

**WP2 – Dissemination:** WP2 has documented all the achievements and progress made by the different WPs, using the project's internet platform (<http://www.sine2020.eu>). This platform went on-line in January 2016 and has received about 1000 visitors/month on average. It announces the periodic calls for industrial experiments, neutron schools, job offers, and other such events.

**WP3 – Training neutron scattering, e-learning and schools:** WP3 hosts and develops the specialized e-learning portal for neutron scattering and complimentary techniques, such as muon spin rotation. The portal registered 1400 visits by March 2017. WP3 has also launched two calls for support for introductory and advanced neutron schools in the first reporting period.

**WP4 - Industry Consultancy:** WP4 visited as many as 22 events in the first 18 months. Discussions with industrial researchers were constructive and have led to test experiments at some of the facilities. WP4 is assisted by an international industry advisory board; representatives from key technological and industrial sectors support its activities and decisions.

**WP5 – Deuteration.** The WP5 partners have successfully produced a wide variety of both routine and non-routine deuterated precursors and surfactants (STFC Deuteration facility), small deuterated molecules, precursors for the first target molecule lactic acid (D 5.4, DEULAB at ESS), and the commercially and technologically important isoprene (D5.3) and polyhexylthiophene (P3HT) polymers (D5.5, FZJ). The partnership has created the DEUNET platform coordinated by ESS, for networking, dissemination and outreach.

**WP6- Macromolecular crystallogenesi.** In WP6 the ILL has principally investigated the feasibility of designing and implementing automated robotic approaches for the growth of large macromolecular crystals. ILL is testing magnetic alignment in strong magnetic fields (17T). The ESS is investigating strategies for large crystal growth based on vapour-diffusion and dialysis, with temperature as a major parameter. FZJ has studied the crystallisation process with light scattering techniques, to understand the importance of the early phase of crystallisation for the later size of protein crystals.

**WP7 – Sample Environment.** The central task of WP7 has been the development of standards to facilitate communication between the instrument control workstation and sample environment equipment. ICMA has developed a simulation code to reduce parasitic background from sample environment devices; this has been successfully tested against real experiments. Several techniques to improve time efficiency have been implemented, such as remotely controlled goniometer heads inside dilution fridges (PSI) and reduced cooling times for furnaces (ISIS). Various designs for new pressure cells are on the way, including a piston cell for muon instruments with an expected 50% pressure increase.

**WP8 - Instrumentation – e-tools:** WP8 works to develop novel software tools by exploiting synergies among existing instrument- and neutron source simulation packages (MS2). Main Task 1 results for P2 in this area includes a report on an improved solution for supermirrors in MCNP (D8.3), a report from benchmarking experiments at BOA PSI (D8.4) and the release of improved material description for high-energy neutron transport (D8.9). A key activity for Task 2 is the development and assessment of novel materials for instrument shielding (D8.6). Finally for Task 3, we report on new concepts for Larmor labelling using compact instrument (D8.7).

**WP9 – Detectors:** As an example of the progress made by all the partners we can cite the work achieved at LIP, where two neutron-sensitive resistive plate chambers (RPCs) have been designed and constructed

(T9.4.1). The detector characteristics have been measured in collaboration with TUM; they show neutron detection efficiency of 12.5% at 4.7 Å and impressive spatial resolution better than 0.25 mm.

**WP 10 –Data Treatment:** The software requirements of all the facilities have been identified. They were presented at the General Assembly meeting in Portugal. Common guidelines (Task 10.2) have been established and were presented during *Workshop II* at ILL on 24 and 25 April, 2017 (D10.1).

Progress beyond the state of the art, expected results until the end of the project and potential impacts (including the socio-economic impact and the wider societal implications of the project so far)

*Update this section.*

The tasks of all work packages have **been** given clearly defined objectives, with an impact beyond the time horizon of the SINE2020 project. Whilst preparing and reinforcing the European community for the scientific opportunities to be **provided** by the ESS, this project also develops the potential of Europe's large-scale neutron facilities for innovation beyond 2020. The benefits of the technical improvements and training opportunities proposed will impact on the quality of the experiments and subsequent publications at the ESS and other large-scale neutron facilities in Europe. The commitment of all the partners to their tasks demonstrates the renewed and long-term **capacity for innovation inherent to the neutron sector** and its **capacity to adapt to today's societal challenges**:

- Different platforms (**e-neutron**, **DEUNET**) have been defined and deployed by the SINE2020 project. These platforms play an important role in terms of outreach and long-term availability of the results obtained through the cooperation of our partners.
- During the initial period, our Industry Consultancy group has elaborated a **strategy for addressing industrial partners**; it will present a **business model for industrial liaison** in due course (M46).
- we can cite a selection of technical tasks expected to lead into innovation: the use of deuterated, biologically relevant, unsaturated lipid membranes for investigations into the **functionality of cell membranes and membrane proteins**, providing avenues for research into **health and disease** (D5.9, D5.10), the synthesis of tailored polylactic acid polymers, to elucidate the properties of this **important biodegradable plastic with biomedical and technological applications** (D5.11), the development of neutron furnaces with cooling rates superior by a factor of 5, increasing sample through-put on the instruments and **reducing costly instrument down-time** caused by sample manipulation (D7.9, D7.22), the development of 700 bar hydrogen containers to measure hydrogen diffusion in metal-hydride-based materials, promising **more efficient materials for energy storage** (D7.11).
- SINE2020 has also been involved in the design and deployment of state-of-the-art software and virtual instruments for the community. This is seen as an important dimension of the programme, contributing to its influence on the experimental process and overall societal impact.

Please fill in your WP specific objectives, progress and impact

## 1. Explanation of the work carried out by the beneficiaries and Overview of the progress

*Explain the work carried out during the reporting period in line with the Annex 1 to the Grant Agreement.*

*Include an overview of the project results towards the objective of the action in line with the structure of the Annex 1 to the Grant Agreement including summary of deliverables and milestones, and a summary of exploitable results and an explanation about how they can/will be exploited<sup>1</sup>.*

*(No page limit per work package but report shall be concise and readable. Any duplication should be avoided).*

### 1.1 Objectives

*List the specific objectives for the project as described in section 1.1 of the DoA and described the work carried out during the reporting period towards the achievement of each listed objective. Provide clear and measurable details.*

#### **WP8 INSTRUMENTATION - E-TOOLS:**

The work of WP8 is three-fold and will further harvest synergies from between the development of

- Task 8.1 New software tools for simulating beamlines from source to detector including estimates of background. The software tools will receive validation input from Task 8.2.
- Task 8.2: Development of innovative shielding concepts and materials for future instruments. The developed concretes will be tested experimentally and performance estimated using the software tools developed in Task 8.1.
- Task 8.3: Development of compact Instrumentation for Larmor Labelling applications at the ESS. The task is developing future instrument concepts that will benefit from both the new simulation possibilities of Task 8.1 and the improved shielding of Task 8.3.

Further, an overall task for all partners is to publish and participate in networking and dissemination of the WP results whenever possible. In the last period, material developed in the WP has been presented at several workshops and meetings, e.g. the MDANSE school organized as a WP3 school event.

We expect to have at least one open, project-wide workshop during 2019 where we will present highlights from the work in all of the WP tasks. Also, 3-5 new publications are expected based on the work carried out in PR2.

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<sup>1</sup> Beneficiaries that have received Union funding, and that plan to exploit the results generated with such funding primarily in third countries not associated with Horizon 2020, should indicate how the Union funding will benefit Europe's overall competitiveness (reciprocity principle), as set out in the grant agreement.

## 1.2 Explanation of the work carried per WP

### 1.2.1 Work Package 8

*Explain the work carried out in WP1 during the reporting period giving details of the work carried out by each beneficiary involved.*

**Task 8.1: E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing** (*Responsible: DTU, Partners: PSI, ESS,NPI, ESS-Bilbao and MTA-EK*)

The task is developing software E-tools for *integrated simulation* using neutronics and Monte Carlo ray-tracing, i.e. will implement 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 (including high-energy neutrons and other particles) through moderators and reflectors and (b) Monte Carlo ray-tracing, e.g. McStas and RESTRAX, which in the range of cold and thermal neutrons can describe transport along guides and neutron interaction with other optical elements and samples.

The combination of these two types of code is necessary to allow optimising instruments and experiments from the source to the sample, including shielding. Including shielding allows estimating background, thereby increasing realism of instrument simulations – and for the first time express *instrumental signal to noise* by simulation techniques.

### **Deliverable 8.3 – Computational tests, multiple platforms** (*ESS-Bilbao, DTU*),

*The original thought behind the deliverable title of “Computational tests, multiple platforms” was to ensure basic platform portability of the developed McStas-MCNP interchange software (MCPL), see Deliverable report D8.2. During WP discussion it however became clear that the scope of work could be lifted to a higher level and we have therefore adjusted the scope of D8.3 to cover exciting new work on combined support for supermirrors and standard variance reduction techniques within the MCNP6 code:*

In this work ESS-Bilbao have spearheaded an evaluation of a patch for MCNP6<sup>2</sup> which allows to describe neutron optical devices such as guides. Further, ESS-Bilbao together with the PSI have developed enhancements to improve the statistics in the computationally difficult problem have been introduced, e.g. a deterministic mechanism for transporting reflected and transmitted neutron rays respectively. Also, the developed solution has been rigorously compared to legacy implementations. In the deliverable report (D8.3) it is shown how the resulting tool can be applied with standard Variance Reduction techniques such as the so-called *DXTRAN Sphere*<sup>3</sup> method, e.g. to the geometry of the future

<sup>2</sup> MCNP6: T. Goorley, M. James, T. Booth, F. Brown, J. Bull, L.J. Cox, J. Durkee, J. Elson, M. Fensin, R.A. Forster, J. Hendricks, H.G. Hughes, R. Johns, B. Kiedrowski, R. Martz, S. Mashnik, G. McKinney, D. Pelowitz, R. Prael, J. Sweezy, L. Waters, T. Wilcox, and T. Zukaitis, “Initial MCNP 6 Release Overview”, LA-UR-11-07082, Los Alamos National Laboratory, also Nuclear Technology, 180, pg 298-315 (Dec 2012).

<sup>3</sup> Dxtran is a deterministic transport method typically used for increasing the sampling in a spherical region that would otherwise not be adequately sampled because the probability of scattering toward the region is often very small. Essentially, the dxtran method splits the particle into two pieces at each source or collision point: a piece that arrives (without further collisions) at the dxtran sphere and a piece that does not.

MIRACLES backscattering spectrometer for the ESS. The results present breakthrough in shielding analysis for long guides, as integrated, one step shielding calculation is now feasible even for very long guides.

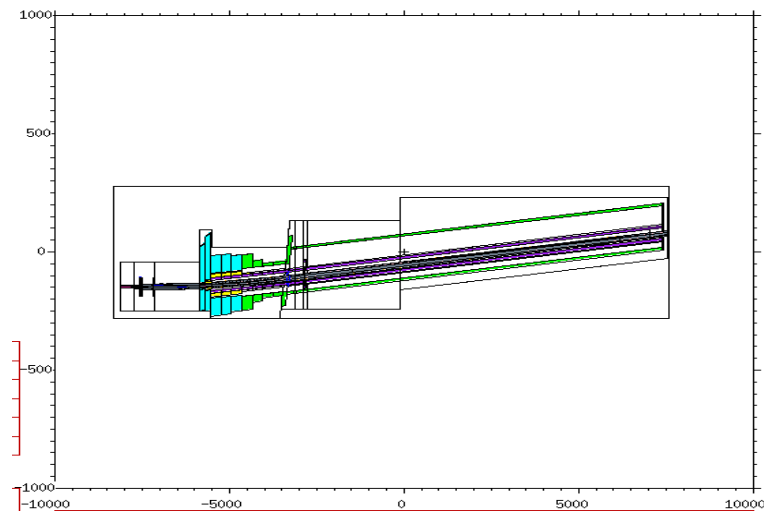


Figure: MCNP model for MIRACLES. Axes are in cm, and the X axis has been compressed by a factor of 10 for convenience.

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From: Monte Carlo Variance Reduction Using Nested Dxtran Spheres. Available from:

[https://www.researchgate.net/publication/283167788 Monte Carlo Variance Reduction Using Nested Dxtran Spheres](https://www.researchgate.net/publication/283167788_Monte_Carlo_Variance_Reduction_Using_Nested_Dxtran_Spheres)

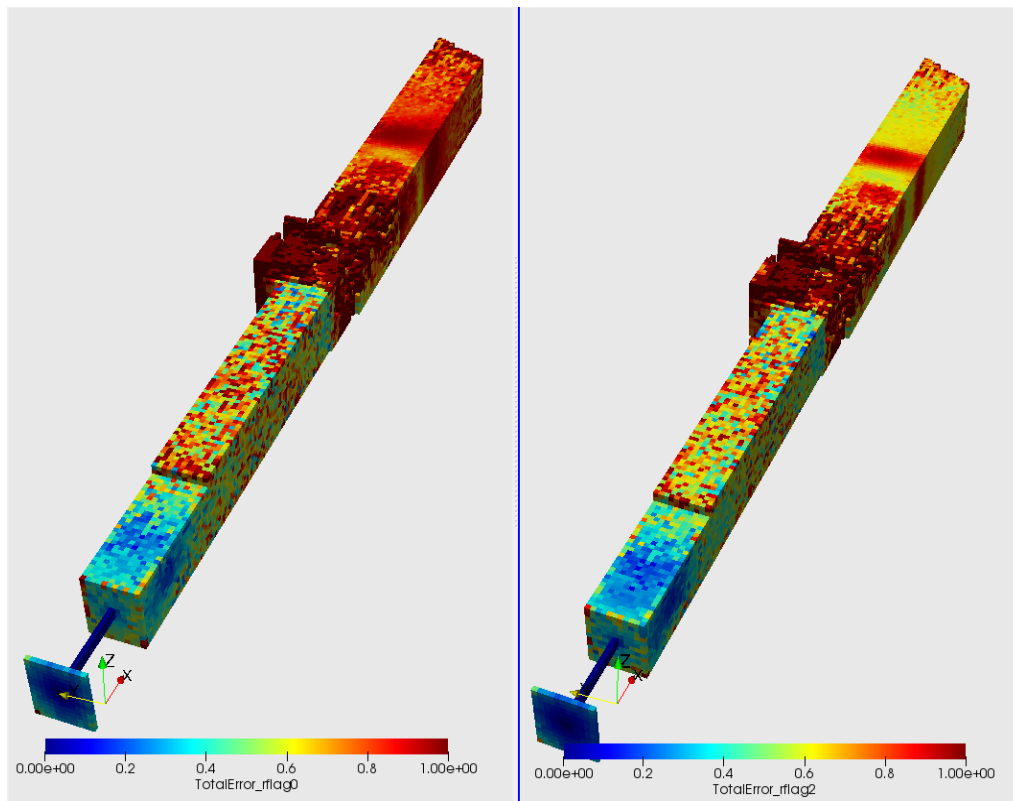


Figure: Comparison of default stochastic transport (left) Vs deterministic guide reflection (right) in the ESS MIRACLES geometry.

**Deliverable 8.4 – Experimental tests (DTU with PSI),**

For D8.4, two benchmark experiments were performed during back-to-back beamtimes at BOA (PSI) in August/2017. The first set of BOA measurements consisted in the investigation of neutron transport through a simplistic setup with direct, attenuated and beams reflected on a supermirror. Further, the measurements have been compared with simulated experiments in augmented versions of MCNP and McStas, as well as MCNP and McStas connected. The software additions and connections enable a qualitatively good agreement between simulation and experiment.

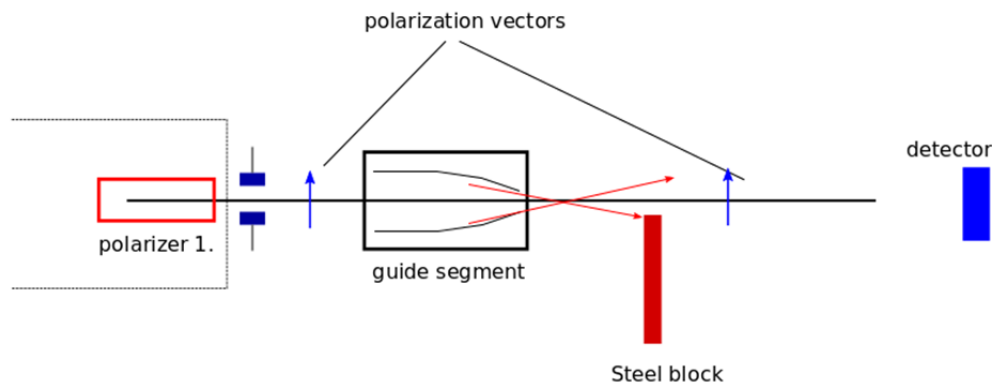


Figure: Sketch of a geometry utilized in the first experiment

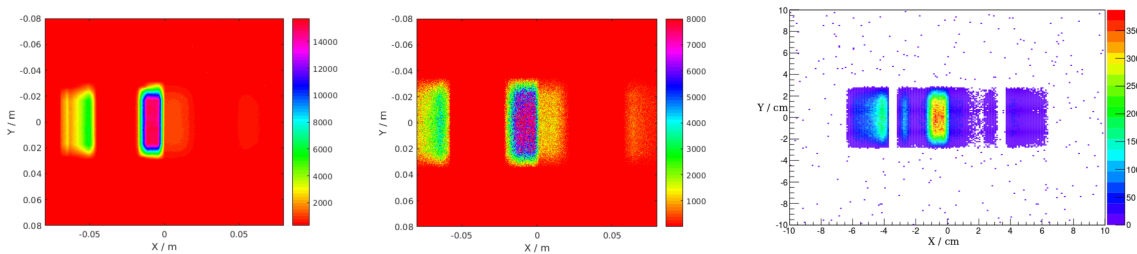


Figure: Left: Raw experimental detector image. The steel block is set to block appr. half of the direct beam. Detector in the "near" position, catching all 3 beam paths. Middle: Simulated beampaths in McStas. Right: Simulated beam paths in MCNP.

For the second experiment, a polarized neutron experiment at BOA (PSI) in August/2017 was performed. This experiment was a calibration measurement intended to provide a validation for the effect of partially polarized beams impinging on a polarization dependent supermirror(ref). This often-ignored situation has needed careful validation for several years. The early analysis of the data indicates that the data is useful and thus the experiment was a success.

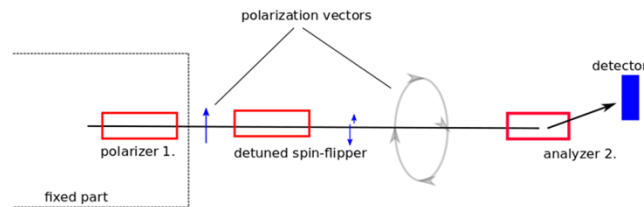


Figure: Sketch of the partial polarization experiment.

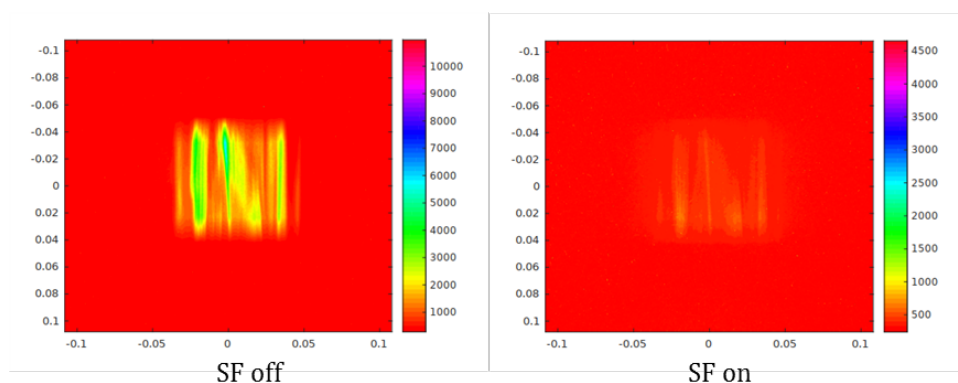


Figure: Experimental detector images. Left: spin flipper off. Right spin-flipper on. There are clear signs of structure coming from the analyzer blades.

### Deliverable 8.9 – Improved description of materials for high-energy neutron transport (ILL)

For D8.9, the ILL has developed a new algorithm-framework which allows to extract material physical quantities from experiments with improved accuracy by the coupling of the data treatment with molecular/atomistic and instrument modelling.

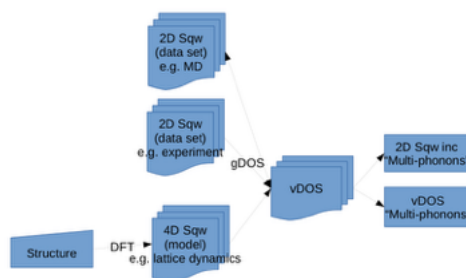


Figure: Illustration of how the so-called *generalized density of states* (vDOS) is centrally connected both to quantities that can be measured at facilities, and those that can be estimated using e.g. atomistic modelling.

Knowing a material to be used in nuclear facilities allows to measure and/or compute a number of physical quantities. The chemical formula (and space group) allows to compute the structure factor, which represents the spatial arrangement of atoms in space. In addition, that same information can be used to get an estimate of the density of states using a molecular/atomistic modelling. This information quantifies the typical vibrational energies of movements in the material, which are responsible for the moderation of neutrons.

The neutron scattering technique permits to measure the structure factor, using neutron diffraction, and the phonon spectrum, using inelastic spectrometers. However, as any measurement, data treatment must be carried out to extract the theoretical information, removing e.g. instrumental effects, including resolution, and additional contributions to the measured signal.

Existing methodologies date from 30 years ago, and thanks to progresses in computational physics, it is now feasible to extract the material physical quantities with improved accuracy by coupling the data



treatment with molecular/atomistic and instrument modelling. Then, it is expected to better estimate important data such as the neutron scattering cross section, especially in the low energy region ( $\omega < 100$  meV) which determines the spectral characteristics of the final moderation process events.

Since the release of the D8.6 report, the algorithm has been released through version 2.0 of the iFit software package<sup>4</sup>.

**Task 8.2: Innovative Shielding Concepts and Materials** (*Responsible: PSI, Partners: ESS, STFC, ESS-Bilbao, TUM, MTA-EK and DTU*)

The main focus of Task 8.2 in WP8 is the research into new concrete mixes and the optimisation of laminate shielding structures, including the development of heavy concrete mixes or comparable materials, for effective shielding of neutrons is spear-headed by the PSI.

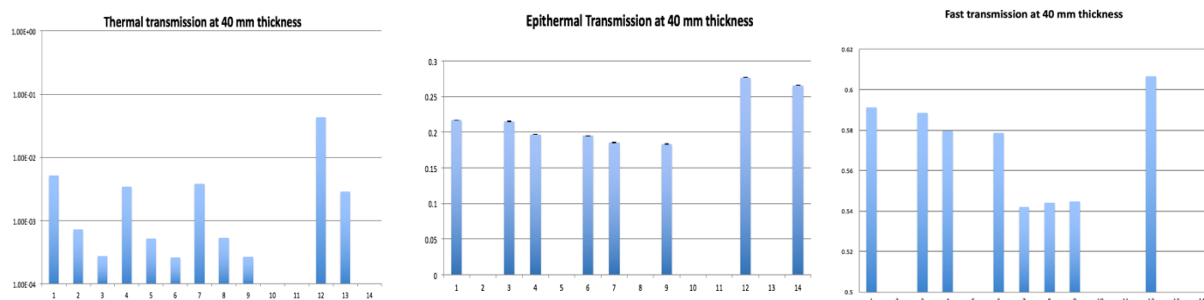
**Deliverable 8.6 – Developing special heavy concretes for fast neutron shielding (PSI),**

In connection with D8.6, special mixtures of mineral cast (material comparable to normal heavy concrete) was developed. The new materials shows shielding characteristics closed to heavy concrete mixtures. The mineral casts were developed in collaboration with the Rampf System company (Germany). Furthermore, several heavy concretes were composed and tested. The heavy concretes were produced by Alpha Beton AG (Switzerland). All of the developed compositions are new product developments which are presently not available for order.

calculated density [kg/dm <sup>3</sup> ]	5.000	4.800	4.800	4.800	4.800	4.800	4.800
effective measured density [kg/dm <sup>3</sup> ]	5.200	4.850	4.770	4.880	4.860	4.890	4.740
	sample 1	sample 2	sample 3	sample 4	sample 5	sample 6	sample 7
	[kg]	[kg]	[kg]	[kg]	[kg]	[kg]	[kg]
Barite							
Magnetite							
Hematite							
Fe-granulate St. 37							
Fe-granulate St. 37							
Fe-granulate, stainless , 1.4301							
Boron-carbide 5%							
measured attenuation factor [1/cm]	0.313	0.213	0.204	0.213	0.208	0.217	0.207

Table: Overview of the investigated heavy concrete compositions

<sup>4</sup> For download installation and documentation, see <http://ifit.mccode.org>



**Figure: Comparison of thermal, epithermal and fast neutron transmission for samples of the developed mineral casts.**

The performed measurement have show that heavy concrete composition no. 1 and mineral cast composition no. 6 have the best shielding characteristics.

Finally, the heavy concrete no. 1 was compared to mineral cast no. 6 and to a standard concrete composition.

The result is that the mineral cast and the heavy concrete are better as standard concrete in all three comparisons. The heavy concrete has the best shielding properties for fast neutrons but the mineral cast is very close.

A cost comparison makes the mineral cast very attractive. The price of the mineral cast is close to that of standard concrete, whereas the heavy concrete is at least 5 times more expensive.

As a follow-up development, the PSI expect to adapted the mineral cast with a higher epoxy content (from 7 to 9 %wt), and it is expected that the fast neutron shielding behaviour will be further improved.

### **Task 8.3: Compact Instrumentation for Larmor Labelling applications at the ESS** (*Responsible: TU-Delft with observers: DTU, STFC, MTA-EK and ESS*)

Larmor labelling is widely used to increase the resolution of neutron scattering both in energy (Neutron Spin Echo spectroscopy<sup>5</sup>) and momentum transfer (Spin Echo SANS<sup>6</sup>, Larmor diffraction<sup>7</sup>). Since these techniques do not require highly monochromatized and collimated neutron beams they do not trade resolution for neutron flux. However, the effective neutron count rate is effectively reduced because of the use of polarised neutron beams and because the Larmor precession areas cannot be combined with neutron guides. Furthermore, most existing instruments are relatively long, due to homogeneity requirements for the precession areas. This in fact collimates the beam and significantly reduces the neutron flux.

<sup>5</sup> F. Mezei; Neutron Spin Echo, Lecture Notes in Physics, **128**, Springer, (1980), 3.  
Mezei, F.; Pappas, C.; Gutberlet, T; Lecture Notes in Physics, **601**; Springer (2003).

<sup>6</sup> M.T. Rekveldt; *Nucl. Instrum. Methods Phys. Res. B*, **114** (1996) 366.

<sup>7</sup> M.T. Rekveldt; W. Kraan; T. Keller; *J. Appl. Crystallogr.*, **35** (2002) 28.

### Deliverable 8.7: Compact Instrumentation for Larmor Labelling applications at the ESS (TUDelft)

The deliverable report presents a rigorous investigation of the available parameter space for several instrument options (symmetric, asymmetric magnet layout), supplemented by realistic magnetic field calculations for such setups. Finally the report presents and evaluates the possibility of a compact SEMSANS add-on for SANS and imaging instruments.

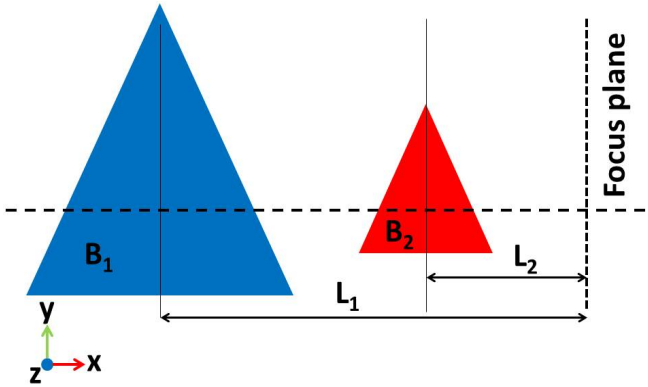


Figure: Schematic representation of the SEMSANS field configuration considered in this study.  $B_1$  and  $B_2$  are the respective magnetic fields of the first and second triangular field regions. The focus plane indicates the plane, where all cumulative precession phases interfere constructively. Ideally the focus plane should also be the detector plane.  $L_1$  and  $L_2$  are the distances of the focus plane from the magnetic centres of region 1 and 2 respectively. In the calculation, we have considered only those neutron trajectories that cross both triangular field regions

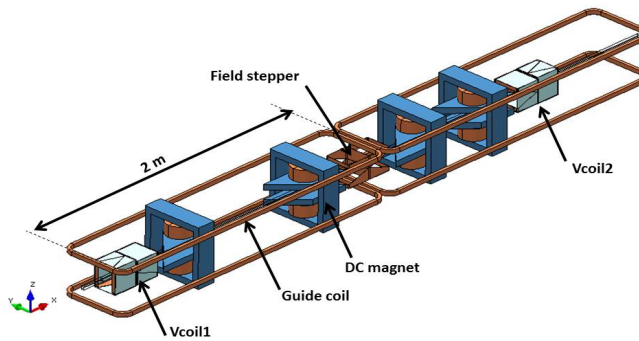


Figure: Schematic drawing of SEMSANS arrangement considered for the magnetic field calculations. The white boxes illustrate the Vcoils, which act as  $\pi/2$  flippers, the blue components are DC magnets with parallelogram shaped pole shoes, the central coil is a field stepper. The long upper and lower create a homogenous magnetic field, which guides the beam polarisation.

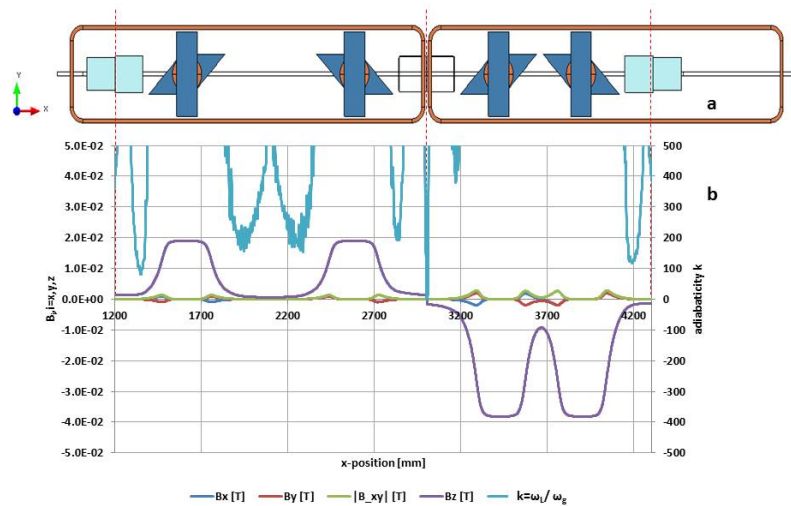
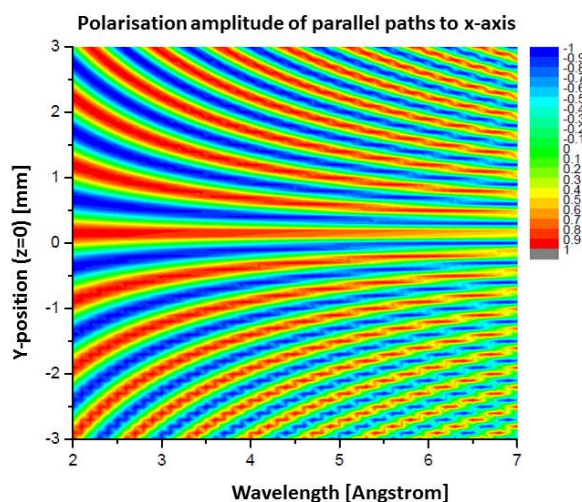


Figure: Top view of the SEMSANS setup (a) and (b) the corresponding magnetic field components and adiabaticity parameter  $k$  for a path parallel to the symmetry x-axis and with an offset of  $y=5$  mm and  $z=5$  mm.



**Figure:** Contour plot of the spin echo modulation  $P_{NSE}$ , calculated for neutron trajectories parallel to the central one. The next step was to consider the effect of the beam divergence.

Deliverable 8.3 represents and reports on the bulk work performed in Task 8.3 and elegantly demonstrate that the development of modular, compact Larmor setups are indeed both feasible and attractive as inserts for the future ESS instruments.

#### **Publications:**

As the report show, progress is good on the deliverables of the WP. Several publications are planned, based on the above deliverables and manuscripts are in the making.

#### **Status on other incoming deliverables:**

- Deliverable 8.11 “Improved user interface”: DTU reports good progress on a proposed method for automatic transfer of geometrical information from MCNP to McStas. Initial prototype software looks promising and the remaining work will be performed during the fall of 2018.
- Deliverable 8.12 “Software documentation and report on combined RESTRAX + McStas simulations”: NPI has reported on excellent progress already in connection with the first PR. Other staff obligations and technicalities however makes it unrealistic to write the report before early 2019.
- Deliverable 8.13: “Optimization study of a selected instrument using CombLayer and McStas-MCNPX”: Work will be carried out during the fall of 2018 as it relies on the now delivered D8.3 and the forthcoming D8.11.
- Deliverable 8.14: “Investigation of effective shielding concepts for high energy particles”: Essential work has already been performed, and finalization plus reporting is expected during the fall of 2018.
- Deliverable 8.15: “Recommendations for ESS instruments”: The underlying work has been carried out and is available documented in D8.7 as seen in the PR. Write-up of the formal D8.15 report will happen during the fall of 2018.
- Deliverable 8.16: “Activation studies, radiation resistance”: MTA-EK has reported good progress already in connection with the first PR. The final work and simulation benchmarking will be carried out with DTU during the fall of 2018.

#### **Delayed deliverables and milestones for WP8:**

- Deliverable 8.8 “Port of selected scattering kernel code from McStas to RESTRAX” is delayed due to availability of key staff. The essential work has been done and only the reporting remains, expected fall 2018.
- Deliverable 8.10 “Several background measurement series at different facilities in Europe” is delayed due to availability of key staff and delayed access to the experimental facilities. The experiments have now been performed and only the reporting remains, expected fall 2018.
- Milestone MS4 “Completion of validation campaign”: Depends on D8.14 and is hence expected during fall 2018.

Date	Meeting/workshop	Location	Who participated
04/07/2017	Mid-Term Review	Brussels, B	WP leader
22-25/01/2018	WP8-WP3 software meeting	Grenoble, FR	WP leader, ILL observer E Farhi, WP3 software developer J Garde
05-06/06/2018	2 <sup>nd</sup> General Assembly	Parma, IT	WP team
23-29/09/2018	MDANSE school	Orotava, E	WP leader, DTU developer E Knudsen, ILL observer E Farhi
18-19/10/2018	McStas workshop	ORNL, US	WP leader, ILL observer E Farhi
22-25/10/2018	NOBUGS meeting	BNL, US	WP leader

### 1.3 Impact

*Include in this section whether the information on section 2.1 of the DoA (how your project will contribute to the expected impacts) is still relevant or needs to be updated. Include further details in the latter case.*

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## 5. Deviations from Annex 1 and Annex 2

*Explain the reasons for deviations from the DoA, the consequences and the proposed corrective actions.*

The complete list of changes in the description of Work of SINE2020 approved during our last General Assembly/ Board meeting in June in Parma this year, is to be found below.

Some are minor and might not even request an official approval, whereas others might require official approval. As the project advances, we felt the need for some budget shifts in order to still be able to offer the European Commission the best value for money in terms of scientific or technical output.

The requested changes are listed in **the below tables**. All changes are approved by the respective teams involved in the work package. The current deliverable status and those currently delayed are mentioned. To resume there are also the tables of the new budget distribution per WP. They reflect the budget after changes after the 2<sup>nd</sup> General Assembly, as adopted during the SINE2020 Board meeting, held on 6<sup>th</sup> June 2018 in Parma.

### 5.1 Tasks

*Include explanations for tasks not fully implemented, critical objectives not fully achieved and/or not being on schedule. Explain also the impact on other tasks on the available resources and the planning.*

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Further explanation may be found in the WP dedicated text under section 1.2.

### 5.2 Use of resources

*Include explanations on deviations of the use of resources between actual and planned use of resources in Annex 1, especially related to person-months per work package.*

*Include explanations on transfer of costs categories (if applicable)*

Include explanations on adjustments to previous financial statements (if applicable).

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#### Changes as approved during SINE2020 Board meeting (6<sup>th</sup> June 2018)

WP	Explanation for changes	Requested changes
WP3	CEA highlights the fact that the budget foreseen for specialized schools may not be spent by the end of the project. WP3 leader currently develops the possibility to convert	40k EUR can be transferred from CEA to UCPH and DTU budgets → roughly 9 person months

	the remaining to staff cost in order to bring forward the 'virtual facilities' development	
WP4	STFC and TUD declared themselves unable to spend till the end of the project; HZB - after discussion - will declare the resources as foreseen.	<p><b>MTA EK</b> -- 22k EUR staff cost and 22.7k EUR other cost increase</p> <ul style="list-style-type: none"> <li>other cost items: 18k for industry event &amp; 16k for neutron hands on training (remaining budget as of end of 2017: 11.3k) <math>\rightarrow (18+16)-11.3=22.7k</math> EUR</li> <li>staff cost request: PostDoc recruitment for the last year &amp; feasibility study support</li> </ul> <p><b>TUM</b> -- 19k EUR staff cost increase</p> <ul style="list-style-type: none"> <li>staff cost request: WP4 and WP2 are strongly linked and during the last year of the project the dissemination activities require an extra effort</li> </ul> <p><b>ILL</b> -- 84k staff cost and 38k other cost increase for ILL</p> <ul style="list-style-type: none"> <li>Staff cost request: 6 additional PM for ILU till the end of the project, especially for the dedicated event in the Lyon Region and report writing (business plan etc) &amp; scientists accompanying feasibility study and development of easy to use software tools</li> <li>Other cost items: 30k for a Synergi event in Lyon 2019; 8k roadshow Austria; 6k for SANS movie</li> </ul>
WP7	<p>Task 7.4: The in-situ NMR system has been developed and two experiments have been performed at the LLB. At ISIS, a post-doc is developing in-situ muonium chemistry and has already made great progress. Due to the difficult recruitment of this post-doc, we have decided to postpone D7.12 by 6 months and D7.13 by 12 months.</p> <p>The feasibility study on anvil cells for muons (D7.8) has demonstrated that the development of this cell is technically too challenging. Its future success depends among others on instrument upgrades, which exceeds the timeframe of the SINE2020 project.</p>	<p>Delay for two deliverables</p> <p>D7.12 from M30 to M36</p> <p>D7.13 from M36 to M48</p> <p>Deletion of one deliverable:</p> <p>D7.16 has to be abandoned. The resources are reallocated to remaining tasks within the workpackage.</p>
WP8/9	ESS-B requests to contribute also to WP9 at no additional cost.	<p>ESS-B proposes to contribute additionally to WP9, without damage to WP8, as the PM cost are lower than estimated during the proposal preparation:</p> <p>Staff cost/mth estimated vs real: 6350 vs 4700 € over 12mths 20k to allocate in WP9</p>

WP9	In order to maintain the current staff at LIP, the WP has decided to transfer 30k EUR.	LIP budget increase of 30k EUR / decrease STFC Knowledge transfer budget
WP9	FZJ allocated amount of 16k EUR of direct cost to be moved to staff cost	Cost neutral.

#### Update on deliverables schedule & submission:

81 deliverables were due till month 32 (May 2018). Next time limit will be month 36 (September), coinciding with the next periodic report. **SINE2020 has delivered 86%** of its due reports, i.e. 71 deliverables have been submitted and 10 are delayed for acceptable reasons (i. e. maternity leave, recruitment difficulties, instrument shutdown period etc).

The delayed deliverables are listed below:

#	Title	Responsible	Initial delivery date	Forecasted delivery date
D3.4	Development of virtual instruments	DTU	24	48
D6.7	Report on prototype, its control, and performance	ILL	32	36
D6.8	Overall report on temperature, precipitant, nucleation & vapour diffusion studies	FZJ	32	40
D7.12	Report on testing sample cell, sample environment and RF cavity	STFC	30	36
D8.3	Computational tests (multiple platforms)	ESS_B	18	36
D8.8	Port of selected scattering kernel code from McStas to RESTRAX	DTU	24	33
D8.10	Several background measurement series at different facilities in Europe	PSI	24	36
D10.3	SASView ready for user test	ESS	30	34
D10.4	BornAgain ready for user test	FZJ	30	36
D10.5	MuhRec/KipTool ready for user test	PSI	30	33



## Updated budget table after budget changes

3 TRAINING: E-LEARNING & SCHOOLS											
Acronym	Staff effort charged to project (man months)	mean staff cost/months	Staff cost	Sub-contract	Consumables	Travel	Equipment charged to project	Total Direct cost	Overhead Costs	EU contribution	
UCPH	48	6,666	359,968	0	11,000	10,000	0	380,968	95,242	476,210.00	
DTU	24	6,250	150,000	0	1,000	10,000	0	161,000	40,250	201,250.00	
STFC	2	6,096	12,192	0	0	3,000	0	15,192	3,798	18,990.00	
PSI	1	7,400	7,400		0	3,000	0	10,400	2,600	13,000.00	
CEA	9	5,907.02	53,163.20		1,000.00	4,000.00		58,163.20	14,540.80	72,704.00	
MTA EK	NaMES					210,000		210,000	52,500	262,500.00	
CEA	NaMES					100,000		100,000	25,000	125,000.00	
TUM	Observer										
TOTAL	84		582,723	-	13,000	340,000	-	935,723		1,169,654.00	

4 INDUSTRY CONSULTANCY											
Acronym	Staff effort charged to project (man months)	mean staff cost/months	Staff cost	Sub-contract	Consumables	Travel	Equipment charged to project	Total Direct cost	Overhead Costs	EU contribution	
HZG	48	6,250	300,000		217,128	30,000		547,128	136,782	683,910	
ILL	50	6,250	309,375		58,000	20,000		387,375	96,844	484,219	
HZB	12	6,250	75,000		20,000	5,000		100,000	25,000	125,000	
TUD	12	6,250	30,000		2,000	5,000		37,000	9,250	46,250	
STFC	12	6,250	10,000		5,000	5,000		20,000	5,000	25,000	
CEA	12	6,250	75,000		20,000	5,000		100,000	25,000	125,000	
MTA EK	18	3,675	66,150		42,697	5,000		113,847	28,462	142,309	
NPI	12	3,675	44,100		20,000	5,000		69,100	17,275	86,375	
TUM	observer	6,250	18,750					18,750	4,688	23,438	
TOTAL	176		928,375	-	384,825	80,000	-	1,393,200	348,300	1,741,500	

8 INSTRUMENTATION - E-TOOLS											
Acronym	Staff effort charged to project (man months)		Staff cost	Sub-contract	Consumables	Travel	Equipment charged to project	Total Direct cost	Overhead	EU contribution	
DTU	21	6,250	131,250	0	12,000	20,000	0	163,250	40,813	204,063	
ESS	9	7,000	63,000		4,000			67,000	16,750	83,750	
PSI	15	10,249	153,735		4,000			157,735	39,434	197,169	
STFC	3	7,479	22,437		4,000			26,437	6,609	33,046	
TUD	12	6,250	75,000		4,000			79,000	19,750	98,750	
NPI	6	3,000	18,000		4,000			22,000	5,500	27,500	
TUM	3	6,710	20,130		4,000			24,130	6,033	30,163	
ESS-B	12	6,350	56,200		4,000			60,200	15,050	75,250	
MTA EK	6	3,675	22,050		4,000			26,050	6,513	32,563	
ILL	Observer										
UCPH	Observer										
TOTAL	87		561,802	0	44,000	20,000	0	625,802	156,451	782,253	

9 INSTRUMENTATION - DETECTORS											
Acronym	Staff effort charged to project (man months)	mean staff cost/months	Staff cost	Sub-contract	Consumables	Travel	Equipment charged to project	Total Direct cost	Overhead	EU contribution	
STFC	25	4,744	118,600	0	31,000	12,000	0	161,600	40,400	202,000	
ILL	23	6,250	143,750		20,000	8,000		171,750	42,938	214,688	
FZJ	16	6,807	124,912		0	8,000		132,912	33,228	166,140	
TUD	9	5,640	50,760		7,000	8,000		65,760	16,440	82,200	
ESS	4	7,000	28,000		0	8,000		36,000	9,000	45,000	
LIP	15	5,000	105,000		10,000	8,000		123,000	30,750	153,750	
PSI	16	7,400	118,400		15,000	12,000		145,400	36,350	181,750	
CEA	13	5,848	76,024		10,000	8,000		94,024	23,506	117,530	
TUM	3	6,710	20,130			8,000		28,130	7,033	35,163	
ESS-B			20,000					20,000	5,000	25,000	
TOTAL	124		805,576	0	93,000	80,000	0	978,576	244,644	1,223,220	

**NEW BUDGET AFTER CHANGES**

#	Participant short name	MGT WP1 management	COORD WP2 dissemination	COORD WP3 training	COORD WP4 industry	RTD WP5 "sample" deuteration	RTD WP6 "sample" crystal	RTD WP7 sample environment	RTD WP8 "instrument" E- tools	RTD WP9 "instrument" detectors	RTD WP10 data treatment software	TOTAL
1	ILL	610,369			484,219	311,250	311,250	391,250		214,688	388,889	2,711,914.00
2	ESS	4,375				532,500	203,750	228,750	83,750	45,000	492,361	1,590,486.00
3	STFC	4,531		18,990	25,000	200,630	-	263,250	33,046	202,000	351,961	1,099,408.75
4	PSI			13,000				391,250	197,169	181,750	434,250	1,217,418.75
5	TUM	5,625	339,450		23,438			60,688	30,163	35,163	5,000	499,525.00
6	FZJ	3,750				173,603	293,606			166,140	380,261	1,017,360.00
7	CEA			197,704.00	125,000.00			204,166.00		117,530.00	53,000.00	697,400.00
8	TUD				46,250				98,750	82,200	5,000	232,200.00
9	HZB				125,000			179,800			5,000	309,800.00
10	HZG	3,750			683,910			67,375				755,035.00
11	CSIC							119,800				119,800.00
12	UCPH	1,350		476,210								477,560.00
13	DTU	2,500		201,250					204,063		5,000	412,812.50
14	NPI				86,375			43,650	27,500			157,525.00
15	ESS-B								75,250	25,000		100,250.00
16	MTA EK	3,750		262,500	142,309				32,563			441,121.25
17	LIP									153,750		153,750.00
18	UNIPR										87,500	87,500.00
TOTALS		640,000	339,450	1,169,654	1,741,500	1,217,983	808,606	1,949,979	782,253	1,223,220	2,208,223	12,080,866.25

*5.2.1 Unforeseen subcontracting (if applicable)**Specify in this section:*

- a) the work (the tasks) performed by a subcontractor which may cover only a limited part of the project;*
- b) explanation of the circumstances which caused the need for a subcontract, taking into account the specific characteristics of the project;*
- c) the confirmation that the subcontractor has been selected ensuring the best value for money or, if appropriate, the lowest price and avoiding any conflict of interests.*

*5.2.2 Unforeseen use of in kind contribution from third party against payment or free of charges (if applicable)**Specify in this section:*

- d) the identity of the third party;*
- e) the resources made available by the third party respectively against payment or free of charges*
- f) explanation of the circumstances which caused the need for using these resources for carrying out the work.*