple different platforms (avoid as much as possible compiler-specific and platform-specific problems) – month 18  Subtasks 5-6: 'Actual' tests: 2 full simulations of experimental set-ups. The BOA beamline should be one of them, as we have both a new updated MCNP model (up to the zapfen unit), and a new tested McStas instrument for the banker interior – month 18  Subtasks 7-8: Proceed with the interface (within the improved interface) of a different combination of softwares (e.g. proof-of-concept inclusion of GEANT4 and RESTRAX) – month 24  Subtask 9: Identify overlapping functionalities within partners and software – month 3  Subtask 10: Workshop “*Requirements/Development for a reverse Monte Carlo variance reduction method applied to neutron beamline transport systems*” Keywords: Variance reduction, optimizers, knowledge transfer between, RESTRAX, CombLayer, McStas/iFit – month 9  Subtask 11: Port of selected scattering kernel code from McStas to RESTRAX – month 36  Subtask 12: Release of McStas components based on RESTRAX code (e.g. monitors for ToF diffraction incl. time modulation) – month 12  Subtask 13: Release of RESTRAX/SIMRES program including binding with McStas –month 36  Subtask 14: SW documentation and report on combined RESTRAX + McStas simulations – month 36  Subtask 15: An initial look at how interoperability between CombLayer and McStas-MCNPX can be achieved – month 24  Subtask 16: Optimization study of selected, either existing or close-to-compleed instrument (e.g. at ISIS or PSI) using CombLayer and McStas-MCNPX – month 36  Subtask 17: Improved description of materials for high-energy neutron transport codes (e.g. water, D2, H2, ...). – month 24  Subtask 18: Workshop on use of the developed integrated e-Tools for instrument simulation – month 48  **Task 2: Innovative Shielding Concepts and Materials,**  Subtask 1: Evaluation of detectors  Subtask 1a Evaluation of detectors for fast neutron and gamma spectroscopy – mainly for background measurements  Subtask 1b: Evaluation of neutron dose rate meters for fast neutrons  subtask 1c: test measurements at different facilities  Milestone: after 9 months - report  Subtask 2: Several background measurement series at different facilities in Europe (PSI, ISIS, TUM)  Subtask 2a: Background measurements  Subtask 2b: Validation of the measured data with MC simulations  Milestone: after 18 months – 1st measurement report  Milestone: after 30 months – 1st validation report  Milestone: after 36 months – 2nd measurement report  Milestone: after 42 months – 2nd validation report  Milestone: after 48 months – final report  Subtask 3: Investigation of effective shielding concepts for high energy particles  Subtask 3a: Simulating laminate shielding concepts  Subtask 3b: Investigation of a test setup at ISIS and/or PSI  Subtask 3c: Validation of the measurements by Monte Carlo Simulations (at least with two different MC codes)  Milestone: after 24 months - status report  Milestone: after 30 months – laminate test setup  Milestone: after 48 months – final report  Subtask 4: Developing special heavy concretes for fast neutron shielding  Subtask 4a: Evaluation of possible compositions  Subtask 4b: Investigation of different test samples at ISIS and/or PSI and/or FRM-2  Subtask 4c: Validation of the measurements by Monte Carlo Simulations (at least with two different MC codes)  Milestone: after 24 months - status report  Milestone: after 30 months – measurement report about test samples  Milestone: after 48 months – final report  General milestone: after 24 months: Presentation & publication of the results  **Task 3: Compact Instrumentation for Larmor Labelling applications at the ESS.**  Subtask 1: Analytical calculation of magnetic field configurations for compact Larmor schemes for ESS instruments  Subtask 2: Evaluation of implications on the design of both inelastic and static neutron scattering generic instrumentation  Subtask 3: Recommendations for ESS instruments, possibly also with the help of simulations. |

**Table 3.1: List of Deliverables: (numbered WP.task.deliverable-no.subdel)**

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| **Deliverable (number)** | **Deliverable name** | **Work package number** | **Short name of lead participant** | **Type** | **Dissemination level** | **Delivery date** |
| 8.1.1 | Parallelism for McStas-MCNPX coupling | 8b | DTU | OTHER | PU | 3 |
| 8.1.2 | Streamlining McStas-MCNPX event transfer | 8b | DTU | OTHER | PU | 6 |
| 8.1.3 | Improved user interface, prerelease | 8b | DTU | OTHER | PU | 12 |
| 8.1.4 | Computational tests (multiple platforms) | 8b | ESS-Bilbao | R | DEM | 18 |
| 8.1.5 | Experimental test A - “BOA@PSI”, collaboration w task 2 | 8b | PSI | R | PU | 18 |
| 8.1.6 | Experimental test B - “ChipIR@ISIS” ”, collaboration w task 2 | 8b | ISIS | R | PU | 18 |
| 8.1.7 | Improved user interface, proof-of-concept inclusion of RESTRAX functionality | 8b | DTU | OTHER | PU | 24 |
| 8.1.8 | Improved interface, proof-of-concept inclusion of other high-energy transport, e.g. Geant4 | 8b | DTU | OTHER | PU | 24 |
| 8.1.9 | Identify overlapping functionalities within partners and software | 8b | ILL | R | PU | 3 |
| 8.1.10 | Workshop: "Requirements/Development for a reverse Monte Carlo variance reduction method applied to neutron beamline transport systems". Keywords: Variance reduction, optimizers, knowledge transfer between, RESTRAX, CombLayer, McStas/iFit | 8b | DTU/ISIS/ILL | DEC | PU | 9 |
| 8.1.11 | Port of selected scattering kernel code from McStas to RESTRAX | 8b | DTU/NPI | OTHER | PU | 36 |
| 8.1.12 | Release of McStas components based on RESTRAX code (e.g. monitors for ToF diffraction incl. time modulation) | 8b | NPI | OTHER | PU | 12 |
| 8.1.13 | Release of RESTRAX/SIMRES program including binding with McStas | 8b | NPI | OTHER | PU | 36 |
| 8.1.14 | SW documentation and report on combined RESTRAX + McStas simulations | 8b | NPI | R | PU | 36 |
| 8.1.15 | An initial look at how interoperability between CombLayer and McStas-MCNPX can be achieved | 8b | ISIS | OTHER | PU | 24 |
| 8.1.16 | Optimization study of selected, either existing or close-to-compleed instrument (e.g. at ISIS or PSI) using CombLayer and McStas-MCNPX | 8b | DTU/ISIS | R | PU | 36 |
| 8.1.17 | Improved description of materials for high-energy neutron transport codes (e.g. water, D2, H2, ...). | 8b | ILL | DEC | PU | 24 |
| 8.1.18 | Workshop on use of the developed integrated e-Tools for instrument simulation | 8b | DTU | OTHER | PU | 48 |
| 8.1.19 | Final release of all software | 8b | DTU | OTHER | PU | 48 |
| 8.2.1 | Evaluation of detectors for fast neutron and gamma spectroscopy – mainly for background measurements | 8b | PSI | R | PU | 9 |
| 8.2.1a | Evaluation of neutron dose rate meters for fast neutrons | 8b | - | - | - | 9 |
| 8.2.1b | Detector test measurements at different facilities (PSI, ISIS, TUM) | 8b | - | - | - | 9 |
| 8.2.2 | Several background measurement series at different facilities in Europe (PSI, ISIS, TUM) | 8b | PSI | R | PU |  |
| 8.2.2a | Background measurements | 8b | - | - | - |  |
| 8.2.2b | Validation of the measured data with MC simulations | 8b | ESS-Bilbao | OTHER,R | PU |  |
| 8.2.3 | Investigation of effective shielding concepts for high energy particles | 8b | PSI | R | PU |  |
| 8.2.3a | Simulating laminate shielding concepts | 8b | ESS-Bilbao | OTHER,R | PU |  |
| 8.2.3b | Investigation of a test setup at ISIS and/or PSI | 8b | ISIS/PSI | R | PU |  |
| 8.2.3c | Validation of the measurements by Monte Carlo Simulations (at least with two different MC codes), collab with task 1 | 8b | PSI | R | PU |  |
| 8.2.4 | Developing special heavy concretes for fast neutron shielding | 8b | PSI | R | PU |  |
| 8.2.4a | Evaluation of possible material compositions | 8b | PSI | R | PU |  |
| 8.2.4b | Investigation of different test samples at ISIS and/or PSI and/or FRM-2 | 8b | ISIS/PSI/TUM | R | PU |  |
| 8.2.4c | Validation of the measurements by Monte Carlo Simulations (at least with two different MC codes) | 8b | ESS-Bilbao | OTHER,R | PU |  |
| 8.3.1 | Analytical calculation of magnetic field configurations for compact Larmor schemes for ESS instruments | 8b | TU Delft | R | PU | 12 |
| 8.3.2 | Evaluation of implications on the design of both inelastic and static neutron scattering generic instrumentation | 8b | TU Delft | OTHER | PU | 24 |
| 8.3.3 | Recommendations for ESS instruments, possibly also with the help of simulations. | 8b | TU Delft | R | PU | 36 |

**KEY**

*Deliverable numbers in order of delivery dates. Please use the numbering convention <WP number>.<number of deliverable within that WP>.*

*For example, deliverable 4.2 would be the second deliverable from work package 4.*

**Type:**

*Use one of the following codes:*

R: Document, report (excluding the periodic and final reports)

DEM: Demonstrator, pilot, prototype, plan designs

DEC: Websites, patents filing, press & media actions, videos, etc.

OTHER: Software, technical diagram, etc.

**Dissemination level:**

*Use one of the following codes:*

PU = Public, fully open, e.g. web

CO = Confidential, restricted under conditions set out in Model Grant Agreement

CI = Classified, information as referred to in Commission Decision 2001/844/EC.

**Delivery date**

Measured in months from the project start date (month 1)

**Table 3.2a: List of milestones (task.milestone-no.)**

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| **Milestone number** | **Milestone name** | **Related work package(s)** | **Estimated date** | **Means of verification** |
| 1.1 | Basic upgrade of McStas-MCNPX interface | 8b.1.1-2 | Month 6 | A functional software prototype delivering subtasks 1.1 and 1.2 |
| 1.2 | Prerelease, advanced gui for McStas-MCNPX | 8b.1.3 | Month 12 | Software prototype released to community, relating to 1.3 |
| 1.3 | Completion of validation campaign | 8b.1.4-6 | Month 24 | Availability of reports on experimental and computational tests. |
| 1.4 | Inclusion of other codes | 8b.1.7-8 | Month 30 | Software prototype released to community, relating to 1.7-8 |
| 1.5 | Networking on optimization | 8b.1.9-10 | Month 9 | Workshop held |
| 1.6 | Simulation of complete instruments combining RESTRAX, McStas and MCNP | xxx | Month 36 | SW release with runnable virtual instruments and documentation |
| 1.7 | CombLayer features for use with McStas-MCNPX | 1.15-1.16 | Month 36 | Report on optimization study for ESS instruments using CombLayer and McStas-MCNPX |
| 1.8 | Improvement to neutronics-code description of material | 1.17 | Month 24 | Availability of new scattering kernels for MCNPX |
| 1.9 | Finalization of task 1 | 1.18-19 | Month 48 | Workshop held and software finalized |
| 2.1 | Report on detector evaluation | 2.1 | Month 9 | Report available |
| 2.2 | 1st measurement report on backgrounds | 2.2 | Month 18 | Report available |
| 2.3 | 1st validation report on backgrounds | 2.2 | Month 30 | Report available |
| 2.4 | 2nd measurement report on backgrounds | 2.2 | Month 36 | Report available |
| 2.5 | 2nd validation report on backgrounds | 2.2 | Month 42 | Report available |
| 2.6 | Final report | 2.2 | Month 48 | Report available |
| 2.7 | Status report | 2.3 | Month 24 | Report available |
| 2.8 | Laminate test setup | 2.3 | Month 30 | Test setup physically mounted |
| 2.9 | Final report | 2.3 | Month 48 | Report available |
| 2.10 | Status report on concretes | 2.4 | Month 24 | Report available |
| 2.11 | Measurement report on test samples | 2.4 | Month 30 | Report available |
| 2.12 | Final report | 2.4 | Month 48 | Report available |
| 2.13 | General milestone | 2.x | Month 34 | Presentations and publication of the results |
| 3.1 | Publication on Larmor concept for ESS instruments | 3.x | Month 24 | Publication submitted |
| 3.2 | Workshop on Larmor concepts for ESS | 3.x | Month 36-48, pending timeline of the ESS project | Workshop held |

**KEY**

**Estimated date**

*Measured in months from the project start date (month 1)*

**Means of verification**

*Show how you will confirm that the milestone has been attained. Refer to indicators if appropriate. For example: a laboratory prototype that is ‘up and running’; software released and validated by a user group; field survey complete and data quality validated.*

**Table 3.2b: Critical risks for implementation**

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| **Description of risk** | **Work package(s) involved** | **Proposed risk-mitigation measures** |
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1. Please indicate one activity per work package:

   MGT = Management of the consortium; COORD = Networking activity; RTD = Joint research activity. [↑](#footnote-ref-1)
2. MCNP = Monte-Carlo N-Particle, developed at Los Alamos National Lab <https://mcnp.lanl.gov> [↑](#footnote-ref-2)
3. McStas = generic Monte-Carlo ray-tracing code for neutron scattering instruments, <http://www.mcstas.org> [↑](#footnote-ref-3)
4. RESTRAX = Monte-Carlo ray-tracing code for neutron scattering instruments, <http://neutron.ujf.cas.cz/restrax/> [↑](#footnote-ref-4)
5. CombLayer is a modelling architecture for preparing MCNP input files for complex-geometry systems. [↑](#footnote-ref-5)