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

1.1 Objectives

1.1.1 Context of the project:

Societal challenges such as energy and environment, healthcare, information technology or even cultural heritage depend among others critically on the development of new materials and processes. This in turn requires precise insight into the structure and dynamics of materials starting from the atomic level.

Neutrons at large scale facilities are predominantly used as a subatomic sized probe for the characterisation of solid and liquid materials. Neutrons deliver structural information of objects from the atomic length scale up to micrometre size and explore the dynamics of these objects in a time window from picoseconds (atomic movements, lattice vibrations) to microseconds (movement of macromolecules, domain walls). With these properties neutrons are thus one of the most incisive experimental tools for understanding and modelling new functionalities of materials.

Neutron scattering experiments are reserved to large scale facilities, either spallation sources (e.g. ISIS, ESS) or research reactors (e.g. ILL, FRM-II, LLB). The efficient connection of these facilities to academic and industrial research (user community) and the broader non-scientific public in general is important for the scientific and cultural progress in Europe.

SINE2020 - *S*cience and *I*nnovation with *N*eutron in *E*urope – unifies 18 partners from large scale facilities, universities and other research centres in Europe around two central issues:

- Preparing the European neutron community for the unique opportunities at the European Spallation Source (ESS).
- Developing the innovation potential of present neutron large scale facilities.

To achieve these objectives SINE2020 is structured into 10 work packages. WP1 to WP4 aim on common objectives to foster collaboration among the present user community and to address and to form future generations of neutron users form academia and industry. WP5 to WP10 concentrate on specific technical tasks identified as key ingredients for future scientific challenges explored by neutron scattering.

1.1.2 Overview of the project objectives:

The main objectives of every WP are given in the following:

WP1 - Project management ensures smooth cooperation within all partners and supports the governance instances, which are Board, Advisory Committee and international observers.

WP2 – Dissemination supports the SINE2020 project by (1) providing tools and materials for internal and external communications, (2) fostering collaboration between SINE2020 WPs, and (3) outreaching to scientific communities and the broader public.

WP3 – Training neutron scattering, e-learning and schools emphasizes the training of new generations of neutron users, which is crucial for the future scientific impact generated by neutron scattering techniques. SINE2020 supports the training of new and advanced users by a) freely accessible, e-learning modules with online experiment simulation sessions in a specialized platform and b) European neutron schools which generally include hands-on sessions at Large Scale Facilities.

WP4 - Industry Consultancy aims on raising the awareness and strengthening the cooperation between European industry and neutron research facilities. WP4 is accompanied by an international industry advisory board (IAP) with representatives of different technological and industrial key sectors assists WP4 in its activities and decisions.

WP5 – Deuteration develops new synthesis and purification methods of per-deuterated materials, which are rarely available from commercial suppliers except through costly custom synthesis. This limits the experiments that can be performed, and forms a bottleneck for advancing the applications of neutron scattering, particularly in the areas of soft condensed matter, functional materials and the biomedical sciences. To broaden the range of compounds available, and to provide a cost-effective service and coordinated user access, WP5 proposes to establish a European platform for chemical deuteration (DEUNET) in the form of a network between the ESS, ILL, STFC, and FZJ, with the Australian National Deuteration Facility at ANSTO as an observer.

WP6- Macromolecular Crystallogenesis develops systematic approaches for the characterisation and optimisation of crystallization for large crystal growth ($\approx 1\ mm^3$), specifically for applications in neutron protein crystallography.

WP7 – Sample Environment aims to improve the environment surrounding samples both on neutron and muon experiments, thus improving data statistics and opening new fields of science. Thanks to close collaboration fostered by SINE2020, each member's developments will be useful for the other facilities.

WP8 - Instrumentation – e-tools helps to plan and optimise neutron sources of the present and future (neutronics), design complete instruments and simulate experiments. This instrumentation task embraces e-science related tasks 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).

WP9 – Detectors aims at developing fast, high-resolution neutron detectors for reflectometry applications, which are able to cope with requirements of the ESS, where neutron rates will be up to 100 times faster than at present neutron sources. In addition high timing resolution and high rate detectors will be developed for MuSR. As the need for high rate, high-resolution detectors is common to all neutron and muon sources, WP9 is of wide synergetic benefit across the European neutron and muon facilities.

WP 10 –Data Treatment aims at providing software for straightforward generation of scientific results for non-expert and industry users that are either directly publishable or can be used for creating new innovative products. Specifically, data treatment software is developed for users at ESS in 2020 - users will be familiar with the software and able to produce high-impact results from day one.

Table: Status of deliverables first period

Del. no.	Deliverable name	Delivery date (proj.month)	delivered	New date
1.1	Agenda General Assembly & Minutes of the Board meeting (Kick-off meeting)	3	Y	
1.2	Agenda General Assembly & Minutes of the Board meeting (First annual meeting)	16	Y	14
1.3	1st Periodic report	18	Y	
2.1	Report on outreach activities	12	Y	
2.2	SINE2020 internet portal	12	Y	
3.1	Investigation of e-learning tools with respect to student performance and assessment	12	delayed	30
3.2	Reports on introductory schools year one	12	Y	
4.1	Concept for trade fairs/conferences/workshops/roadshow and first dates	6	Y	
4.2	Content requirements for practical courses adapted to industrial users	10	Y	13
4.3	Case Studies about selected measurements from first call	10	Y	18
5.1	Webpage and user portal established for DEUNET	9	Y	14
5.2	Synthesis of precursors to surfactants, lipids and polymers	12	Y	14
5.3	Novel route for isoprene synthesis	15	Y	
5.4	Synthesis of of L- and D-lactic acid	18	delayed	24
6.1	Report on completion of conceptual design of robot module	12	Y	14
6.2	Report on phase diagram characterisation approaches	12	Y	14
6.3	Report on initial temperature, precipitant & nucleation studies	12	Y	14
7.1	Routines for optimising equipment with McStas	18	Y	
7.2	Concept design for goniometer	18	Y	
7.3	Concept design for improved µSR piston cell	18	Y	
7.4	Concept design for 700 bar hydrogen container	18	Y	
7.5	Concept design for novel neutron clamp cell	18	Y	
7.6	Concept design for in-situ muonium studies	18	delayed	24
7.7	Concept design for in-situ NMR setup	18	Y	
8.1	Evaluation of detectors for fast neutron and gamma spectroscopy – mainly for background measurements	9	Y	
8.2	Improved code interface, pre-release	12	Y	
8.3	Computational tests (multiple platforms)	18	delayed	24
8.4	Experimental test A - "BOA@PSI" & Experimental test B - "ChipIR@ISIS", T8.1+2	18	delayed	24
8.5	Simulating laminate shielding concepts	18	Y	
9.1	First extended RTD meeting	18	delayed	21
9.2	Initial WLS fibre detector hardware	18	Y	
10.1	Guidelines and standards	18	Y	

Table: Status of milestones

No in GA	Lead	Milestone name	Work packages	Expected date		Means of verification
1	ILL	SECoSP protocol defined to allow its implementation	7	36		Description of the standard protocol agreed by all partners
2	DTU	Workshop: "Requirements/Development for a reverse Monte Carlo variance reduction method applied to neutron beamline transport systems".	8	9	6-Sep-16	Workshop agenda, participants list, presentations (T8.1)
3	DTU	Prerelease, advanced gui for McStas-MCNPX	8	12		Software prototype released to community, relating to Task 8.1, D8.3 (pending)
4	DTU	Completion of validation campaign	8	24		Availability of reports on experimental and computational tests, relating to T8.1+2, D8.4 (pending), D8.5 (done)
5	DTU	Workshop on Larmor concepts for ESS	8	36-48		Workshop agenda, participants list, presentations, relating to T8.3
6	DTU	Workshop on use of the developed integrated e-Tools for instrument simulation	8	46		Workshop agenda, participants list, presentations (T8.1)
7	ESS	Workshop I	10	7	4-5 April 2016	Report with first set of prioritized activities as well as compiled input from user community
8	ESS	Workshop II	10	19	24-25 April 2017	Report and demonstrated software can be found on project website and downloaded and compiled
9	ESS	Workshop III	10	31		Report and demonstrated software can be found on project website and downloaded and compiled
10	ESS	Workshop IV / Virtual experiment	10, 3, 8	44		Demonstration at SW Workshop 4 of a virtual experiment with analysis that can be used for e-training

1.1.3 Overview of project results achieved so far toward the objectives:

Management, outreach, education and industrial liaison (WP1 to WP4):

In the first period of the SINE2020 project from 1 October 2015 until 31 March 2017 the 18 partners recruited additional work force in their research units and initiated work according to the respective objectives of the work packages and according to the list of deliverables, Table 1.3.2 of the DoA.

The official kick-off took place at month 3 (D1.1) during the first general assembly. A second general assembly was held in Coimbra, Portugal, in September 2016. (D1.2).

All achievements and progress of the different WPs have been documented by a project **dedicated internet platform** (http://www.sine2020.eu), which went on-line in January 2016 (D2.2). For the moment it counts **about 1000 visitors/month in average**. It announces periodic calls for e.g. industry experiments and neutron schools, job offers and neutron related events. Material published on the website feeds into our periodically distributed electronic newsletter (7 so far, see teaser samples below).

This outreach activity is complemented by social media accounts relying on experience of the previous EU supported project NMI3. SINE2020 is present on Twitter, Facebook and LinkedIn under “EU Neutron”. Equally, we take advantage of the European Commission’s news website CORDISwire, where we post relevant press releases.

As part of the activities of **WP3** we host and develop a **specialized e-learning portal** managed by DTU (D3.7, due date 36 months). Until March 2017 **we registered 1400 visits** with impact across the boarders of Europe, especially in North America. Apart from the running maintenance and update of the software used in the portal, **three online tools have been developed** within the project so far: one to improve the online visualisation of virtual experiments, a second one to enable cloning of the e-neutrons course for local adaptation and a third one to enable teachers to upload their own virtual instruments for their locally adapted e-learning courses.

We provide on-demand self-enrolment in an introductory neutron training course with 10 topics including lessons based on collaboratively written WIKI-book material, video-lessons and screen-casts as well as learning quizzes with feedback (UCPH). The quizzes are important cornerstones of the e-learning modules. They are developed in close collaboration with experts and are used in many different ways depending on the didactical purpose. Furthermore we have within this project opened the e-learning portal to include e-learning courses on important complimentary techniques to neutron scattering such as muon spin rotation (ISIS), as foreseen for deliverable D3.3 (due date 24m).

As second important task of **WP3** we **support the organization of introductory schools**, managed by MTA-EK, and advanced neutron schools, managed by CEA. In order to obtain a fair evaluation of schools applying for support, the two subtasks have set a common international evaluation panel consisting of 10 recognized scientists of different countries representing the major fields of activities in neutron scattering. Two calls have already been opened; one for introductory schools and one for advanced schools. A report on introductory schools was sent by MTA and CEA (D3.2).

In their outreach activities the **WP4** partners visited **as much as 22 industry relevant events in the first 18 months**. Discussions with industrial researchers were constructive and partially concluded in concrete test experiments at different facilities. WP4 was presented by an exhibition booth and/or poster/oral presentation for 14 of these events. The outreach activities were complemented by our SINE2020 web portal, and specially adapted public relation material (brochures leaflets, roll-ups, mobile trade fair booth).

In the first period of the project a concept was developed for specific Training and Education activities offered to industrial scientists. Specially designed e-learning courses (in cooperation with **WP3**) complement on-site training from instrument scientists, e.g. during test measurements on their samples (Task 4).

Special attention is paid to elaborate strategies and facilitate 'direct access' (i.e. without intermediate third part participant) to neutron facilities for European industry. Open calls for feasibility studies resulted in **17 applications by industry**.

Based on this first successful launch, a more specific elaboration of the direct industrial access model is presently in progress. Emphasis is put on access modalities to neutron facilities, the level of service to provide by the facilities and IP policy. To outreach to industry, **WP2** works closely with **WP4** on Industry Consultancy. We have provided a webpage at sine2020.eu/industry containing basic information on neutron scattering as well as instructions on how industry can benefit from free measurements and feasibility studies funded by the project.

Scientific progress and technical developments – Joint Research Activities (WP5 to WP10):

Within **WP5** the STFC Deuteration Facility regularly **produces a large number of deuterated precursors** through catalytic deuterium hydrogen exchange, including aliphatic hydrocarbons such as fatty acid, bromoalkanes, and organic ligands. A wide variety of both routine and non-routine deuterated precursors and surfactants (listed in section 1.2.1.) have been synthesized for non-UK users (D5.7) and DEUNET partners (D5.1), and have resulted in **several successful neutron experiments at ISIS**, with publications in preparation.

At ESS, a new laboratory (DEULAB) has been set up for the synthesis of small deuterated molecules (Task 5.3) and precursors to the first target molecule lactic acid (D 5.4) and the polymer supports for enzyme catalysis have been synthesized and characterized.

At FZJ, deuterated isoprene (D5.3) and polyhexylthiophene (P3HT) (D5.5) have been synthesized via new, improved routes allowing better control of the polymerization and therefore the properties of the commercially and technologically important polymers to be investigated by neutron scattering. An investigation into the synthesis of polylactic acid (D5.8) from the lactic acid synthesized at ESS via lactide has been carried out that will enable the synthesis of designer biodegradable plastic polymers for neutrons scattering studies.

The partnership has had several **networking, dissemination and outreach activities** of the platform (**DEUNET**) coordinated by ESS (D5.5), including visits to discuss collaborations, design of our own web-portal - deuteration.net (D5.1), a user survey and organization of a joint user workshop in Oxford 15-17th

May 2017 (https://indico.esss.lu.se/event/756/) that will form the basis of collecting the research community's input into the scope and strategy for DEUNET (D5.6). **WP5** disseminates our member's capabilities, on-going work and new/events through regular blogs on our website and via Twitter, with links to other user sites including neutronsources.org, the SINE2020 project home page and more to come. DEUNET has been publicized by our members in presentations at conferences and seminars both, in Europe and overseas.

The dissemination activities have led to interest from external groups wishing to obtain services from DEUNET, as well as to contribute specialty deuterated products such as ionic liquids, and our plans for a database of deuterated chemicals and their producers on deuteration.net have received very positive feedback from user groups.

Several approaches to tackle the challenge of macromolecular crystallogenesis are being explored by the various partners concerned within **WP6**. The ILL has principally investigated the feasibility of designing and implementing automated robotic approaches to aid in the growth of large macromolecular crystals. Design concepts have been produced for a robotic system (D6.1), which will enable the crystallisation of macromolecules within quartz crystallisation wells surrounded by aluminium blocks, which can be thermally regulated using Peltier elements. This can be fixed to a translational stage attached to a microscope and digital camera to allow for the monitoring and recording of crystal growth over time to obtain optimal results. Microfluidic technologies, which can be integrated into this system to further regulate the growth conditions, are also currently being explored.

Additionally, investigations are being pursued in the areas of magnetic alignment of multi crystal arrays within a gel medium. Preliminary studies have been carried out in partnership with the University of Birmingham School of Physics and Astronomy department. High magnetic fields (up to 17T) are used to orient microcrystals of model systems within a gel medium, which is maintained in a liquid state at slightly elevated temperatures. As the crystals become aligned, the temperature of the system is reduced, cooling and solidifying the gel to keep the crystals fixed in their current orientation.

The ESS investigations in this WP focus on phase diagram characterization of protein solubility and crystallization, and to investigate strategies for scaled-up crystallogenesis using methods based on vapor-diffusion and dialysis with temperature as a major parameter to vary in promoting large crystal growth (D6.2). Principally, we have focused on target identification, purification, and characterization. This included plasmid design, expression trials, preparing of deuterated versions of the target proteins, and purification and characterization with SDS-PAGE, size exclusion chromatography, and activity assays as applicable.

Several target systems have been identified: 1) Human carbonic anhydrase IX mimic, HCA IX mimic (both hydrogenous and perdeuterated), 2) Bovine Cu/Zn superoxide dismutase, SOD 3) Full length native human carbonic anhydrase IX, native HCA IX. Screening and optimising of conditions to map out the phase diagram for these targets is underway.

FZJ studied the crystallisation process with light scattering techniques in order to understand the influence of the early phase of crystallisation for the later size of protein crystals. Although numerous light scattering experiments are reported in literature, no specific attention has been paid on the relation between resulting crystal size and initial crystallisation process. As case study, FZJ measured the nucleation of lysozyme crystals over time by dynamic light scattering. These measurements were corroborated with *in situ* small angle neutron scattering to monitor the nucleation process.

A central task in **WP7** is to develop standards to facilitate the communication between the instrument control workstation and the sample environment equipment. Currently, to be able to remotely control temperature, pressure or humidity during an experiment, scientists need to write pieces of code that are specific to the equipment available at each facility. We have started defining two standards: *what* we communicate (metadata) and *how* we communicate information (protocol).

We have worked towards an efficient sample environment for neutron research. One aim is to reduce as much as possible parasitic background produced by the environment around the sample. We are now completing the development of software, which is able to simulate the used environment and to give a quantitative estimate of the background (D7.1). We are presently developing a remotely controlled goniometer inside a dilution fridge, which enables position correction of samples at low temperatures (D7.2). This correction can save up to 24 hours of beam time and avoids stressing samples due to heating cycles.

The third task of **WP7** is to **build a new generation of pressure cells** from new materials and designed from novel geometries to boost the capabilities of neutron scattering and muon spin relaxation. We performed preliminary calculations and prototyping from which we expect a 50% pressure increase. As a first step we have started to improve the piston cell for muon instruments. Based on this experience we design a new-generation high-pressure cell (D7.5) that we could use both in neutron and muon instruments.

The **WP8** partners have exchanged at multiple workshops and meetings, especially the *Neutrons: Cradle to Grave workshop*, Coimbra, Portugal, September 6th 2016" in connection with the first SINE2020 General Assembly (MS2). The workshop discussed possible synergies among existing simulation tools. Especially the implementation of the Monte Carlo variance reduction method, as used in the codes CombLayer and RESTRAX, into McStas was discussed. This method is known to be extremely efficient in **optimizing neutron beam-line transport systems**. All talks from the meeting were recorded and are available for viewing at http://coimbra2016.essworkshop.org.

Further main results so far are:

- Evaluation of detectors for fast neutron and gamma spectroscopy, including improvement of expansion of the so-called *Bonner Sphere* spectrometer at PSI (main input to deliverable D8.1)
- The release of the MCPL library software for interchange of event data between neutronics and instrument simulation packages, see https://mctools.github.io/mcpl/ and T. Kittelmann et.al., http://arxiv.org/abs/arXiv:1609.02792, accepted for publication in Computer Physics Communications. MCPL is developed in collaboration between DTU and ESS (and is the main input to deliverable D8.2).
- A report on the achievements in simulating laminar shielding concepts by EES-Bilbao (D8.5)
- Early progress on porting methodology from RESTRAX to McStas for "reverse direction neutron propagation" from sample to source, contributed by NPI. To become part of report for deliverables D8.8 and D8.12.
- Early progress on shielding material development and characterisation, to become part of the report for deliverable D8.6. Joint effort of ESS and PSI.

In accordance with the timeline of the DoA the first extended work package meeting of **WP9** has been arranged for 13-14 June, including industry partners (D9.1).
ISIS has designed and produced a scintillation detector based on ZnS:Ag/^{6}LiF coupled to multi-anode photomultiplier tubes (MA PMTs) with wavelength shifting (WLS) fibre, (D9.2). The position resolution is 0.7 mm FWHM and pixel to pixel uniformity is ± 20%. Further characterization of the detector is ongoing.
Jülich has designed and produced a scintillation detector based on GS20 glass where each detector pixel is read out by an individual pixel of a 64-channel multi anode PMT, (D9.3, due date M24). Optical isolation of the scintillator pixels has been achieved. An electronics readout system has been constructed to evaluate the detector and the development of a new readout system with higher rate capability is underway.
ILL has designed and constructed a 3He microstrip gas chamber (MSGC) with resistive electrodes, (D9.6, due date M24). This enables two-dimensional position sensitivity to be obtained from these detectors. First results have been obtained and are being analysed.

LIP has designed and constructed two neutron-sensitive resistive plate chambers (RPCs), (T9.4.1). Detector characteristics have been measured in collaboration with TUM, and include a neutron detection efficiency of 12.5% at 4.7 Å and a very impressive spatial resolution of better than 0.25 mm FWHM as presented by Professor Fonte from LIP at the Coimbra meeting. Work is now proceeding on the design and construction of a stack of double gap RPCs to improve neutron detection efficiency.

PSI has designed and produced two types of two-dimensional position sensitive scintillation detector read out with SiPMs, (T9.4.2). The detectors are based on ZnS/^{6}LiF and each detector type uses a different method for achieving position sensitivity. Initial results have been obtained and work is continuing to optimise the performance of both types of detector.

ISIS and PSI are evaluating the use of silicon photomultipliers (SiPMs) for muon spectroscopy, (T9.4.3). A Monte Carlo simulation programme has been developed and together with laser stimulation experiments and muon experiments, is being used to evaluate a range of the latest commercial SiPMs.
CEA have designed and simulated a neutron sensitive Micromegas detector based on microbulk micromegas detector technology, Task (9.4.4). Simulations show that such a detector could achieve a neutron detection efficiency of 40% at 1.8 Å. Construction is in progress.

Communication and coordination between partners, led by the WP leader ESS, is central to achieve the objectives of **WP10.** To this end annual workshops are organized (Task 10.1). *Workshop I* took place at PSI April 4th and 5th, 2016 with 26 participants from all partner facilities and the two observers DTU and HZB. The aim was coordination and knowledge transfer between the different facilities. Software requirements of every facility have been captured in the following and presented at the General Assembly meeting in Coimbra.

In order to coordinate software development at different facilities, common guidelines (Task 10.2) have been established and presented at *Workshop II* at ILL April 24th and 25th, 2017 (D10.1). Guidelines will enable different software components to be linked together in an interoperable manner (plug and play) and facilitate joint development, within and beyond the WP. The guidelines were established on the basis of a questionnaire, surveying the different techniques for software development of the partners.

1.2 Work carried out per WP:

1.2.1 WP1 - Management:

The SINE2020 consortium held its kick-off meeting on the 16th October 2015 in Copenhagen. A detailed description is available on our web site: http://www.sine2020.eu/news-and-media/140-scientists-met-in-copenhagen-for-the-nmi3-and-sine2020-meetings.html

The project manager takes care of the daily follow-up of the deliverables and milestones, meetings minutes and all issues related to budget questions, which appeared during the first period. The project management team is now composed of Miriam Förster as project manager and Martin Böhm as project coordinator since October 2016. The change of coordinator was necessary, as Mark Johnson, former coordinator, has accepted the position of Associate Director of the ILL in October 2016. This change has been adopted during the second General Assembly, held in Coimbra, Portugal, in September 2016. (D1.2). See below the link to our web page for this event : http://www.sine2020.eu/news-and-media/95-scientists-met-in-coimbra-for-the-sine2020-general-assembly.html?search_highlighter=Coimbra

The governance bodies, such as Advisory Committee and Board members have been set-up in the first Board meeting and updated in each Board meeting.

In between the reporting period we request every six month monitoring reports from all WPs in order to be able to detect problems which may cause delay early on. We also have frequent telephone conference calls with individual WP leaders in order to have an informal exchange on the collaborations.

The periodic report for the first 18 months has required quite some substantial work in requesting, collecting and assembling the contributions from WP leader as well as finance departments of the 18 beneficiaries. In order to have a sensible overview of the progress in relation to spending (be it in person month or Euros) it was necessary to request an extra table of spending of each beneficiary per WP, as this information cannot be retrieved anymore from the cost statements. It was also necessary to request an extra dissemination activity table per WP, as we need to enter this information now globally and not only for the dissemination work package. We would like to state here that the dissemination table in the Participants Portal only adds up numbers, which we believe do not make many sense in itself without a proper explanation.

Overall, the project is on track with some minor delays, most often due to late recruitment or maternity leave. We have no doubt that the project will achieve its objectives in the 48 month' duration. The consortium has worked together for many years, involved staff is renewed, but the overall goal is clear and we all strive to make the future European Spallation Source a successful facility thanks to a continuously trained user community.

1.2.2 WP2- Dissemination:

WP2 is managed by the information officer Ines Crespo placed at TUM in close collaboration with the WP4 coordinators, as well as the Project Manager and Coordinator. Unfortunately, Ines Crespo did leave TUM for a non-fix-term contract. Regarding **task 2.1** of WP2, our objective was to have an internet portal adapted to the needs of the scientific community, with relevant information to the project members and outside world. **Task 2.2** aims to foster collaboration among work packages. As for **task 2.3**, we aim to create and disseminate material to promote the project's activities both within and beyond the project's own community.

Task 2.1: Tools and material for internal and external communications *(TUM, M1-48)*

a. Templates for posters and presentations have been designed for the use of the project members.

b. The project's website, available at sine2020.eu, went online in mid-January. For the moment it counts with an average of about 1000 visitors/month. The website has a private area where we store templates, important documents and presentations for project members as well as the Advisory Committee.

c. The website is updated whenever there is new material on the project's activities, such as calls for industry experiments, for schools, interviews with WP coordinators and scientists, job offers, events, etc. Efforts have been made to link related information and news items within the website in order to make it more dynamic and attract visitors to other pages. Material published on the website feeds into our electronic newsletter. Annex I lists the material produced in this period.

d. We have created an electronic newsletter to send the latest news and events published on the website to anyone who wants to subscribe. In this period we have sent seven newsletters (teaser samples below) to over 700 people. The e-newsletter has proved successful to attract visitors to our website.

Task 2.2: Fostering collaboration between SINE2020 work packages *(TUM, M1-48)*

a. Industry: We regularly advise the Industry WP on design and content of brochures, cards, posters, website, social media, etc. to be used in outreach events to attract industry to use neutron scattering facilities.

b. Services and R&D: We have produced a number of overview articles about the project's WPs so that the neutron community is aware of tools that will be available for their use at the neutron facilities in the future.

c. Training: On our website, we promote the schools supported by the project as well as developments of the e-learning platform to attract people to SINE2020's Training activities.

Task 2.3: Scientific and public outreach *(TUM, M1-48)*

a. It has been decided to "recycle" the NMI3's social media accounts for SINE2020. We have thus renamed the Twitter, Facebook and LinkedIn accounts into "EU Neutron" where we post all the material published on the website.

b. We take advantage of the European Commission's news website CORDISwire where we post relevant press releases.

c. The project was presented at the JCNS LabCourse, with focus on the factors more relevant to the students: where they can find further information about neutron scattering, schools, and the e-neutrons e-learning platform. The number of "likes" on our Facebook page increased 700% after the presentation. Slides were also presented at the Italian Neutron School by the organisers, and we regularly sent them to relevant events.

d. To promote the project and participating facilities, we publish a series of SINE2020 advertisements on the back cover of each issue of the journal *Neutron News* (4 per year), each issue corresponding to a different partner facility which covers the respective costs. They are coordinated by the Information Manager and were designed by the MLZ Designer.

e. The website Neutronsources.org is a project supported by a network of European press officers. The website went live in July 2013 and counts now with around 2000 visitors/month. Social media accounts for about 12% of the website visits. Our aim is that the website becomes a sustainable option, where neutron-related material is posted independently to any project, so that it lives beyond the project's life-time. A working-student, financed by the FRM II, assists in uploading information to the website.

f. In summer 2015 the European Neutron Scattering Association (ENSA) has published a new brochure on Neutrons for science and technology to illustrate the scope and potential of neutrons. A second, improved edition of the brochure was prepared with some support from the SINE2020 Information Manager and MLZ Designer. The aim is to distribute copies to scientists from other fields, in order to attract new users to the technique. This is done in collaboration with the national user associations.

g. To outreach to industry, WP2 works closely with WP4 on Industry Consultancy. We have provided a webpage at sine2020.eu/industry containing basic information on neutron scattering as well as instructions on how industry can benefit from free measurements and feasibility studies funded by the project. We support them actively on social media as well.

h. We have identified and liaised with other projects and institutions who share the same interests with the aim of fostering collaboration. Thanks to these contacts:

- we can now post some of our news on the ESFRI website,
- we published an article on "Neutrons for research and ongoing international collaboration" on the e-EPS (European Physical Society) newsletter on November 24, 2016,
- we published an editorial on "Communicating Neutron Scattering" on the journal *Neutron News*, published on January 24, 2017,
- we were involved in the publication of two articles (one on Neutronsources.org and the other on the journal *Neutron News* – upcoming) on the contribution of neutron scattering to validate the predictions of the 2016 Nobel Prize laureates in Physics,
- interaction with other facilities and projects on social media has increased,
- the project was presented at the MaMaSELF (Master in Materials Science Exploring Large Scale Facilities) status meeting on May 10-13, 2016,

- SINE2020 flyers and Neutron brochures will be distributed at the MLZ stand in the German Neutron Scattering Conference, and at the IAEA General Conference.

i. Given that there are a number of common members with the project brightnESS, we thought it made sense to organise a joint communications meeting with all the facilities press officers. We met on March 7, 2016 in Lund, to present the two projects, foster collaboration between the 32 attendees, and run two small media-related workshops.

j. Native Scientist: The Information Manager was part of the "Native Scientist" activity in Munich, where she went to a school with another three scientists to explain neutron scattering to 10-year olds in Portuguese, which is hers and their mother tongue. The initiative aims to bring science to schools while at the same time giving the opportunity to students who live in foreign countries to speak in their mother tongue.

k. With the aim of reaching University students, we have contacted a number of people who teach neutron scattering at universities so that they tell their students about all the information that might be useful for them (e.g. the schools we fund; the e-learning portal; Neutronsources.org). While it is out of our control whether they showed our slide, we have received positive replies from a number of them. Neutron schools have also been contacted with a positive feedback.

Annex I: List of dissemination publications on sine2020.eu – months 1-12

1	Interviews with students of the MATRAC2 school	31/03/2017
2	Boosting innovation with neutrons	30/03/2017
3	NOW opening: FREE analysis of your material or device at European neutron research facilities	30/03/2017
4	Neutrons for science and technology: second edition of the ENSA Brochure	28/03/2017
5	Deuteration User Survey	27/03/2017
6	JOB: We're looking for an Information Manager	23/02/2017
7	40 participants met in Lund to discuss the SINE2020 Sample Environment collaboration	15/02/2017
8	Registrations open for CETS2017	13/02/2017
9	Registrations open for the JCNS Laboratory Course Neutron Scattering	07/02/2017
10	Haldor Topsøe uses neutrons to improve performance of cells for hydrogen production	07/02/2017
11	Apply now to the Oxford School on Neutron Scattering	01/02/2017
12	Improved formulation for STEPAN surfactants	27/01/2017
13	Communicating neutron scattering on Neutron News	25/01/2017
14	High pressure research using muons at PSI	24/01/2017
15	The first year of SINE2020 support of neutron and muon schools	16/01/2017
16	Neutrons: Cradle to Grave workshop - slides and videos available	14/12/2016
17	MCPL: a new format that simplifies data interchange between applications	13/12/2016
18	Improving the fitting in Mantid for neutron and muon data	05/12/2016
19	Neutrons on the e-EPS	24/11/2016
20	Release of SasView 4.0.1	23/11/2016
21	What if neutron scattering uses the same type of detectors used to look into space?	11/11/2016

22	Funding available for Neutron and Muon Advanced Schools	02/11/2016
23	New Interactive Brochure: NMI3 – A successful European collaboration for science	25/10/2016
24	NEW VIDEO: 1 Year of SINE2020	20/10/2016
25	The new Industry brochure	19/10/2016
26	New Management team at ILL as of October 1, 2016	11/10/2016
27	Where is the muon? A review of simulation methods	30/09/2016
28	Job: Postdoc Scientist in Muonium Chemistry at ISIS	29/09/2016
29	NOW opening: FREE analysis of your material or device at neutron research facilities	28/09/2016
30	SINE2020 funds metallurgy, surfactants, microelectronics, and fuel cells experiments	28/09/2016
31	26 students attended the Italian Learning Days School	27/09/2016
32	Martin Böhm is the new SINE2020 Coordinator	27/09/2016
33	Apply to the Berlin School on Neutron Scattering by October 15	22/09/2016
34	95 scientists met in Coimbra for our General Assembly	15/09/2016
35	Q&A: Enhancing cooperation between industry and neutron facilities	13/ 09/2016
36	Sample Environment: Interview with the coordinator	30/ 08/2016
37	Funds for post-grant FP7 publications	01/ 08/2016
38	Project administrators met EC auditors to help secure eligibility of H2020 funding	01/ 08/2016
39	SINE2020 facilitates the study of the human body	11/ 07/2016
40	The CETS School 2016: a summary	05/ 07/ 2016
41	Chemical Deuteration: interview with the coordinator	29/ 06/ 2016
42	New MicroStrip Gas Chamber to be produced within the SINE2020 Detectors WP	14/ 06/ 2016
43	Workshop I of the SINE2020 WP on Data Treatment	14/ 06/ 2016
44	ILL is looking for a Head of the Computing for Science Group	08/ 06/ 2016
45	Registration to the SINE2020 General Assembly is open	23/ 05/ 2016
46	Job offer: Postdoc in Biology, Biochemistry or Biophysics	23/ 05/ 2016
47	ESFRI report alerts to risks of shutting down neutron facilities in Europe	20/ 05/ 2016
48	The ESS View on SasView	19/ 05/ 2016
49	John Womersley to be the next ESS Director General	12/ 05/ 2016
50	PSI is looking for a Director of the neutrons and muons division	27/ 04/ 2016
51	Helmut Schober to be the next ILL Director	18/ 04/ 2016
52	SINE2020 has a new Industrial Liaison Officer	23/ 03/ 2016
53	Schools to receive SINE2020 support announced	22/ 03/ 2016
54	NOW opening: FREE analysis of your material or device at neutron research facilities	17/ 03/ 2016
55	Neutrons for Industry: SINE2020 aims at increasing industrial use of European neutron sources	16/ 03/ 2016
56	Communicating collaboration – communications officers met in Lund	11/ 03/ 2016
57	Mark Johnson to be next ILL UK Associate Director and Head of Science	09/ 03/ 2016
58	Neutron scattering e-learning platform now online	09/ 03/ 2016
59	Explaining neutron scattering to children in their mother tongue	02/ 03/ 2016
60	Job: Post-Doctoral Fellow in Biochemistry at the ILL	26/ 01/ 2016
61	Call for proposals for funding of neutron and muon introductory schools	02/ 12/ 2015
62	Job: Three Scientific Software Programmers at the ILL	20/ 11/ 2015
63	Job: Deuteration Chemist to ESS	18/ 11/ 2015
64	140 scientists met in Copenhagen for the NMI3 and SINE2020 meetings	29/ 10/ 2015
65	Vacancy for SINE2020 Postdoc in Biophysics	02/ 11/ 2015
66	Post-doc position funded by SINE2020 offered at the University of Parma	07/ 10/ 2015

Annex II: Meetings/events within WP2 – months 1-12

Date	Place	Topic of meeting	Who participated
16/11/2015	Copenhagen	Joint Business Communicators meeting	Industry WP leader Information Manager
16/09/2016	ESS	SINE2020 and brightnESS joint industry outreach meeting	Industry WP leader Information Manager
7-9/09/2016	Uni. Coimbra	- General Assembly, Board and WP meetings - Meeting with local press officers - Interview to Detectors WP	All project
23-27/07/2016	Manchester Complex Centre	- EuroScience Open Forum (ESOF2016) - H2020 Science Communication meeting	Information Manager
13-22/07/2016	Rhine-Waal Uni.	STEAM Communications Summer School	Information Manager
7/03/2016	ESS	SINE2020 and brightnESS joint communications meeting	Information and Project Manager
27/10/2015-06/11/2015	ILL	- Interviews to WPs - Communication strategy for SINE2020 - Collaboration with Neutron News, Neutronsources.org history pages, and Press Officers from ILL and ESRF	Information manager Project manager Project coordinator
14-15/10/2015	Copenhagen University	General Assembly, Board and WP meetings	All project

1.2.3 WP3 - Training neutron scattering, e-learning and schools:

Task 3.1: Development of e-learning platform (e-neutrons.org)

In SINE2020 we have further developed and expanded the neutron e-learning platform (http://www.e-neutrons.org, see fig 1), which was developed and launched through NMI3-II in FP7. The platform currently includes an introductory neutron scattering course in two formats (high-guidance self-study and no-guidance pick-and-choose) as well as an introductory course in muon spin rotation. It is possible to sample the learning material without a registered account via the e-neutrons front page tasters (see fig 1 bottom).

Within the current project we have especially worked on improving the user administration and experience as well as developing tools for cloning the e-learning material produced by the e-neutrons team to personalized courses for use in blending learning in connection with on-site schools. Furthermore we are in the process of expanding the e-neutrons learning material with ESS relevant activities.

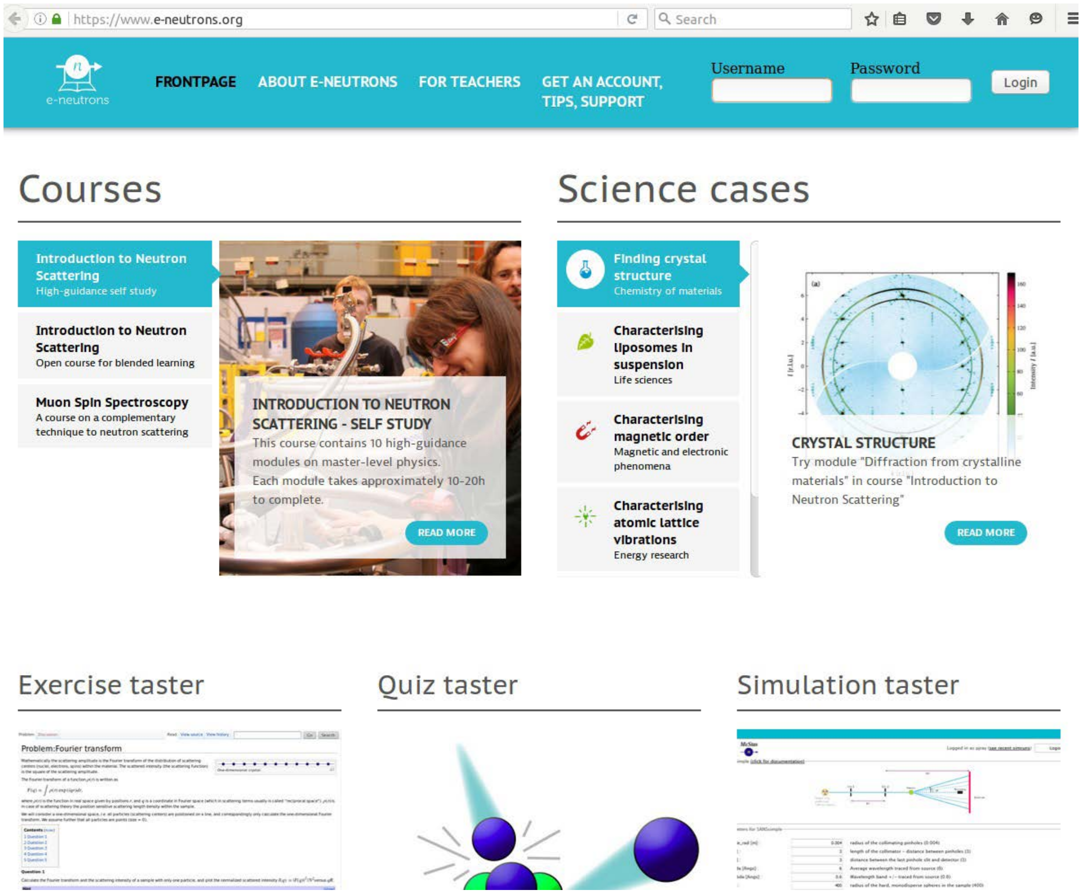

Fig 1: screenshot of the e-neutrons frontpage with sign up, tasters etc

Task 3.1.1: Coordination & management *(UCPH M1-48) 10 PM*

We carry out monthly 1-day meetings on coordination and development of e-neutrons with the rest of Danish WP3 team. We also recently had an online WP3 meeting with TUM participants identifying the need for closer collaboration, better communication tools and a student worker dedicated to e-neutrons at TUM. The job will be posted as soon as possible in the Spring of 2017 and we will decide on a collaboration platform Summer 2017.

Task 3.1.2: Platform development *(DTU M1-48) 4PM*

New users can sign up independently to one or more courses via http://www.e-neutron.org or can be bulk enrolled via a web-tool, which has been developed in PR1.
A new 3D visualization tool of simulated rays has been developed for the online simulator mcweb at e-neutrons. It allows student to follow the neutron propagation from source though instrument to detector and view the process dynamically from all angles, see Fig 2.
A web-tool for cloning the master copy of the introductory neutron scattering course was also produced within this project period. The course clone is administered by e.g. an organizer or teacher, who adapts it to suit their needs in blended learning, e.g. which topics to include, the pacing and which students to

enroll. It is also fully open for the teacher to remove or add new teaching material to the lesson plans in their clone. A web-tool has been developed to upload new McStas instruments so that teachers can also create their own personalized simulation quizzes. The wiki textbook remains the common teaching material for all clones and is thus not copied but referred to via links when appropriate. So far the course clones are hosted by the e-neutrons development server at DTU. We are working on a solution for hosting and administration of the copies at TUM.

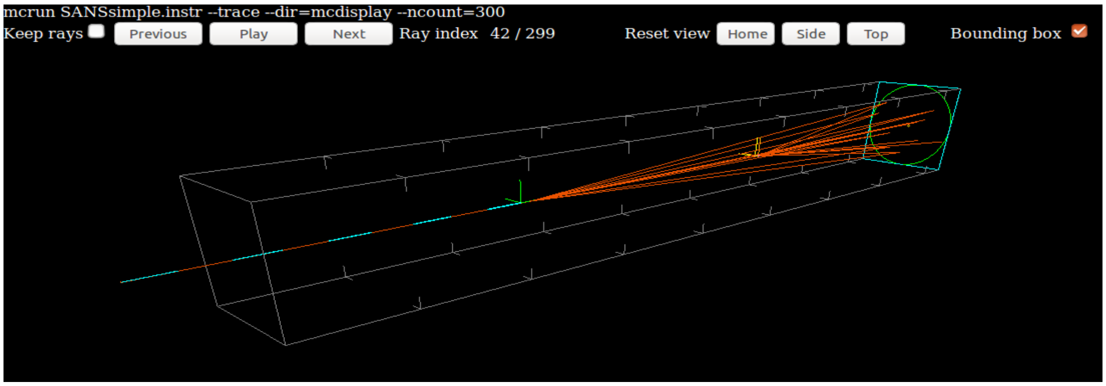

Fig. 2: Screenshot of the 3D visualization tool for online neutron simulation

Task 3.1.3: Student assessment & evaluation *(UCPH M1-48) 10PM*

The quizzes at e-neutrons have been developed with the purpose of providing each student with a tool for active learning and self-assessment rather than certification of competences such as ECTS points. We will evaluate the use of these didactical tools and make recommendations on how to include certification in an e-neutrons course.

Task 3.1.4: Evaluation/production of learning material *(UCPH M1-36) 12 PM*

We are currently analyzing user data from WIKI textbook in order to identify typical user behavior; the results and evaluation will go in a written document [*Student interaction with online textbooks: What can be learned from serverlogs*, J. Bruun and L. Udby, in preparation 2017].

We are continuously expanding the learning material in the wiki and have implemented student-activated hints and solutions to most wiki exercises.

Two new learning quizzes have been finished and implemented which connect the neutron scattering techniques diffraction and inelastic scattering by using the same sample material (nickel) as a science case.

Task 3.1.5 Formatting/implementing learning material *(UCPH M1-36) 6 PM*

We have hired a part-time student assistant for 1 year to update existing learning material and implement version control. He will also make a report of which features are used, when and how in the various e-learning material at e-neutrons (D3.1). We intend to use this overview to define and discuss the e-neutrons software requirements in task 3.2.1.

We have also uploaded material in the e-neutrons library section from all the on-site schools, which have received funding though WP3.

Task 3.1.6: Muon e-learning (ISIS) *(ISIS M1-24) 2 PM, (PSI M1-24) 1 PM*

An e-learning course regarding muon spin rotation (Introduction to muon spin rotation) was developed and finished with two modules, one regarding cosmic ray muons and another regarding muon data analysis (D 3.3). Both were implemented with great success in the ISIS muon training school 2016.
Most students are not familiar with the basic concepts needed for muon spectroscopy, so they need an introduction module. For this purpose we converted original material from an ISIS-Diamond training school for graduate students using an undergraduate demonstration practical. This uses cosmic rays, cosmic ray muons and a simple experimental setup for muon data collection (like one detector on an instrument). The e-learning module teaches key theories and skills and implements end of topic quizzes to further aid understanding. A part of this quiz module is shown in Fig.3.
All the lectures given at the on-site ISIS muon training school 2016 were filmed and made available together with the e-learning modules mentioned above in the e-neutrons course "Introduction to muon spin rotation". The course is available on demand for all registered users of e-neutrons.

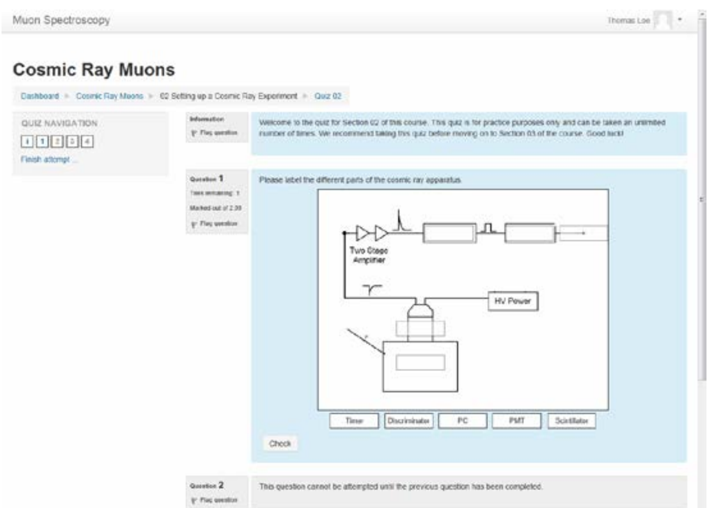

Fig.3: Screenshot of a quiz module for mons.

Task 3.2: Development of a virtual neutron facility and training material

We have decided to include up to 4 ESS instruments with samples in the virtual neutron facility. We have discussed the step-wise procedure to construct the virtual experiments. Two science cases for two VE have been selected for reworking into VE instruments and corresponding learning material.

Task 3.2.1: Virtual ESS instruments *1 (DTU, CEA M1-24) 19 PM*
In order to complement the existing virtual neutron instruments at e-neutrons we have decided to include up to 4 ESS instruments with samples to represent the major neutron techniques and research fields which will be used in real experiments at ESS (D3.7). We have decided to construct a neutron imaging instrument representing the instrument ODIN at ESS as our first virtual instrument, following a stepwise approach

Fig 3: Screenshot of part of a quiz module in "Introduction to muon spin spectroscopy" from a simple template instrument to a more complex one optimized to include specific variable parameters which are important for the student learning experience.

Task 3.2.2: Corresponding training material *(UCPH,DTU M1-36) 10 PM*
In order to enable the student to achieve the optimal learning outcome of the virtual experiments, learning material needs to be constructed, which couples the virtual instrument, virtual sample and adjustable parameters to a corresponding real experiment and the data, which are obtained therefrom (D3.7). Our approach is to develop a quiz from a specific science case as the first part of the learning material to set the learning objectives. Once the quiz is finished we will embed it in an e-learning module and provide the appropriate background reading material for the student from self-written or freely available open online sources. Currently we are constructing the first quiz module regarding imaging on a cultural heritage object in collaboration with specialist Anna Fedrigo (ESS).

Task 3.2.3: Implementation online and blended *(UCPH, DTU M36-48) 10 PM*

The simulation quiz module will be implemented online at e-neutrons and tested in a blended learning setting when it is finished.

Task 3.3: Enhancing coordination for Pan-European neutron training Schools *(CEA, MTA EK M12-48)*
CEA and MTA-EK have setup of a common international evaluation panel between introductory and advanced school. The neutron schools were revieved recently (March 2017) by the chair of the evaluation panel, Julian Oberdisse, including recommendations for future schools.

MTA-EK has organized a call of support for the organization of introductory schools. 11 school organizers applied and 8 schools were elected for support based on assessment from the international evaluation panel. The ranking and funding of the schools is shown in the table below.
The learning material from all funded schools has been uploaded to the e-neutrons.org library.

School	Requested 2016 (EUR)	Requested 2017 (EUR)	Received 2016 (EUR)	Received 2017 (EUR)	School Attendees
01. JCNS Laboratory Course on Neutron Scattering, Jülich (2016, 2017)	10 000	10 000	8 000	8 000	54
02. Berlin School on Neutron Scattering (2016, 2017)	9 800	9 800	9 800	9 800	29
03. CETS, Central European Training School, Budapest (2016, 2017)	10 000	10 000	8 000	8 000	31
04. Hercules2016, Grenoble (2016, 2017)	10 000	10 000	7 500	7 500	80
05. ISIS Muon Spectroscopy Training School (2016)	10 000	-	10 000	-	31
06. Oxford School on Neutron Scattering (2017)	-	10 000	-	7 000	After PR1
07. Giornate Didattiche, Italy (2016, 2017)	-	-	7 000	7 000	26
08. PSI Summer School (2017)	-	10 000	-	10 000	After PR1

09. School on Scattering Methods Applied to Soft Condensed Matter, ILL (2016)	-	-	-	-	
10. Fitting and modelling Inelastic Neutron Scattering Data, PSI (2016)	-	-	-	-	
11. COST School on Surface Analytical Techniques, Jülich (2016)	-	-	-	-	

CEA organized a call of support for the organization of advanced schools: 7 schools applied, 6 were elected for support, based on assessment from the international evaluation panel as shown in the table below:

School	Requested 2016 (EUR)	Requested 2017 (EUR)	Received 2016 (EUR)	Received 2017 (EUR)	School Attendees
01. Matrac 2 Matrac 1 + special focus on Fundamental Aspects of Materials	-	2500	-	2500	44
02. SonS The neutron precession techniques	-	8700	-	8000	To be announced
03. Matrac 1 Application of Neutrons and Synchrotron Radiation in Engineering Materials Science	-	3 000	-	3 000	44
04. SISN Neutron scattering data handling	-	10 000	-	5000	To be announced
05. Bombannes 2016 Scattering Methods Applied to Soft Condensed Matter	8 000	-	5000	-	42
06. Bombannes 2018 Scattering Methods Applied to Soft Condensed Matter	-	8 000	-	5000	To be announced
07. Frontiers of Condensed Matter Physics	-	1000	-	-	-

1.2.4 WP4 - Industry Consultancy:

Task 4.1: Network coordination and management *(HZG M1-48) PM18*

As coordinator of WP4, the ILO at HZG was responsible of the project management tasks. This contained coordination of personal and video meetings, reporting to the SINE2020 project management and the cooperation between WP4 and WPs 2 and 3 as well as, externally, with as well as other activities for industry outreach like Science Link Network or the INTERREG Baltic Sea Region Project Baltic TRAM.

The HZG ILO was also responsible for the communication of the project activities to the Industry advisory board (IAB) and the implementation of their comments and advice in the WP activities.

Within the first 18 months three work package meetings were organised: Grenoble (F), 01-26-2016, Coimbra (P) 09-07-2016, and Garching (D), 03-30/31-2017, which defined the general strategy among the partners towards industrial liaison. The meeting in March 2017 emphasized on the coordination with the members of the international advisory board (IAB), who work together with WP partners on chosen tasks.

The central management task of WP4 is the coordination of the work of the project partners, especially of the two full time employees (at HZG and ILL) and the communication with WP2 (Communication) and WP1 (Management). Important information was shared with the WP partners in conference calls on a regular basis (7 meetings in 18 months).

Task 4.2: Information and outreach *(HZG, TUM M1-48) PM50*

The HZG ILO designed, together with the communication officer from WP2, the content of the industry section of the SINE2020 homepage by creating to the general concept of the pages. Industry relevant methods and examples of successful cooperation available at the partner facilities were edited in the form of easy accessible case studies (pdf version on http://www.sine2020.eu/industry.html).

In addition, information about the service offered to industry by SINE2020 was disseminated by electronic four newsletters, two press releases and in social networks (Twitter, LinkedIn).

The partners participated in various events (cf. Table 4.1) to inform industry about the offer by SINE2020 and the opportunities for innovation and research. The SINE2020 partners visited 22 events to meet industrial researchers and inform them about the SINE2020 offer. On 14 events SINE2020 WP4 was presented by an exhibition booth and/or poster/oral presentation.

Table 4.1: Participation in Events

	Event	Date	Location	Participation	external Partners	SINE2020 beneficiaries
1	Nanotechnologies and Advanced Materials	2016-03-23	The Hague (NL)	Visitor + meetings + breakout session	-	TUD
2	Business Rendez-Vous Ostrava 2016	2016-05-23	Ostrava (CZ)	Networking, poster	-	NPI
3	Fuel Cell and Hydrogen Conference	2016-05-23-25	Birmingham (UK)	Stand	-	ILL
4	High time for Beam Time Information Event	2016-06-07	Szeged (HU)	Presentation	Science Link Network	NPI
5	High time for Beam Time Information Event	2016-06-07	Dolní Břežany (CZ)	Presentation	Science Link Network	MTA-EK, NPI
6	World Conference on Non-Destructive Testing	2016-06-13/17	Munich (D)	visitor	NFFA	HZG
7	Industrial Technologies – Creating a Smart Europe	2016-06-22/24	Amsterdam (NL)	Presentation	NFFA	TUD, HZG
8	Journées territoire et Hydrogène	2016-06-29/30	Grenoble (FR)	Visitor	-	ILL

9	Imaging - Pushing the Limits	2016-07-04	Hamburg (D)	Presentation	Baltic TRAM	HZG
10	DGM-FA-Aluminium	2016-07-07	Hamburg (D)	Presentation	Science Link Network	HZG
11	VDI-TUM Expertenforum	2016-09-15/16	Garching (D)	Visitor + poster	-	HZG
12	Industry Space Days	2016-09-20/22	ESTEC Noordwijk (NL)	Stand + meetings	-	ILL, TUD
13	World of Tech & Science	2016-10-4/7	Utrecht (NL)	Stand	-	TUD, HZG
14	3D print Exihibition	2016-10-4/5	Lyon (FR)	Stand	-	LLB, ILL
15	Rendez-vous Carnot	2016-10-5/6	Lyon (FR)	Stand + meetings	ESRF/IRTnano/NFFA	ILL
16	AUTOMOTIVE Hungary 2016	2016-10-19/21	Budapest (HU)	Stand, Satellite workshop	-	MTA-EK, HZB, ILL
17	Re-IndusEU2016	2016-10-26/28	Bratislava (SLK)	Stand, Satellite workshop	Science Link Network, ESRF, CALIPSO, CERIC	MTA-EK, HZG, NPI
18	Baltic TRAM Conference	2016-10-26	Hamburg (D)	Presentation (with ESRF)	Baltic TRAM	HZG
19	London Space week	2016/11/15-16	London (UK)	Visitor + meetings	-	STFC
20	TechInnov	2017-02-23	Orly (FR)	Visitor + meetings	-	ILL
21	Innovation for Health	2017/02/16	Rotterdam (NL)	Visitor	-	TUD
22	Materials2Industry	2017/03/22	Hamburg	Visitor	-	HZG

We also prepared and designed a series of material (hardware) to support outreach activities at events, conferences or workshops:
- A mobile booth and 2 roll-ups for trade fairs, accessible to all partner.
- 13 case studies (in a form of a double sided A4 sheet) taken from scientific experiments which are relevant to industrial companies.
- A print (and web) brochure to be handed out at events together along with printed versions of the above mentioned case studies.
- Promotion materials like pens, postcards and folders for the information brochures and case studies.

WP4 developed a concept for outreach activities to establish efficient neutron research centre-industry interaction (D.4.1). Following this concept SINE2020 hosted focused satellite workshops to bring together participants from industry, science and politics, to discuss cooperation between industry and academic science at large scales facilities in general and neutron facilities in peculiar. Further events are in planning. A large event will be organised in Amsterdam on March 8/9, 2018.

Task 4.3: Education and Training *(HZG, TUM M1-48) PM50*

An industrial adapted approach to the technic has been elaborated with the IAB (D4.2). It was concluded that the emphasis has to be put in a first stage on general information (4.2) and easy access (4.4) in close collaboration with instrument scientists. Once direct access has been established, specific industrial adapted education tools as developed in WP3 are necessary for efficient training of industrial scientists.
It was agreed with WP3 to utilise e-neutrons.org's web infrastructure to launch dedicated short courses for industry. WP4 will create content in the form of videos/animations and text to explain solutions for typical problems in different industry sectors. A first concept was developed during the WP4 meeting on March 30/31, 2017.

In the framework of the EU-project BrightnESS related to the future European Spallation Source, industrial R&D managers and researchers have been interviewed in order to collect their requirements for neutrons measurements, access to the facilities and training/education. The results of this survey have been shared with SINE2020. The analysis of the BrightnESS study and the creation of a concept for further steps in education and training were done in cooperation between ILL and HZG.
A concept for practical training, which should be focused on providing the basics of neutron techniques, is described in detail in Deliverable D4.2.

Task 4.4: Access *(HZG, ILL M6-48) PM52*

SINE2020 launched two direct calls for industrial applications to measurements. The first call was open from March 28, 2016 – June 30, 2016, the second call from September 28, 2016 to January 21, 2017. We are using dates for communication purposes only and requests are processed continuously (on the flow). Up to now, 17 applications (Fig. 4.1) have been be reviewed by a board of experts consisting of staff members of the participating neutron centres. From these applications, 11 could be accepted (the other six being either from academic users or not feasible for neutron techniques, Fig. 4.2). On average, one day of neutron beam time is granted to the applicants.

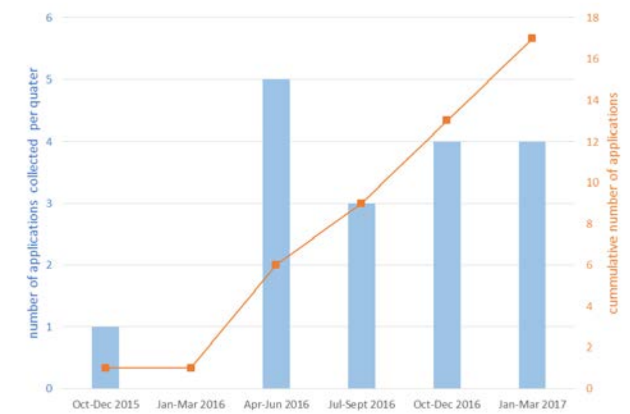

Figure 4.1: Number of received applications per quarter since the start of SINE2020.

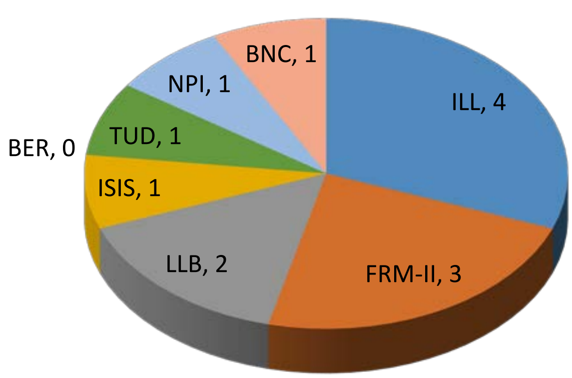

Figure 4.2: Distribution of test measurements per facility (total number is 13, since two of the eleven selected studies were conducted complementary at two facilities).

In the frame of Deliverable 4.3 the results of the first two calls and the already conducted measurements were summarized and transferred in case studies to be used as information material both on events and the project website.

The industrial liaison officer (ILO) at ILL treats the incoming applications. This task includes the collection and follow-up of the requests from companies as well as of the measurements themselves (including reporting) and further feedback from the companies. It also includes first contacts with applicants to request further details in order to ease the decision process for each WP partner.
In case of the ILL the ILO and instrument scientist are responsible for the conduction of the measurement, data analysis and reporting.

1.2.5 WP5 - Deuteration:

Task 5.1: Chemical deuteration by catalytic H-D exchange and synthesis of surfactants *(STFC M6-30) 24 PM*

The STFC Deuteration Facility receives two proposal calls annually for deuteration compounds from the UK and international ISIS neutron user community and also through ILL neutron proposal calls. The STFC Deuteration Facility regularly produces a large number of deuterated precursors through catalytic deuterium hydrogen exchange, including aliphatic hydrocarbons such as fatty acid, bromoalkanes, and organic ligands. A wide variety of compounds (also the corresponding protonated versions if not commercially available) has been synthesized, for example, in 2016 we received 83 requests, of which 63 were supported. For the work in WP5 (Tasks 5.1) Dr. Kun Ma was recruited on a fixed term at the end of October 2016 (M13) and has so far fully supported four proposal requests, including one from the ESS in Sweden. He has produced 11 deuterated surfactants in for user beam time and produced four deuterated fatty acid precusors.

The following projects have been supported by the STFC Deuteration Facility through SINE2020 WP5 funding in period 1 (M1-18):

a. A large quantity of perdeuterated ligands (>25gram in total) for Professor P Santini (Università di Parma, Italy), for a project on Spin dynamics of the Mn12 prototype nanomagnet unravelled by 4-dimensional inelastic neutron scattering (D5.2, D5.7). The experiment is part of an ILL PhD studentship pf Simon Ansbro and the national Italian FIRB project "New challenges in molecular nanomagnetism: from spin dynamics to quantum information processing". The experiment was a success, and a publication is currently in preparation.
b. The routine deuterated CTAB, SDS, AOT and nonionic surfactants(C12E6) for non-UK users of ISIS (D5.7), including Andrew Jackson (ESS) for applying self-assembly in deep eutectic solvents to templated ionothermal synthesis; a joint PhD project of Adrian Sanchez-Fernandez with Professor Karen Edler (University of Bath).
c. 11 surfactants with different counterions for non-UK users (ESS) (D5.7) for beamtime on the SANS2D instrument, which was completed.
d. Synthesis of several non-routine compounds to non-UK users (D5.7), for example deuterated Triolein, and Tween 80 detergent for Tommy Nylander (Lund University).
e. Deuterated resorcinol, urea, benzyl alcohol and choline chloride Mr F D M del Monte, CSIC, Instituto de Ciencia de Materiales de Madrid, Spain (D5.7) for the study of deep eutectic solvent

dilutions: nanometer size domains and molecular reorganization for an experiment on NIMROD that was successfully completed.

f. Deuterated trimethylglycine for Professor M Ricci (Università di Roma Tre, Italy) (D5.7) for an experiment on the SANDALS instrument scheduled in early 2017.
g. Method development and synthesis of 15g of deuterated quinolin-8-ol ligand for Prof. Caretta Stefano (Italy) (D5.7) and Richard Winpenny for ISIS experiments.
h. Deuterated chemicals for DEUNET partner laboratories (D5.2), such as deuterated pentadecanoic acid as precursor to methyl pentadecanoate to be used as internal GC standard in lipid analysis for Hanna Wacklin (ESS) and help with deuterated factty acids (Rachel Morrison, ILL).
i. The facility is currently optimising the unsaturated fatty acid synthesis (D5.7) and has produced intermediates.

The STFC Deuteration Facility is co-organizing the STFC Deuteration User meeting jointly with the DEUNET workshop at the Oxford Spires Hotel, 15-17 May 2017.

Task 5.2: Extraction and purification of small molecules from deuterated cell cultures *(ILL M6-42) 36 PM*

Work at ILL has started on preparing deuterated lipids derived from cell cultures. Initially we investigated the adaption of three acetobacter stains to perdeuterated media, however, the bacteria did not grow to high enough cell densities in either hydrogenated or deuterated media and therefore it was concluded that these strains are not useful for the large-scale production of lipids. Additionally, the fatty acid profile of the lipids produced by the bacteria was not as we had hoped for, as they did not produce any lipids with oleic acid chains – instead a different isomer (vaccinic acid – 7-cis octadecenoic acid) is produced by these bacteria.

We have therefore decided to return to the yeast strain that we have previously used for lipid extraction as we know this strain can successfully grow in deuterated media. We had previously found that while phospholipid class homeostasis was maintained, the composition of fatty acids was impacted with significantly higher C18:1 produced under deuterated conditions (De Ghellinck. *et al.* PLoS One, 9 (2014) 9). We are currently studying how the growth conditions of the yeast affects the type of lipids produced to enable more comparable hydrogenated and deuterated lipids to be produced. Preliminary results have indicated that both the growth temperature and carbon source have an effect.

We have also investigated methods for the separation of phospholipids. We were initially interested in the molecular species separation of the lipids, however, after reviewing the literature and discussing with several experts in the field we have since decided that this is not practical due to the difficulty and small amount of material which would be recovered. We are therefore going to focus on separation based on either chain length or saturation level which we believe will be easier to achieve. We also hope that by ensuring that both the hydrogenated and deuterated samples are equivalent then less separation would be required.

Rachel Morrison visited ESS to learn lipid extraction and separation techniques in February 2017. She also attended a course run by the James Hutton Institute on Fatty acids and lipids which gave a good overview of the field and an insight into different techniques which can be used for lipid analysis.

Task 5.3: Synthesis of complex deuterated molecules *(ESS M6-42) 48 PM*

D5.4 Synthesis of L- and D-lactic acid

ESS has made considerable progress within Task 5.3 towards completing deliverable D5.4, including:

a) Synthesis and characterisation of a deuterated precursor to the enzymatic reaction for producing lactic acid (sodium pyruvate-d_3).[1-2]

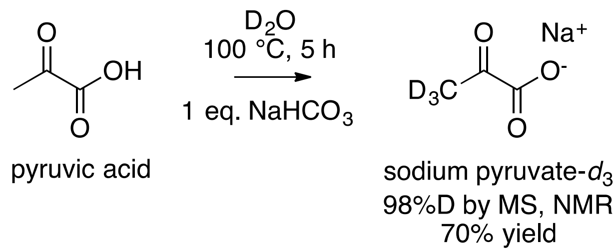

Fig. 5.1: Production of sodium pyruvate-d_3 from pyruvic acid in D_2O.[2]

b) Synthesis of the monomer acryloxysuccinimide for co-polymerisation with acrylamide.
c) Synthesis of the polymer to serve as support material for the enzymatic reaction (poly(acrylamide-co-*N*-acryloxysuccinimide) (PAN). The reported initiator AIBN is no longer available so an alternative catalyst (ACHN) was used, which required some changes in reaction conditions. The literature method[3] and the method we employed are summarised in Fig. 5.2.

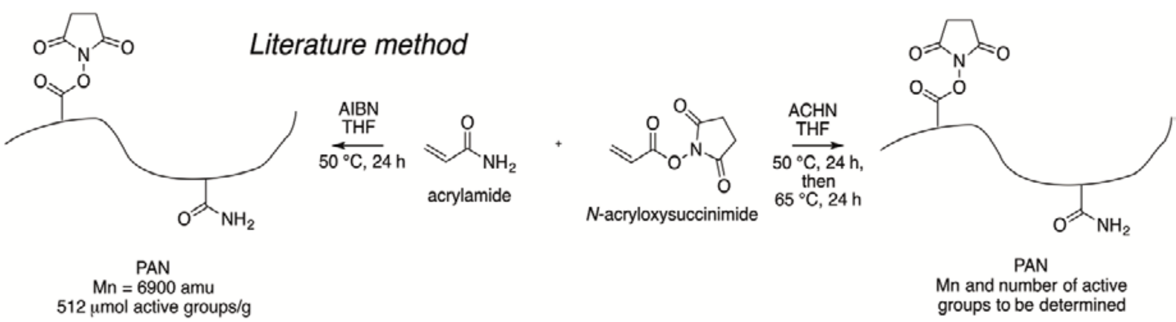

Fig.5.2: (Left) Literature method for the synthesis of PAN with Mn = 6900 amu and 512 μmol active groups/gram;[3] (right) the method employed in our laboratory.

The effects of changing catalyst and reaction temperature on the polymer product (molecular weight and number of active groups) are being investigated using UV-Visible spectroscopy and Dynamic Light Scattering (DLS) at Lund University, where we have arranged to access analytical equipment not available at ESS. We expect to complete the polymer characterisation and lactic acid synthesis by M24 (September 2017).

An automated flash chromatography system (Biotage Isolera) was procured for the purification of the compounds synthezised. In addition the materials (enzymes, co-factors, hydrogenous test-substrates and reaction vessels etc.) and equipment required for the immobilisation of the enzyme have been procured. The best system for monitoring the reaction progress by pH-STAT titration (Metrohm 907 Titrando) has been identified and will be procured shortly after the end of P1.

We have concluded that a deuterated reaction solvent is not required for the production of per-deuterated lactic acid from pyruvate, reducing the cost of the synthesis significantly. The only deuterated co-factor needed is the formate substrate of the NADH-regenerating enzyme formatted dehydrogenase). This is commercially available but can also be synthesized in-house to reduce the overall cost of lactic acid production.

We will also investigate the physical entrapment of enzymes in dialysis tubing as an alternative method of enzyme immobilisation.

We have begun investigation of the isolation and purification of the lactic acid produced by using a racemic, non-labelled sample of DL-lactic acid (85% solution in H_2O). Continuous solvent extraction has been identified as a suitable method for the isolation of the deuterated enantiopure D- and L-lactic acid from the reaction mixture.

D5.11 Synthesis of novel deuterated lipids and surfactants

For this project, we have begun to set up the analytical equipment and processes to allow us to isolate molecules from cell cultures for further derivatisation by chemical or enzymatic synthesis including

a) Analysis of the composition of unlabelled cell cultures known to contain high-value lipid components;
b) Production of promising cell cultures under deuterated conditions at our collaborating laboratory at Lund University (Lund Protein Production Platform LP3) and analysis/ purification of components
c) Enzymatic conversion of biological lipid mixtures as a potential new route to complex deuterated lipids.

The possibilities of combining chemical synthesis with biological expression have attracted interest from several university collaborators at Lund, Umeå, Oslo and in Canada for deuterated cell components as mixtures, single molecular species, or synthetic derivatives such as for new collaborations that have recently submitted beamtime proposals to ISIS and ILL.

Task 5.4: Polymer synthesis *(FZJ M6-30) 18 PM*

D5.3 Synthesis of deuterated isoprene

The Jülich Centre for Neutron Science as a part of the Forschungszentrum Jülich (FZJ) contributes to the project with its knowledge in the field soft matter. Especially, deuterium labeled polymers are of high importance for science and industry when they are applied in neutron science. The synthesis of such polymers is a complex process, usually starting from the synthesis of monomers. As deuterated monomers are in many cases not commercially available, they have to be synthesized in the laboratories. Moreover, the variety of potential starting materials is scarce and therefore limiting the number of potential chemical transformations. One goal of the project is to develop new synthetic routes to deuterated monomers, important in applications. Exemplarily, isoprene, a monomer for the synthesis of synthetic rubber is highly desired, but cannot be obtained in the required high purity. The synthesis of poly(3-hexylthiophen-2,5-diyl) (P3HT) is another example, a material which is relevant for light emitting diodes (LEDs) and organic solar cells, as well as poly(lactic acid) being relevant as a renewable plastic with high biocompatibility for medical applications.

Synthetic rubber, which is industrially used as a component in rubber tires, can be made of isoprene and is therefore of high relevance for industrial applications and science. To study the polymer (polyisoprene, PI) by neutron scattering, it is necessary to gain access to its deuterated form which is accomplished by the synthesis of deuterated isoprene monomer. There is an established route to this compound, however with certain disadvantages such as multiple steps, low selectivity including a high temperature elimination step. To avoid these circumstances, a new method leading to highly pure, deuterated isoprene was established (D5.3), and is shown in Figure 5.3.

The method starts from the selective α-oxidation of acetone-*d6* to the corresponding diketone typically using selenium dioxide as the oxidant. An access of acetone-*d6*, which can be recovered, is needed to avoid overoxidation to pyruvic acid. Ideally, the next step would be a two-fold Wittig reaction using a deuterated C1 Wittig reagent. Unfortunately, the diketone (methylglyoxal) strongly tends to oligomerisation. This problem was overcome by the use of protective group chemistry allowing a subsequent Wittig reaction after deprotection.

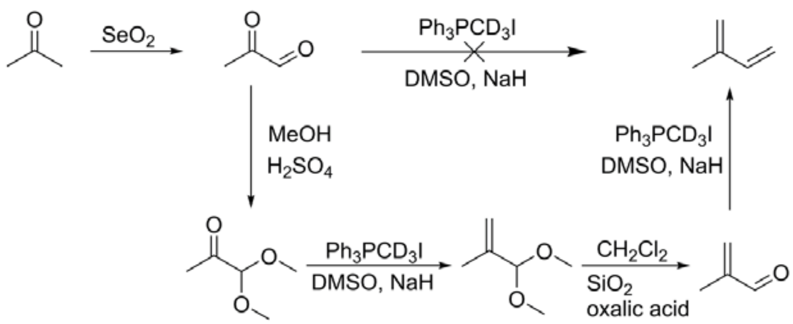

Fig. 5.3: Overall reaction scheme of the synthesis of isoprene-*d8.*

D5.5 Synthesis of P3HT

Poly(3-hexylthiophen-2,5-diyl) (P3HT) is a conductive polymer which can be applied in organic light emitting devices (OLEDs) or organic solar cells and therefore relevant in the field of renewable energy (D5.5). For structural investigations, it is necessary to establish a route for high molecular weight block copolymers consisting of P3HT and polyethylene oxide (PEO). There are some synthetic routes described in literature which may lead to this material, however they were not tested for high molecular weight materials with narrow molecular weight distribution. Therefore, different approaches were screened in laboratory in order to get the best material possible. While the starting material (P3HT) could be synthesized with even better properties than claimed in literature, end-group functionalization, storage conditions and purification needed to be optimized by using special techniques. The synthesis of the block-copolymer (P3HT-b-PEO) was tested by several methods including polymerization from a macro P3HT starting material, Steglich esterification, Suzuki cross-coupling, and click chemistry. While most of the given reactions could not be applied successfully under these conditions, click chemistry showed best results. Azido functionalized PEO (PEO-N_3) was used together with ethinyl-functionalized P3HT in a 1,3-dipolar copper catalyzed cycloaddition (Fig. 5.4).

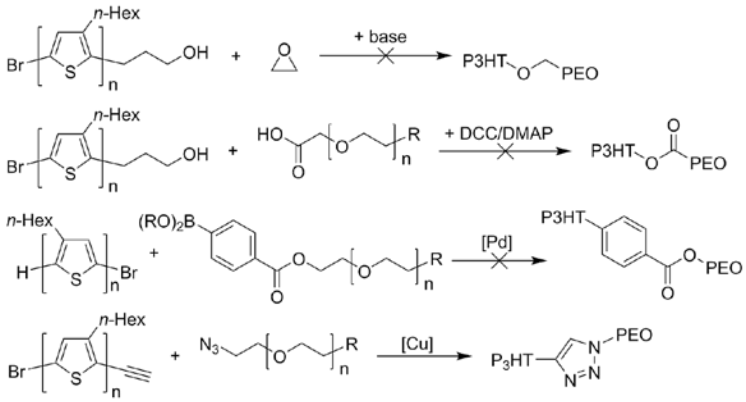

Fig. 5.4: Synthetic approaches to P3HT-b-PEO.

D5.8. Synthesis of deuterated polylactic acid

Poly(lactic acid) (PLA) is relevant for renewable plastics and medical applications. The synthesis of its deuterated form for neutron scattering is planned in cooperation with ESS who will deliver the deuterated chiral lactic acid monomers which are produced by a biotechnological process (D5.11). For the production of PLA with narrow molecular weight distribution, it is necessary to use lactide – the dimeric condensation product of lactic acid. It was found that the lactide formation is usually carried out by an oligomerization-depolymerization process including loss of material and stereoinformation. Especially, the loss of material is highly undesired in the case of deuterated starting materials. Therefore, it was decided to follow a new attempt as reported by B. Sels (Science 2015, 349, pp 78-80). The authors use special zeolites in order to achieve lactide formation under relatively mild conditions. Another advantage would be the ability to recover unreacted material.

Task 5.5: Network coordination and platform activities *(ESS M6-48) 12 PM*

The ESS has coordinated the networking and platform activities during period 1, which have included several dedicated Workpackage meetings (listed in Table 1), and a user workshop to be held in Oxford in May 2017. For disseminating the work done in the WP, we have set up pages for the work-package on sine2020.org, and have started our own website for DEUNET (deuteration.net) to communicate to and connect with the user community (D5.1). To collect input for the scope and strategy of the future user platform DEUNET, we are carrying out an international user survey and have distributed it to the wider network via email, the website and twitter. The Deuteration.net website is being populated with information about the Network members, current projects and news/events (D5.1) and hosts regular blogs, updates and our event calendar. On advice from the user community we are in the process of setting up a deuterated chemicals data base that will enable users to search if the compounds they are interested in have been deuterated before and at which facility or commercial provider.

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1.2.6 WP6 - Macromolecular Crystallogenesis:

Task 6.1.1: Development Of A Robotic System For Large Crystal Growth *(ILL M1-36) 18 PM*

The aim of the ILL in this work package is to provide new automated approaches for macromolecular crystallogenesis, with a specific view to generate large protein crystal growth suitable for structural characterization using neutron diffraction methods. This field of research is beset with the challenge of producing protein crystals of a suitable size (0.5 – 1mm^3) compared to the much smaller size requirement for X-ray studies (~0.01 mm^3) due to the large differences in available flux between the two types of sources. Traditionally this bottleneck has been approached by manual crystallization drop set-ups which is both time and labor intensive. Here we describe the designs for a prototype crystallization robot that employs automated thermal cycling using Peltier elements for temperature control of crystallization wells.

The core set-up for this prototype robot involves a custom plate design mounted on a motorized x-y translation stage (see Figure 6.1). An inverted microscope set-up that is equipped with a high-resolution camera will also be used to image individual well conditions. By combining both the imaging set-up and a programmable x-y stage crystal growth in many experimental conditions can be monitored in an automated fashion during the course of an experiment. Additionally, a temperature control element is incorporated into the custom plate design to provide thermal control of the crystallization wells during an experiment.

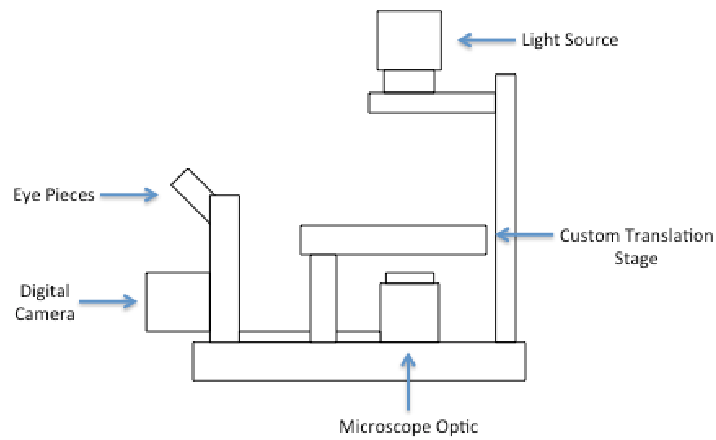


Fig. 6.1: Layout of proposed robotic system

This principle behind the design of this robot is that as protein crystals grow, the saturation level in the protein solution falls as it forms part of the growing crystal(s). At a certain point, this protein solution then becomes under-saturated and crystal growth is halted. By using a temperature control system it is possible to control the solubility of the protein and therefore its saturation level. By increasing a proteins saturation level in solution, crystal growth can resume as it is pushed into the growth region on the phase diagram (see Fig. 6.2). Additionally, by further increasing the temperature it is possible to dissolve excess crystal nuclei back into the well solution. This process followed by slow cooling of the well afterwards can result in the continued growth of a large single crystal.

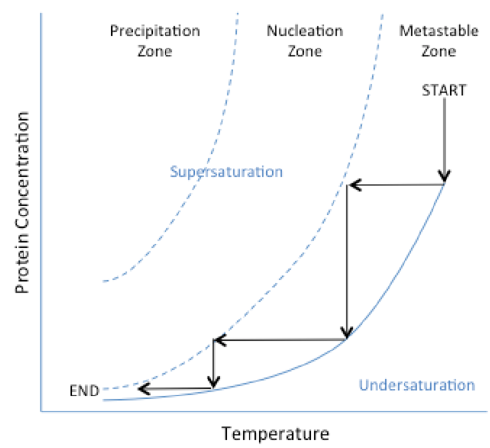


Fig. 6.2: A typical protein crystallization phase diagram. A protein crystal nucleus can be added as a seed at the start position in the metastable zone where growth can occur but there is no spontaneous nucleation. As it begins to grow the protein concentration depletes and growth halts when it reaches under-saturation. By modifying the temperature the saturation level of the protein solution is increased and growth occurs again. This process is repeated until the largest possible crystal is obtained.

The custom plate design is to be comprised of quartz crystallization wells organized into 5 x 4 rows and set into brass heating blocks. Each of these quartz wells is intended for separate crystallization experiment conditions for a total of 20 conditions, which can be screened at a given time. These blocks are to be connected to a Peltier element with a temperature feedback system. This will allow for heating and cooling of the experimental wells to within 0.1°, with a temperature control range of 4 to 60°C (see Fig. 6.3). The individual rows are to be separated from one another by foam insulation so as to thermally insulate the individual heating blocks and ensure correct thermal control is achieved. Typical crystallization experiments are carried out at room temperature as protein degradation typically occurs above 40°C (with some thermally stable exceptions).

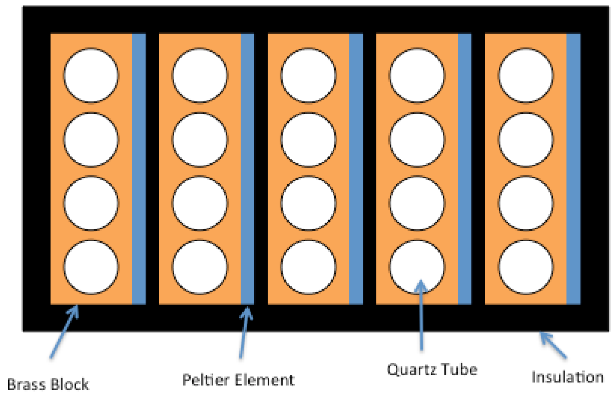


Fig 6.3: Custom crystallization plate design to be fitted to translation x-y stage.

An important aspect of a design for a robotic system for the purpose of protein crystallization will be its ability to run many experiments at once. Given that the time for a crystallization experiment can take anywhere between a few days or several months to complete, high throughput is a necessity. As such the instrument is designed to be scalable to accommodate a set-up involving 3 x 4 custom plates in a tiled set-up on the x-y stage (see Fig. 6.4). This will allow for the simultaneous exploration of up to 240 crystallization conditions for one or multiple proteins of interest at a time.

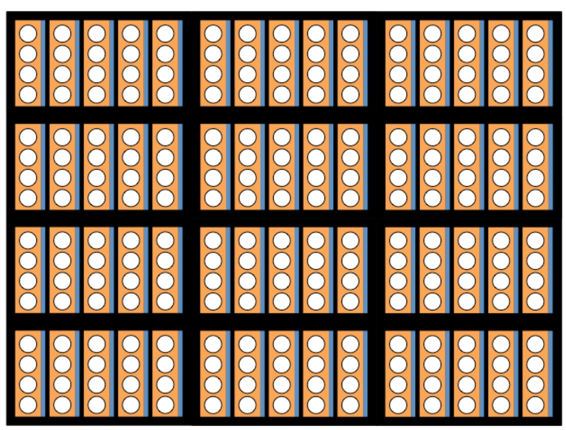


Fig. 6.4: Tiled set-up of individual custom plates arranged in 3 x 4 design on x-y translation stage.

Task 6.1.2: Development Of A Flow Crystallization System *(ILL M1-36) 18 PM*

The ILL is also developing a flow crystallization system, which can be used to encourage the growth of large macromolecular crystals. The intention is that this system would be able to be used independently or, at a later date, in conjunction with a robotic system that is able to control other parameters necessary for controlling crystal growth.

A suitable microfluidic device has been identified for use in these experiments, a Dolomite Mitos P-Pump. This consists of a pressure pump which is connected to an eternal gas supply, in this case nitrogen gas. The pump is then able to regulate the overall system pressure from the supply to pump liquids at extremely low flow rates, between 70 – 1500 nl min^{-1}. We believe that by providing a constant supply of fresh protein stocks and/or precipitating agent over the course of a typical crystallisation experiment we can reduce the contamination of nucleating crystals or existing crystal surfaces with contaminants and degraded material. This should help to promote the growth of larger protein crystals over time as we maintain conditions necessary for crystals growth within the metastable region of the phase diagram. Experiments are currently in progress using model systems including Lysozyme, Rubredoxin, TTR and Thaumatin with the desire to expand into novel systems at a later date.

Further to the investigations carried out in Tasks 6.1.2 and 6.1.2, additional research has been conducted into the magnetic alignment of protein micro crystals using high magnetic fields. Here, large numbers of micro crystals of a target protein are placed within capillaries containing a gel-like medium which remains liquid at 40°C. This crystals suspension is then placed in a high magnetic field (up to 17T) with the temperature maintained at 40°C to keep the gel medium in a liquid state. The micro crystals then undergo bi-axial alignment in the presence of the high magnetic field and are all placed in the same orientation. By reducing the temperature of the sample to 20°C, the gel medium transitions from a liquid to a solid, effectively fixing the crystals in their respective orientations. Due to the high density of the micro-crystals in the sample, and their alignment in the same orientations, the sample effectively becomes one large 'single crystal', which can then be used for diffraction studies.

Initial experiments have been performed in collaboration with Elizabeth Blackburn at the University of Birmingham, school of Physics and Astrophysics department. Here several test samples have been prepared using the model protein Lysozyme and can be seen in Figure 8. Here we can clearly demonstrate the alignment of the Lysozyme crystals within the gel medium contained in the capillary. Repeat experiments are to be performed shortly with other model systems such as Rubredoxin, TTR and Thaumatin. Given the encouraging progress made pursuing this method, we will be asking the scientific advisory board that the focus of Task 6.1.1 be directed towards furthering this method development.

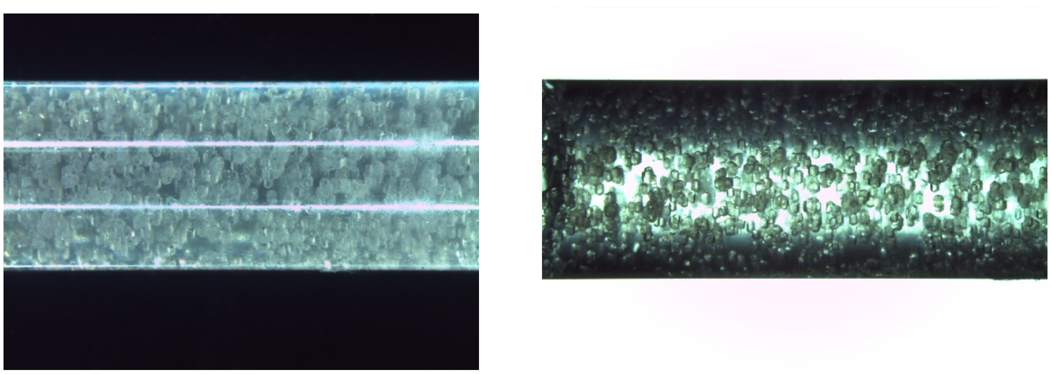


Fig. 6.5: Magnetically orientated lysozyme microcrystals within gel medium in capillaries.

Task 6.2.1: Phase Diagram Characterization For Proteins *(ESS M1-24) 22 PM*

The ESS portion of this WP is to focus on phase diagram characterization of protein solubility and crystallization, and to investigate strategies for scaled-up crystallogenesis using methods based on vapor-diffusion and dialysis with temperature as a major parameter to vary in promoting large crystal growth. For the first period, we focused on target identification, purification, and characterization. This included plasmid design, expression trials, preparing of deuterated versions of the target proteins, and purification and characterization with SDS-PAGE, size exclusion chromatography, and activity assays as applicable. As we are aiming to increase the crystal volume, we should work with known entities that can produce enough of to achieve scale-up and large crystals in a systematic way.

Based on this we narrowed down the targets based on a set of criteria: 1) expression levels, 2) ease of purification, 3) stability, 4) known crystallization conditions.

Our targets that we worked on in this period were as follows: 1) Human carbonic anhydrase IX mimic, HCA IX mimic (both hydrogenous and perdeuterated), 2) Bovine Cu/Zn superoxide dismutase, SOD 3) Full length native human carbonic anhydrase IX, native HCA IX.

For (1) HCA IX mimic, we express the protein in E. coli and do a 2-step purification. The protein is very soluble and we work with 10-35 mg/mL concentrations for crystallization set-ups. We performed phase diagram determination in hanging and sitting drop vapor diffusion set-ups, initially at room temperature. Once the best conditions were determined from the phase diagram, we did temperature ramp experiments to fine-tune protein solubility and crystal growth. We used two approaches; one was sitting drops in the Centeo temperature controlled device with temperatures between 12 and 20 C. The best result was to set-up the drops at 20 C, ramp down to 12°C and keep the temperature there. The resulting crystals were large and single, and increasing the number of ramps did not improve the crystals.

The same approach was used for SOD but with opposite results. SOD is available commercially from Sigma-Aldrich, so we did not have to prepare it in-house. After fine-screening the known conditions using the phase diagram approach, we further optimized using temperature. Here it was best to set-up drops at 12°C, ramp up to 20°C and incubate. This suggests that different protein react differently to changes in temperature and how a particular protein behaves will have to be determined on a case-by-case basis. The Centeo device is very useful for these kinds of experiments, but can only handle small volumes. For scaling up we have to use large programmable incubators that can hold several plates at once. We were able to duplicate the results for both system in drop volumes of 3 uL, 10 uL, and 50uL. We now aim to scale up the volume even more, while using temperature as a variable factor.

During a WP meeting in January 2017, it was pointed out that the most accurate way to determine a phase diagram is to do it under batch conditions. We did not at the time have any batch conditions for any of our proteins, and we recently started working to obtain those. We have started to set up trays screening for batch conditions (microbatch, under oil) using the "condition converter" from Douglas Instruments. We do not at this time have definitive results from the trials yet.

In the first quarter of 2017 we also commissioned a new Oryx8 liquid handling robot from Douglas Instruments. This machine allows us to do a lot more screening (both vapor diffusion and batch) in a large range of volumes, and allows for the ability to seed. We have noticed that for all of our targets, seeding is key to getting improved crystals from the beginning, this is now part of our normal workflow. The Oryx8 is a perfect match to our needs for crystal optimization. We are heavily relying on the robot to help us in the next phase of the project. See Fig. 6.6.

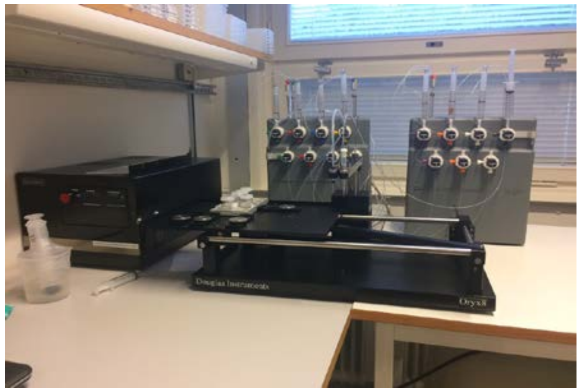


Fig. 6.6: New Oryx8 protein crystallization system.

For the native HCA IX we have made significant progress. This membrane protein is expressed in a baculovirus/insect cell system and we finally obtained enough material to do some initial screens. We have found some hit conditions and are further refining those in the next period.

Our plans for the next phase of the project includes multiple facets:

1) Test X-ray diffraction quality of the crystals we obtained for SOD and both hydrogenous and deuterated HCA IX mimic.

2) Adapt all our vapor diffusion conditions to batch to allow better control and scale-up, including more accurate phase diagram determination.

3) Continue to scale-up our crystallization volumes.

4) Use temperature on large volume set-ups under batch conditions to further improve crystals.

5) Fine-screen and optimize conditions for native HCA IX, with scale-up as the final step.

Task 6.3.1 Phase diagram characterization for proteins *(FZJ, M1-36) 14 PM*

A phase diagram characterization of one of the most studied protein models, the hen-egg white lysozyme, based on neutron and light scattering techniques by using the batch crystallization method, has been performed. The temporal evolution of fractal aggregates during the nucleation process has been described. Those results have been reported in Deliverable D6.3. An interesting challenge is the extension of this phase diagram investigation to other proteins. We therefore tried to search for other proteins which could be successfully crystalized to obtain large ~1 mm^3 crystals. Luckily we found Streptavidin in complex with Biotin to crystalize when lowering the temperature to 8°C. At these conditions, large 2mm by 2mm by 1 mm crystals formed. Unfortunately, the crystals were not stable at room temperature but dissolved in the remaining mother liquor around them. Yet, we were able to record an x-ray diffraction image on those crystals yielding diffraction to 2.5 Å resolution. Attempts to use 30% vol. of deuterated glycerol as a cryoprotecting mother liquor and freezing the crystals in a cryostream always resulted in opaque crystals showing no diffraction any more. The next steps will certainly be a more rigorous search for better crystallization conditions yielding crystals stable at room temperature or more sophisticated techniques to freeze the existing crystals in the cryostream.

For the latter purpose one can think of a crystallization apparatus, where one places the crystal in an optical microscope and adds the deuterated glycerol slowly, step by step in small quantities observing the crystal. A crystallization apparatus, which allows adding and removing the mother liquor around an existing crystal is in the design phase. The previous experiments can also be understood as prerequisites to explore the specifications of such a device. In brief, the concept of such an apparatus bases on two roundish glass slides with a Teflon spacer in between. This serves as the compartment around the crystal. It should be in close thermal contact with a Peltier element for fine temperature control. This in turn is connected to a heat bath which is temperature regulated by a commercial water-cooling unit. An inverted microscope looks through the two glass windows and monitors the crystal size and quality either in light transmission or in crossed polarized mode. Later, dynamic light scattering should be used in order to monitor whether new crystallites or aggregates from in the surrounding mother liquor solution around the crystal.

The Teflon spacer may have only two pipes, one exiting and one for entering the new liquid with close by valves. This corresponds to batch crystallization conditions. When adding a dialysis membrane to one pipe of the spacer one arrives at dialysis conditions. Vapor diffusion conditions can in principle also be realized when one does not fill the whole area around the crystal but leaves some space for vapor to diffuse out at the top end of the spacer.

The next steps on this task will be:

1) Making progress in the design of the crystallization apparatus resulting in first technical drawings.
2) Identifying suitable commercially available Peltier cooling and inverted microscope parts and their implementation into a computer controlled environment.
3) Exploring the limits of large crystal growth using the batch crystallization approach based on the **Task 6.3.2 Application Of Vapor Diffusion Approaches** *(FZJ, M1-36) 13 PM*

Since in the crystallogenesis workshop it was stated that vapor diffusion does not provide good control on crystal growth, more emphasis has been put on the batch crystallization method. In this task, it was decided to use the model system Thermolysin, which is readily commercially available. Several crystallization recipes (with and without added Polyethylenglycol) have been tried out, many of them resulting in the growth of large crystals. A first x-ray characterization gave disappointing results of resolutions of only 4.6 Angstrom at most, although the crystal size was already optimized to around 0.5 mm^3. Here, the conditions need to be optimized in order to achieve a higher resolution. Often this can be reached by a slowing down of the crystallization process. In vapor diffusion techniques, one can easily achieve this by covering the reservoir solution by oil, or by lowering the temperature.

The next steps on this task will be:

1) Assessment whether vapor diffusion methods shall be implemented in the planned crystallization apparatus (see Fig. 6.7).
2) Optimization of the conditions for Thermolysin in order to achieve higher resolutions.
3) Characterization of the Thermolysin crystals with neutron diffraction in order to judge whether the crystal size is sufficient.
4) Streptavidin/Biotin system, a first non-trivial protein to be crystalized.

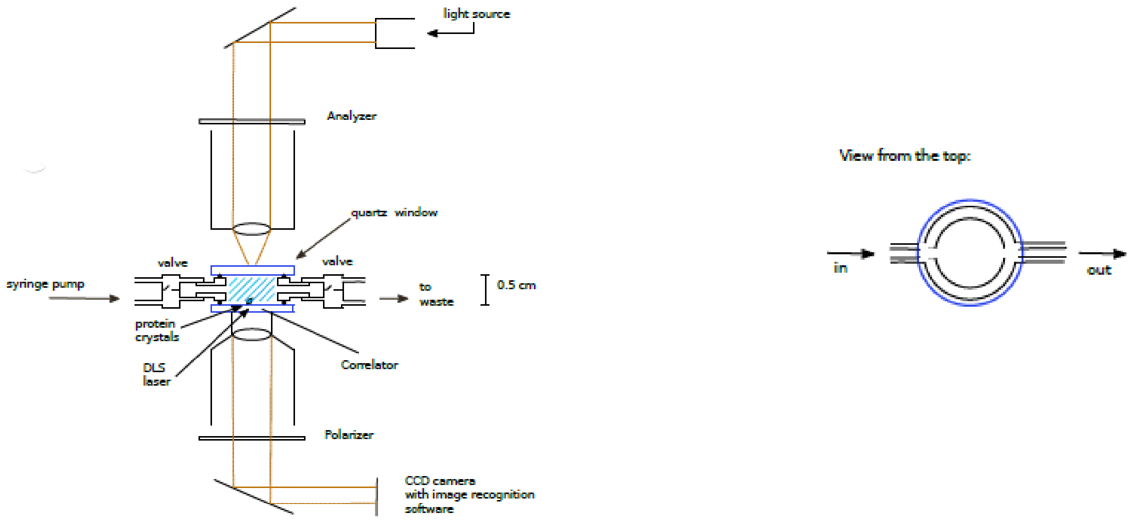


Fig. 6.7: Design for the planned batch crystallization apparatus (left). With other spacers also dialysis or even vapor diffusion methods may be realized (right).

1.2.7. WP7 – Sample environment

Task 7.1: FLOSS software standards for sample environments *(HZB, M6-48) PM 60*

A preparatory work was done in close cooperation with the ISSE International Committee for the Standardization of Sample Environment Communication (https://sampleenvironment.org). This work has been presented and discussed with specialists from European facilities at the HZB in April 2016 and at the ESS in January 2017. Most items were agreed and are now summarised in a draft document describing the SECoP protocol. A demonstration was presented in January 2017 and the team is now contacting industrials with the aim to determine what would convince them to adopt it.

Task 7.2: Towards efficient sample environment for neutron research *(ILL, M6-48) 42 PM*

A new Monte Carlo software has been produced by ICMA to simulate realistically a sample surrounded by sample environment equipment on a neutron scattering instrument. It models elastic scattering, both coherent and incoherent, neutron absorption and inelastic scattering, all taking place in a crystalline medium with three types of microstructures. It has been benchmarked with data collected on ILL instruments. It is now being packaged as a component of the worldly known simulator McStas and will soon be available to the community (deliverable 7.1).

In order to reduce beam-time losses when performing experiments at ultra-low temperatures, a survey was conducted amongst partners to determine the dimensions of dilution refrigerators used at the European facilities. From this survey, three concept designs of a goniometer head have been proposed and discussed with partners (deliverable 7.2). A prototype is now being manufactured at PSI.

Another survey has been organised to determine the current procedures and furnaces that are widely used at European facilities to carry out experiments at high temperatures. Partners have then decided to develop a system for reducing the cooling time in ILL-type furnaces. Tests performed at STFC with different inert gases at different flow rates and from different starting temperatures have allowed to reduce the cooling time from 6 ½ hours to 40 min. ILL and STFC now work on ways to automate the process.

Task 7.3: Next generation pressure cells for neutron and muon research *(PSI, M6-36) PM 75*

A kick-off meeting has been organised at PSI with experts in high-pressure techniques (CSEC and IMPMC third parties) to present a review of the current capabilities at neutron and muon facilities and discuss potential improvements (review published by PSI on high-pressure research with µSR in *High Pressure Research* **36** (2016) 140).

From these discussions, the PSI team started working on the design of a multilayer hybrid piston cell for µSR. They have acquired expertise in high-pressure at CSEC, performed FEA calculations and finally built prototype cells with great success. We now believe that the practical limit of 1.8 GPa for Ø5 mm sample will soon be pushed to 2.5 – 2.8 GPa for a larger Ø6 mm sample (see deliverable 7.3).

A few months after the kick-off meeting, partners met also at ISIS (STFC) to establish whether sufficiently compact anvil cells could be developed for µSR. Implications for beamline and spectrometer design have also been investigated. The outcome of this study will be reported as planned in D7.8 (M24); however, our preliminary conclusions suggest it unlikely a practical cell can be realised, removing the muon contribution from D7.16 (M36). In parallel, the STFC team has launched a feasibility test of the new PSI-like piston pressure cell on the RIKEN-RAL instruments at ISIS. Dummy pressure cells with different sample volumes and matched beam collimators have been prepared. Beam tests are being performed to determine the maximum ratio of sample to background (cell) signal that can be obtained.

On the neutron side, ILL allocated some beam time to IMPMC to identify background sources in diffraction experiments using Paris-Edinburgh anvils and to test new anvil materials. The data have revealed that the TiZr gasket is the major source of background and various ways to reduce gasket-scattering have started and will be pursued when the neutron will restart. Extensive tests were also carried out using sintered diamond anvils and allowed to collect neutron diffraction data to record high pressure (22 GPa) and simultaneously very low temperatures (1.8 K) published by IMPMC in *High Pressure Research* **36** (2016) 73.

In parallel, STFC compiled a review of the current cells available at the European neutron facilities and in particular those that are suitable for inelastic neutron scattering. From this review and considering the results obtained by PSI, partners decided that background and transmission measurements should be carried out on 7 materials before launching FEA calculations. These measurements are almost complete and a meeting is scheduled late April at PSI with CSEC, ILL and ISIS to launch the FEA optimisations of a multilayer hybrid neutron cell (see deliverable 7.5).

From discussions with partners and high-pressure experts, HZG also developed a concept for adapting the prototype high-pressure cell for in-situ XRD studies of solid-state hydrogen storage materials to the requirements of in-situ neutron scattering experiments. Sapphire capillaries have been chosen for their pressure and temperature stability, their transparency to neutron beams, and because they are inert to hydrogen. A prototype 700 bar hydrogen container is being manufactured and beam time has been requested at the MLZ/FRM II to further develop the setup and safety procedures (see deliverable 7.4).

Task 7.4: Complementary in-situ measurements for neutron and muon experiments *(STFC, M6-48) 54 PM*

After two recruitment sessions, a post-doc finally started working in January 2017. A prototype birdcage RF coil is being prepared at ISIS and on-beam commissioning is scheduled in spring 2017 to check the sample stability.

With regard in-situ NMR, the LLB team has designed and tested successfully a probe-head that can be aligned precisely with the magnetic field. The NMR set-up has been tested and used ex-situ on a Food Science case: the porous starch matrix mobility hydration dependence. They have recently performed a test experiment on the IMAGINE station of the LLB and the data analysis is underway (see deliverable 7.7). This experiment revealed some issues related with the alignment of the neutron beam with the NMR field and they are looking for technical solutions.

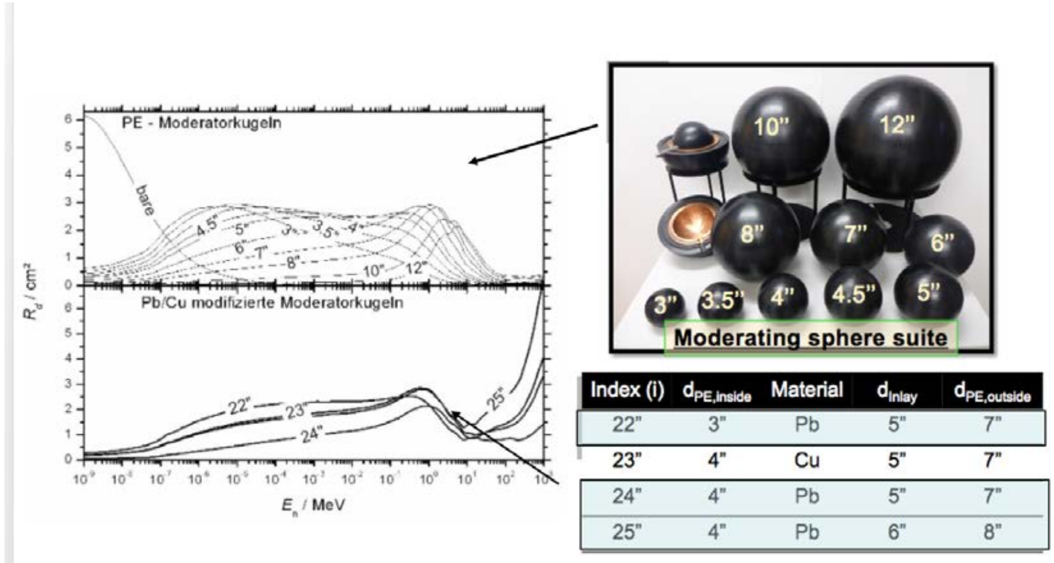
1.2.8 WP8 - Instrumentation – e-tools

The WP8 partners have exchanged at multiple workshops and meetings, including:

- "Neutrons: Cradle to Grave workshop, Coimbra, Portugal, September 6th 2016" in connection with the first SINE2020 General Assembly
- A satellite WP meeting in connection with the ICANS conference in Oxford, April 2016.
- Periodic, coordinating Skype meetings

The main results so far are:

- The above-mentioned "Cradle to Grave" workshop, which fulfils a project milestone (MS2). All talks from the meeting were recorded and are available for viewing at http://coimbra2016.essworkshop.org
- Evaluation of detectors for fast neutron and gamma spectroscopy, including improvement of expansion of the so-called *Bonner Sphere* spectrometer at PSI (main input to deliverable D8.1), see Fig. 8.1.
- The release of the MCPL library software for interchange of event data between neutronics and instrument simulation packages, see https://mctools.github.io/mcpl/ and T. Kittelmann et.al., http://arxiv.org/abs/arXiv:1609.02792, accepted for publication in Computer Physics Communications. MCPL is developed in collaboration between DTU and ESS (and is the main input to deliverable D8.2). See Fig. 8.2.
- A report on the achievements in simulating laminar shielding concepts by EES-Bilbao (D8.5)
- Early progress on porting methodology from RESTRAX to McStas for "reverse direction neutron propagation" from sample to source, contributed by NPI. To become part of report for deliverables D8.8 and D8.12. See Fig. 8.3.
- Early progress on shielding material development and characterisation, to become part of the report for deliverable D8.6. Joint effort of ESS and PSI. See also D.D. DiJulio et. al. NIM A **859**, (2017) pp 41–46. See Fig. 8.4.



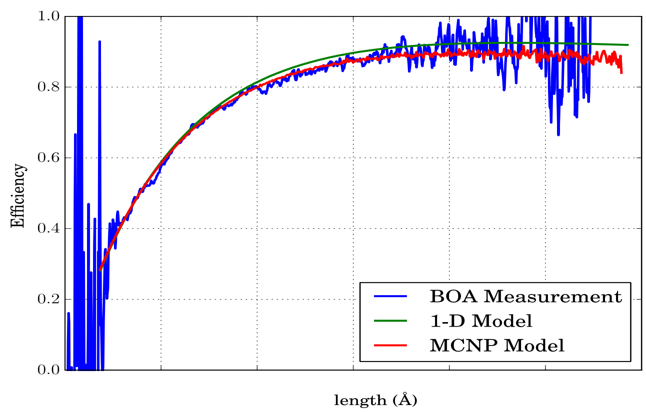


Fig. 8.1: From Coimbra 2016 presentations by Uwe Filges, PSI. Top: Shows how the PSI Bonner Sphere spectrometer has been supplemented with Pb/Cu moderating spheres, for extiension of the dynamic range. Bottom: Comparison between detector efficiency simulated using MCNP and measured at the BOA beamline.

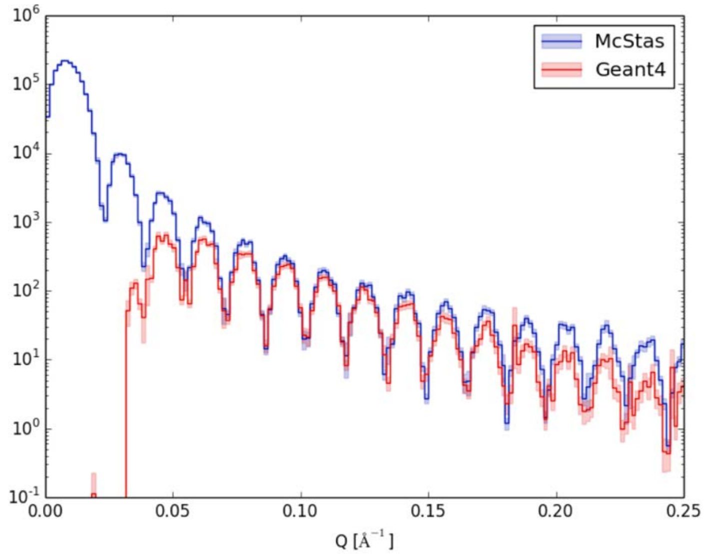


Fig. 8.2: Reproduced from T. Kittelmann et. al.: Illustration of MCPL capabilities. A Geant4 detector simulation of the ESS LOKI Band-Gem detector added to post-sample output from McStas.

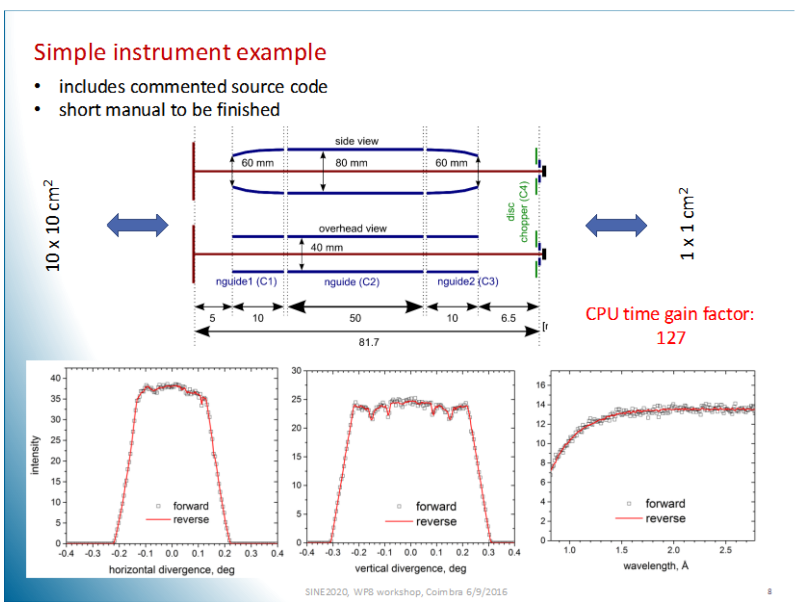


Fig. 8.3: From Jan Šaroun presentation, Coimbra 2016: Illustration of forward and reverse simulation using McStas, demonstrating speed gain factor of 127.

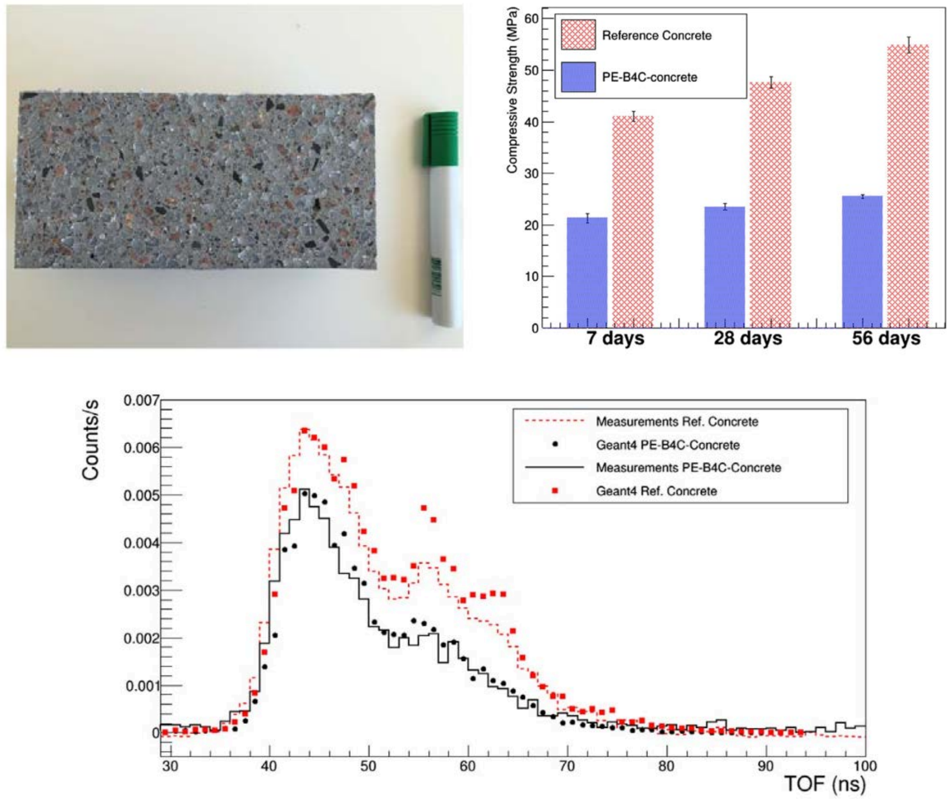


Fig. 8.4: Reproduced from D.D.DiJulio et. al. Top left: Photo of a cross-section of PE-B4C-concrete, the marker is shown for reference. Top right: The compressive strength of the reference concrete and PE-B4C-concrete after 7, 28 and 56 setting days. Bottom: A comparison of measurements and (Geant4) simulations for a reference concrete and the developed PE-B4C-concrete.

1.2.9 WP9 - Detectors

Task 9.1: Involvement of industry and the wider European neutron and detector communities in this WP *(STFC, M1-48)*

This task is the responsibility of all partners. With regard to extended work package meetings to involve industry, the first of these meeting is running later than scheduled and has now been arranged for 13-14 June. At this meeting it is intended to concentrate on inviting members of industry to the meeting who have an interest in detector construction rather than specific component construction, but specific details are still have to be determined.

In inviting people engaged in neutron detector development who are not members of this WP, both the ENEA and UMB presented their work at the work package meeting at Abingdon in January 2017. At the Coimbra meeting professor Fonte from LIP gave an excellent overview of the status of RPCs. Understanding the detector work going at other facilities outside is beneficial to all WP members. The UMB work on the BAND GEM detector is of particular relevance to Task 9.4.4, which faces the same issues of extracting the charge from multiple boron coated layers.

Task 9.2 Development of scintillation detectors with high rate capability for reflectometry

Task 9.2.1: Development of a ZnS scintillation detector with WLS fibre readout *(STFC, M7-48), 28 PM*

ISIS is developing a scintillation detector based on ZnS:Ag/^{6}LiF coupled to multi-anode photomultiplier tubes (MA PMTs) with wavelength shifting (WLS) fibre. Although ZnS:Ag/^{6}LiF scintillator offers high light output and pulse shape discrimination between neutrons and gamma, the afterglow associated with this scintillator limits high rate detector applications. In reflectometry, high intensity data is often limited to one to three lines across the face of the detector. With a conventional xy array of WLS fibres this data ends up in just a few PMT channels and can cause sever detector dead time. To avoid this we are looking at ways of distributing the high intensity data across a lot more of the PMT channels. A design concept has been established and a first detector has been built consisting of 128 0.5 mm diameter fibres covering an active area of 32 x 32 mm^2 and divided into 4096 pixels, Figure 9.1 LHS. The fibre array is coded into two 64 channel MA PMTs, although, to date, only one of these has been equipped with electronic readout channels. The detector has been designed so that the fibre scintillator assembly can be rotated in the neutron beam allowing the image from a slit to be spread across a variable number of PMT channels, Figure 9.1 RHS. The completion of the first detector hardware is deliverable 9.2. Position resolution is 0.7 mm FWHM and pixel to pixel uniformity is ± 20%. Further characterization of the detector is ongoing. In the non 90 and non 0 degree positions, increased ghosting has been observed and work is underway to understand why this is and determine an appropriate solution.

Task 9.2.2: Development of a scintillation detector with direct PMT readout *(FZJ, M1-48) 20 PM*

FZJ is developing a scintillation detector where each detector pixel is read out by an individual photomultiplier tube pixel. This provides excellent light collection and high count rate capability but results in a large number of PMT pixels and associated signal processing electronics. The challenge is to keep the cost of the PMTs and electronics affordable without degrading detector performance. GS20 glass has been selected for the scintillator and the 64 channel Hamamatsu H8500 has been selected for the PMT. GS20 is a fast transparent scintillator and neutron detection efficiency can be optimised according to the thickness chosen for the scintillator. However, to minimise optical cross talk from one detector pixel to the next, it is necessary to optically isolate individual detector pixels from each other. FZJ has developed a technique for grooving the scintillator and filling the grooves with reflector which works well. Figure 9.2 LHS shows a scintillator segmented into sixty-four 6 x 6 mm^2 pixels. A readout electronics evaluation system has been designed and constructed based on the Rosmap ASIC from Ideas, Figure 9.2 RHS. Evaluation and initial operation of the system is underway and the first optical and electronics measurements have been carried out. For final deployment the rate capability of the Rosmap ASIC is too slow and FZJ is developing their own ASIC, which will meet the foreseen rate requirements. Initially this system will give a position resolution of 6 x 6 mm^2. Use of a 256 multi anode PMT will improve the position resolution to 3 x 3 mm^2. With more sophisticated electronics there is the possibility of improving the position resolution further.

Task 9.3 Development of a 3He based microstrip gas chamber (MSGC) with a novel 2D readout *(ILL, M7-48) PM 23*

The ILL is developing a microstrip gas chamber (MSGC) with two-dimensional position sensitivity. MSGCs are intrinsically 1D detectors and additional work is required to provide 2D position sensitivity. One way of doing this is to make the anodes or cathodes resistive and obtain the second co-ordinate by charge division. Previously, the ILL has developed a method of producing a MSGC with resistive electrodes by coating the chromium electrodes with aluminum. When operated in a 3He CF_4 mixture, work in 2011 showed that the detector suffered from severe aging. Although CF_4 is an excellent stopping gas, chemically it is very reactive. As part of task 9.3, the viability of this method has been explored further. A similar MSGC detector was constructed and used with a 3He $ArCO_2$ gas mixture. Although the aging was not a severe as with CF_4, the detector was still not sufficiently stable for long term use on an instrument at the ILL. Work at the ILL has now concentrated on developing an MSGC, which uses pure chromium electrodes. In this device the resistance of the cathodes is determined by their width and an innovative shape is used to maintain the required charge collection area. MSGC plates have been manufactured, assembled into a detector and the first neutron and gamma data has been obtained, Figure 9.3. Analysis and further data collection is proceeding. Once the results are understood the design will be fabricated using Schott 8900 glass and then work will look at increasing the size and resolution of the detector.

Task 9.4: Emergent Detector Technologies for neutron scattering and muon spectroscopy

The ESS provides information on progress of the ESS project and on detector performance requirements at the ESS. This information facilitates the formulation of detector design goals within this work package.

Task 9.4.1: Development of a neutron sensitive resistive plate chamber *(LIP, M1-48) PM 19*

LIP is developing resistive plate chambers (RPCs) for high resolution position sensitive neutron detectors. RCPs have been used extensively as large area position sensitive detectors in High Energy Physics, but have had little impact to date on the neutron scattering community. LIP has designed and manufactured two test detectors, each 7 x 7 cm^2, Figure 9.4 LHS. The design work is supported by Monte Carlo simulations carries out in GEANT4 and ANTS2. One of the challenges is to make these devices neutron sensitive. Neutron sensitivity has been achieved by coating the aluminum electrode of each device with a layer of $^{10}B_4C$. This process was carried out at the ESS Detector coatings workshop in Linköping. Detector characteristics have been measured including a neutron detection efficiency of 12.5% at 4.7 Å and a very impressive spatial resolution of better than 0.25 mm FWHM, Figure 9.4 Centre and RHS. These tests have been carried out at FRM II in collaboration with TUM. Work is now proceeding on the design and construction of a stack of double gap RPCs to improve neutron detection efficiency.

Task 9.4.2: Development of silicon photomultipliers for neutron scattering *(PSI, M1-48) PM 12*

PSI is developing a two dimensional position sensitive scintillation detector read out with silicon photomultipliers, SiPMs. The detectors are based on $ZnS:Ag/^6LiF$. Two different methods of achieving two-dimensional position resolution are being investigated. The first is the "2D pixelated detector" where each detector pixel consists of an individual scintillator connected via WLS fibre to SiPMs, Figure 9.5 LHS and centre. The scintillator is tilted at a shallow angle to the neutron beam to increase neutron detection efficiency. The fibre ends can be xy coded to reduce the number of SiPMs needed to readout the detector array. The second approach is the "light sharing detector" where the light intensity is measured from each end of a row of WLS fibres embedded in a strip of scintillator, Figure 9.5 Bottom and RHS. Position resolution along the length of the scintillator is determined from the relative light intensities at the ends of the fibres and position resolution in the other direction is determined according to which scintillator strip in the detector received at hit. Prototypes of both types of detector have been constructed and initial results have been obtained. Work is continuing to optimize the performance of both types of detector.

Task 9.4.3: Development of silicon photomultiplier based detector technologies for muon spectroscopy *(PSI, M1-48) PM9*

The use of silicon photomultipliers (SiPMs) for muon spectroscopy is being developed jointly by STFC and PSI. The capability of commercial SiPMs has advanced rapidly in recent years. In this sub task the latest SiPM technology for scintillation-based detector arrays for muon spectroscopy is being evaluated with particular regard for fast timing and high rate applications. At continuous sources like PSI, each muon is injected into the sample and decays before the next muon arrives. This allows precise time measurements of the muon decay and the timing resolution of the detector is critical. At a pulsed source like ISIS, 1000s of muons are injected into the sample at each beam pulse. Here the detectors arrays need to measure many muon decays each beam pulse and the dead time of the detectors are critical. ISIS is developing a Monte Carlo simulation programme, which determines detector the number of missed counts as a function of the fraction of cells fired in a SiPM and the number of counts on the detector per beam pulse, Figure 9.6. Recharge time and number of cells fired as a function of photon flux have been determined experimentally from laser stimulation experiments. Simulations using this programme are able to predict the features observed in the experimental muon data at ISIS and are allowing figures of merit to be assigned to the latest SiPM devices for pulsed MuSR detector applications. Detector performance is being compared with similar devices read out with conventional vacuum PMTs.

Task 9.4.4: Development of Micromegas detectors for neutron scattering *(CEA, M1-48) PM 14*

CEA is developing a neutron sensitive microbulk micromegas detector where neutron sensitivity is achieved by coating grids in the micromegas detector with B_4C. This work builds on the development of a neutron sensitive bulk micromegas detector system carried out in NMI3 II. The bulk system has been shown to work and gives good agreement with the results predicted from the modeling carried out in NMI3. However, the meshes used in the bulk micromegas detector are difficult to obtain and difficulties were experienced in maintaining the correct geometry after coating. In addition stacking of the detectors to improve efficiency is limited by the thickness of the PCB layer supporting the readout electrodes. The main advantage of the microbulk detector is that there is no PCB and the readout pads are supported directly on 50 µm pillars, which support the micromesh. Neutron scattering from such an arrangement should be very low and thus it should be possible to stack several layers one behind the other without adversely affecting the incoming neutrons. CEA have carried out simulations of this device and predicted that four back to back units could achieve a neutron detection efficiency of 40% at 1.8 Å, Figure 9.7 Attempts have been made to coat the microbulk material directly with B_4C, but in the initial trials the B_4C has peeled off the microbulk material. Work on this continues. In the meantime a simplified concept is being developed where the mesh of a bulk micromegas detector is replaced by a microbulk layer. This looks encouraging.

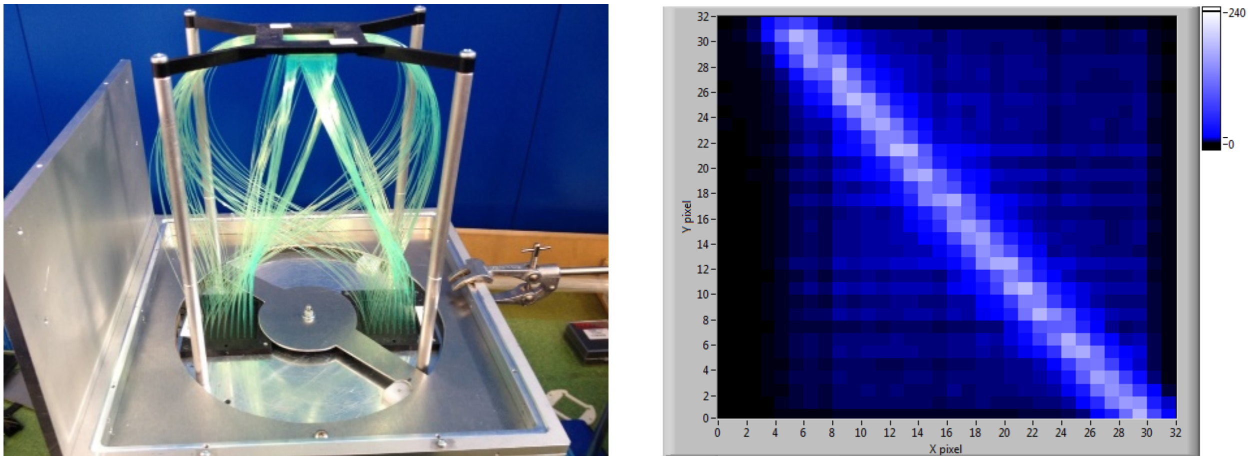


Figure 9.1 LHS: ZnS:Ag/^{6}LiF scintillation detector with wavelength shifting fibres connected to two 64-channel photomultiplier tubes. RHS: Response of detector to vertical slit. Intensity is distributed across all photomultiplier pixels.

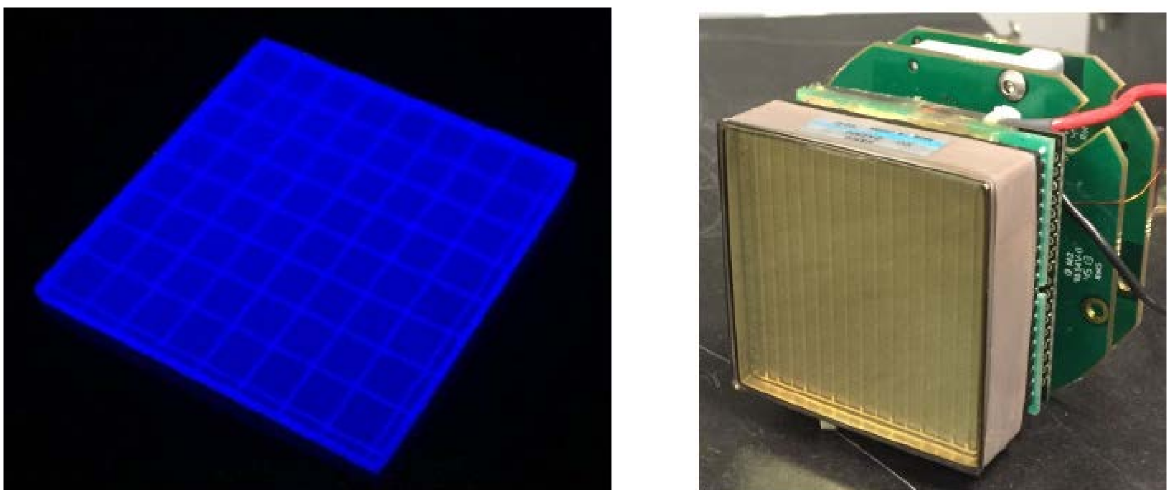


Figure 9.2 LHS: GS20 glass scintillator segmented into sixty-four 6 x6 mm^{2} pixels. RHS: 64-channel photomultiplier tube connected to electronics of direct readout scintillation detector.

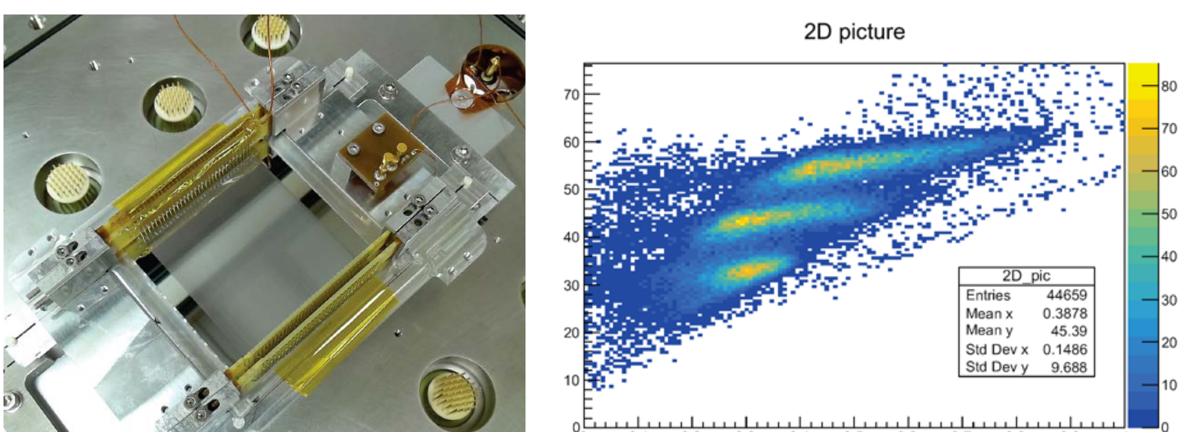


Figure 9.3 LHS: The new microstrip gas chamber with resistive readout which provides two-dimensional position resolution. RHS: The first data from the detector.

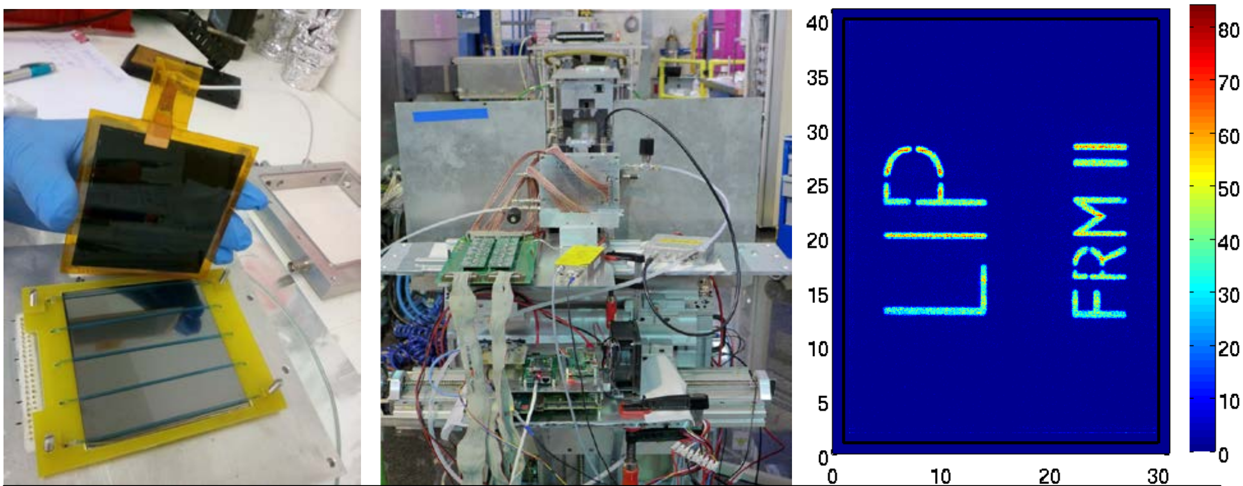


Figure 9.4 LHS: One of the prototype resistive plate chambers with its neutron sensitive coating of $^{10}B_4C$. Centre: The detector on test at the FRM II reactor in Munich. RHS: An image of a cadmium mask captured by the resistive plate chamber. Measurements have shown an image resolution of 0.24 mm FWHM.

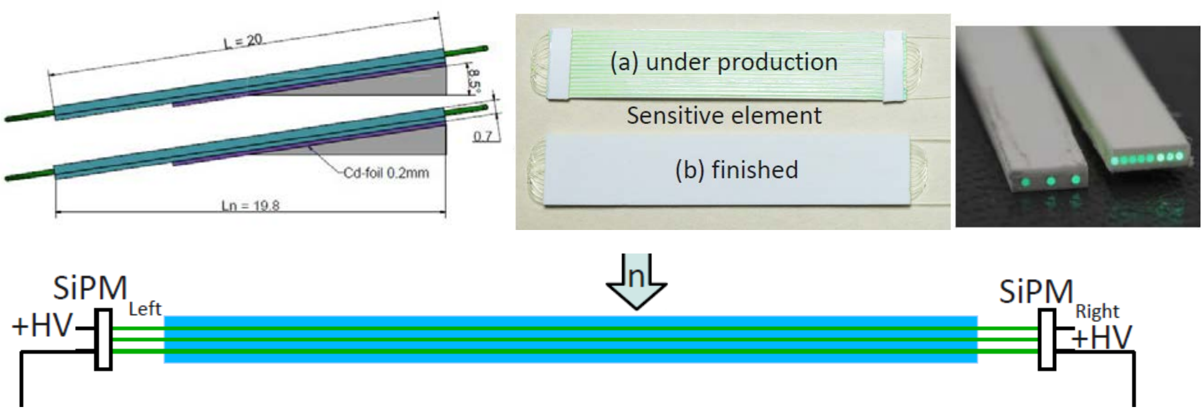


Figure 9.5 LHS: A schematic of two detector pixels of the 2d pixelated scintillation detector being developed by PSI with SiPM readout. Centre: Photographs of a 2D detector pixel in preparation and complete. Bottom and RHS: schematic and photograph of the "light sharing detector."

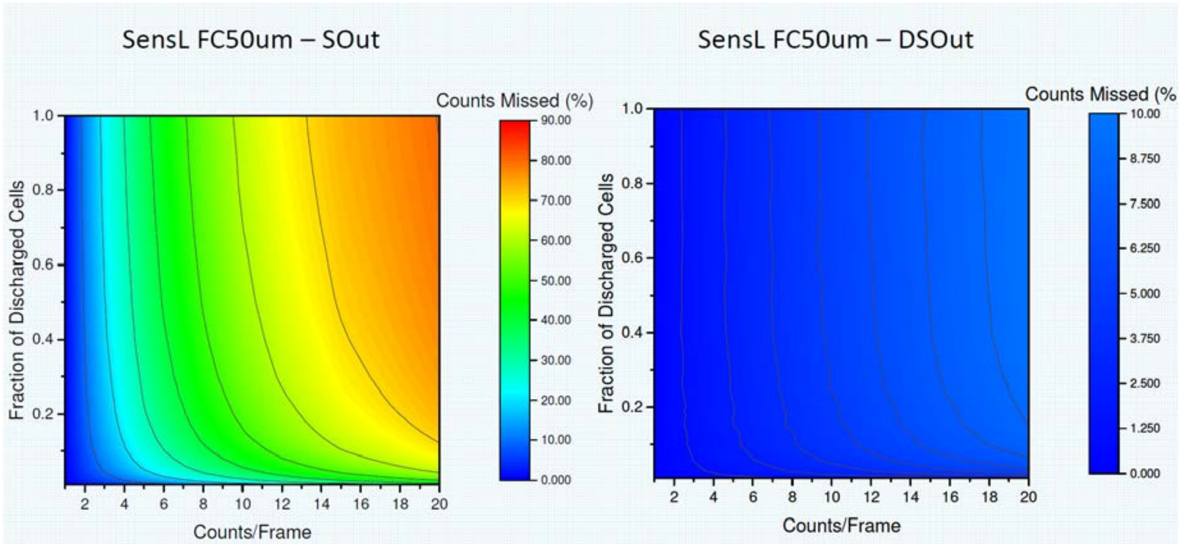


Figure 9.6 LHS: Monte Carlo simulation of a silicon photomultiplier (SiPM) showing the percentage of missed counts as a function of the number of cells in the SiPM which have been discharged and the number of counts on the SiPM per beam pulse. The two pictures are for the same SiPM but in the RHS image the output signal has been differentiated.

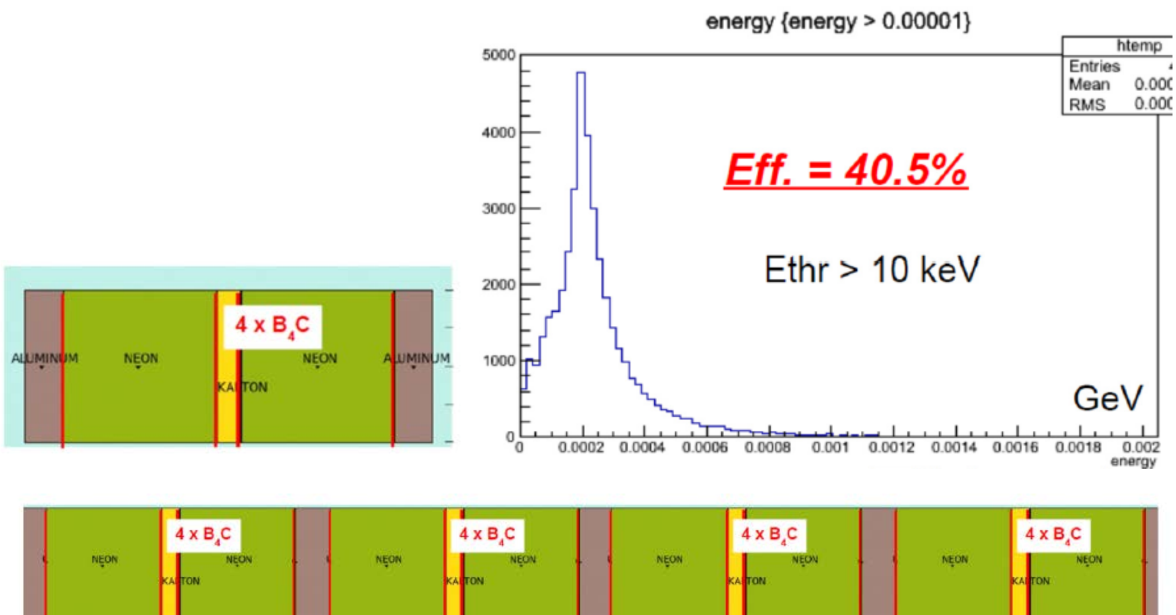


Figure 9.7 LHS: Schematic of a double sided neutron sensitive microbulk Micromegas detector. Bottom: A stack of four such detectors. Top: The simulated neutron detector efficiency of the detector stack at 1.8 Å.

1.2.10 WP10 - Data Treatment

Tasks 10.1 Dissemination and management *(ESS, M1-48)*

Workshop I took place at PSI April 4th and 5th, 2016 (Separate report has been submitted, Fig.10.1). There were 26 participants from all partner facilities and the two observers DTU and HZB. The aim was coordination and knowledge transfer between the different facilities. An action point was that each facility should capture requirements for the considered software and present them at the General Assembly meeting in Coimbra.

Fig. 10.1: Participants in Workshop I in WP10 at PSI

At the General Assembly meeting in Coimbra a parallel session was held for WP10 for the partners not involved in analysis software for imaging. In parallel with this a WP10 meeting was held for the partners involved in analysis software for imaging at the 8th International Topical Meeting on Neutron Radiography (ITMNR-8) in Beijing, China, because most of the imaging participants were already gathered at this conference (Fig.10.2). At both events captured requirements were discussed (A separate report for both events has been submitted).

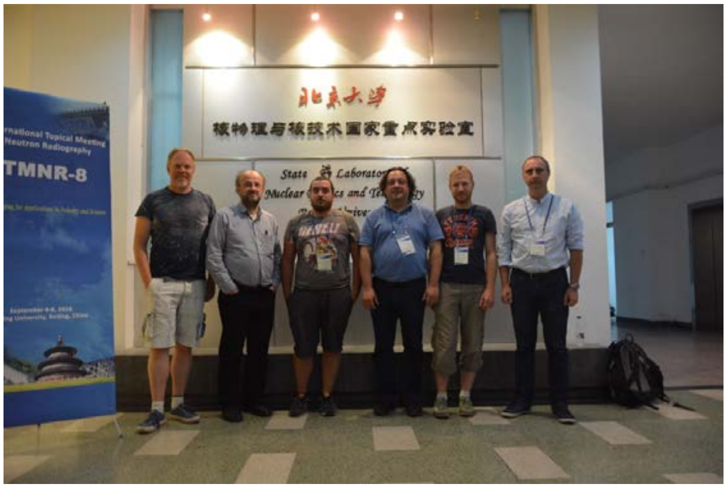


Fig.10.2: Participants in the WP10 imaging meeting at ITMNR-8. From left to right: Anders Kaestner (PSI), Winfried Kockelmann (STFC), Manuel Morgano (PSI), Søren Schmidt (DTU), Michael Schulz (TUM), and Nikolay Kardjilov (HZB).

The locations of the remaining workshops were agreed on at the General Assembly meeting in Coimbra;

- Workshop II will be at ILL April 24th and 25th, 2017.
- Workshop III Spring 2018 at MLZ.
- Workshop IV Spring 2019 at ESS.

Workshop II has been organized. Focus will be on getting feedback and input from expert users and potential contributors to the software considered in this WP. Parallel sessions have been organized for each of the considered software and 58 persons have registered at the indico page: https://indico.ill.fr/indico/event/77/. This includes persons from non-partner facilities (e.g. Oak Ridge National Lab, EMBL, and ESRF) as well as developers of software alternatives to the ones considered in this project. Moreover, the first deliverable 10.1, in WP 10, Standard & Guidelines, will be presented.

We note that Workshop III and IV will focus on non-expert users in conjunction with the remaining deliverables 10.2-8.

Task 10.2 Standard & Guidelines *(STFC, M6-20) PM 59*

This task is led by STFC. Standard & Guidelines is an important tool for facilitating collaboration and inter-operability. A questionnaire has been circulated in order to get an overview of the different techniques that the different partners employ for software development. The Standard & Guidelines, in the form of a report, will be based on the results from this questionnaire. The report will be presented at Workshop II and encompasses Deliverable D10.1.

Task 10.3 Converging on Mantid for continuum sources *(ILL, M6-32) PM 34*

This task is led by ILL, which has been fortunate to also obtain funding for an in kind contribution to this task. Thus, three full time developers have been recruited (Dr. Gagik Vardanyan, Dr. Antti Soininen, and Dr. Verena Reimund) to work on this task at ILL together with a consultant (Dr. Ian Bush) from the company Tesella and ILL staff member Miguel Gonzalez. In addition, one person (Dr. Emmanouela Rantsiou) is working part time at this task at PSI and two persons part time at MLZ/FZJ (Dr. Marina Ganeva and a student).

The following work has been performed at the continuous source partners

ILL:

- Existing ISIS indirect geometry algorithms have been adapted and extended for use at the ILL backscattering spectrometer IN16B. A workflow algorithm and its corresponding interface have been created and Mantid has been already used by the users in the instrument during the first ILL user cycle of 2017 (19 Jan to 8 Mar). Feedback is positive.
- Data reduction for the ILL Time-Of-Flight (TOF) instruments (IN4, IN5, IN6) has been completed and tested. No user feedback yet, as it has been used only by two instrument scientists. We are organizing a training session for the other TOF instrument scientists and plan to deploy Mantid for general use in the 3 instruments for the next cycle (starting on September 1st).
- Loaders and instrument definition files for the reflectometers D17 and Figaro are done. Currently working on the reduction workflow, exploring existing algorithms and interfaces and comparing with our needs. Goal is to have a user interface with similar functionality to the existing one (Cosmos based on IDL/Lamp) by the end of the year. Loaders for the powder diffractometers D1B and D20 are done. Work to manipulate and correct multiple diffraction data sets is on going. The plan is to make first real tests during next cycle after the summer.
- Work on Instrument 2.0 for the instrument description in Mantid in collaboration with ISIS and ESS is quite advanced. Plan to use it to handle the simple scanning instruments here: D2B (powder diffractometer), D4C (liquids and amorphous diffractometer), D7 (polarized diffractometer and TOF spectrometer), and D16 (multipurpose - SANS, reflectivity, diffractometer - instrument). Aiming to be able to treat D2B data together with D1B and D20 in September.

PSI:

- Mantid is being adapted to the reflectometer AMOR at PSI.
- Mantid extensions specifically for the general-purpose test beamline, BOA, are being developed in order to make Mantid the standard data analysis and reduction tool used at this beam line (with the exception of neutron imaging usage of BOA). Mantid is already being used at the BOA beam line at PSI for certain types of measurements.

MLZ/FZJ:

- Mantid is now in routine use at the instrument TOFTOF.
- Development is under way for the forthcoming TOF option of DNS.
- The work will be followed up with an adaptation of Mantid for the diffractometers TOPAS and PowTex.

Task 10. 4: Interoperable data treatment software *(ESS, M6-44) PM 182*

In Task 10.4 the different partners will deliver inter-operable analysis software for specific techniques such that other partners also can employ the software. One analysis program will be supported for each of the considered techniques. At Workshop I in the beginning of the monitoring period it was agreed that involved facilities should capture requirements for the techniques considered. The results of this process were presented at the General Assembly meeting in Coimbra and will again be considered at the relevant parallel sessions at Workshop II.

Small Angle Neutron Scattering (ESS). Two developers (Dr. Piotr Rozyczko and Dr. Wojciech Potrzebowski) have been recruited at ESS for two years to work on SasView, which was selected at the outset of SINE2020 to be the analysis software supported. SasView is already supported by many facilities worldwide, however, it has accumulated some technical debt. In the first 18 months focus has therefore been on setting up an infrastructure for continuous integration testing and on modularization. The modularization is completed, and all models are now contained in an independent model library that also can be used by programs other than SasView. Moreover, as part of this task, it is now possible to use models from the SasFit program from PSI within SasView. The Graphical User Interface (GUI) is also now fully separated from the backend functionality, which in turn can be accessed through an Application Programming Interface (API) enabling multiple user interfaces to co-exist. Work has started on replacing the current GUI with a new one based on the Qt toolkit in accordance with the Standards & Guidelines. Both the model library, the API, and the new GUI will in the future facilitate faster development of new features and will make the codebase easier to maintain. The new GUI will be the new main feature of the upcoming SasView 5.0 release. Integrated testing infrastructure has been designed and is being implemented. This will allow more stringent quality control resulting in higher quality product. Moreover, Dr. Rozyczko and Dr. Potrzebowski have established themselves as central partners in the SasView community, where they actively work on introducing standards for writing cleaner, reliable and maintainable code in line with task 10.2 (Standard and Guidelines) and have participated in SasView Code Camp IV, V, and VI. In addition, Dr. Potrzebowski instructed new users and developers at relevant session during SasView Code Camp VI that took place in Grenoble, April 4th - 11th (http://trac.sasview.org/wiki/DevIntroTutorial).

Reflectometry (FZJ/MLZ):

One person (Dr. Jan Burle) has been recruited to work on the FZJ/MLZ activities in WP10 in collaboration with the FZJ/MLZ scientific computing group. In relation to reflectometry, BornAgain, originally developed for GISAS should be extended to all types of reflectometry. BornAgain already adheres to the Standard and Guidelines, but does miss some features for reflectometry. In the first 18 months, focus has therefore been on supporting multi-layer models and developing a Qt based Graphical User Interface (GUI) in accordance with the Standard and Guidelines and on top of the already existing Python based Command Line Interface (CLI).

Imaging (PSI, CEA/LLB, STFC, ESS):

One person (Dr. Chiara Maria Carminati) has been recuited at PSI for two years, one person at ESS for six months (Dr. Anna FedrigO), and one Master 2 student at CEA for five months (Mrs. Pragya Shekar) to be followed by another Master 2 student (Mr. Pavlo Kosiak) for five months to work on analysis software for imaging. The software that will be supported will be MuhRec and KipTool, which in both cases initially were developed by Dr. Anders Kaestner at PSI.

The partners on imaging have worked on a joint requirement document that was finalized at a meeting in China in connection with the Neutron Radiography meeting in parallel with the General Assembly meeting in Coimbra.

Report from the partners involved in imaging:

PSI: Dr. Chiara Maria Carminati works jointly with PSI staff member Anders Kaestner on the MuhRec/KipTool software. New processing modules and GUI improvements have been implemented for the MuhRec/KipTool codes. The base libraries of the codes have been properly documented and build scripts prepared for continuous integration in a joint effort with ESS who will host the build servers. Latest Windows release in August 2016.

STFC: Dr. Anders Markvardsen and Dr. Federico Montesino-Pouzols have worked on Mantid for imaging: Reconstruction tools from Diamond are being implemented in Mantid and they are working on a GUI for reconstruction through the cluster. Discussions on how to interface MuhRec to Mantid is ongoing.

CEA/LLB: The Master 2 students at LLB has under the supervision of LLB staff member Dr. Frédéric Ott been investigating the possibility around the binary tomogaphy in order to reduce the acquisition time in computed tomography. The most promising algorithm is based on the work S. Roux et al, J. Math. Imag. Vision (2013), which LLB will interface with the MuhRec software of the PSI. An LLB visit to PSI is planned in order to work on this jointly.

ESS: Anna Fedrigo has under the supervision of ESS staff member Markus Strobl worked on data fusion between data from x-ray imaging and neutron imaging. Moreover, ESS (Dr. Wojciech Potrzebowski) has jointly with PSI prepared build scripts for continuous integration.

QENS (ILL): Development activities have not yet started on data analysis for QENS. The best option appears to be to support the efforts that ISIS is pursuing about adding appropriate fitting tools in Mantid. During the WP workshop in April 2017, the requirements from the different facilities will be analyzed and a common strategy adopted.

Atomistic Modelling (ESS, ISIS, UNIPR, ILL) comprises analysis methods for neutron and muon spectroscopy based on atomistic simulation tools, particularly Density Functional Theory (DFT) methods. The related efforts have turned into a cooperation between ESS, ILL, ISIS (STFC), and UNIPR. The Atomic Simulation Environment (ASE) has been proposed as a suitable software framework for Atomic modelling and simulations. This led to the organization of a mini-codecamp focusing on using ASE for requirements from ISIS as well as the muon group. The mini-codecamp was held at ESS in Copenhagen on February 20th and 21st and had participants from the muon group at UNIPR as well as from ILL, ISIS, and ESS (separate report in progress, see Fig. 10.3). Moreover, the ASE lead developer from DTU was invited as well and helped out with questions and issues that aroused during the mini-codecamp. The mini-codecamp exemplified the joint needs for density functional theory calculations to be used for both neutron and muon spectroscopy and resulted in calculations of phonon dispersion curves importable into Mantid as well as a ASE tutorial on how to calculate the potential energy for the absorption of a muon in a material. The tutorial is published on the ASE/GPAW homepage (https://wiki.fysik.dtu.dk/gpaw/tutorials/muonsites/mnsi.html). The conclusion was that the initial impression of ASE was positive and time has now been allocated at workshop II for a discussion of the next step in this regard.

Apart from the above activities, activities at the individual facilities are described below.

ILL: A first round of discussion with the scientists have taken place in order to compile their needs and requirements in terms of software for data analysis in the fields of QENS and INS. The priority of the

Fig.10.3: Participants in the ASE mini-codecamp at ESS. Participants are from left to right: Ifenyai John Onuorah (UNIPR), Roberto De Renzi (UNIPR), Jens Jørgen Mortensen (DTU and ASE lead developer), Thomas H. Rod (ESS), Miguel A. Gonzalez (ILL), Piotr Rozyczko (ESS), Torben R. Nielsen (ESS), and Anders Markvardsen (STFC).

Spectroscopy Group at ILL consists in developing a modern and sustainable phonon tool able to calculate easily phonon dispersion curves and neutron observables (mainly dynamic structure factors and densities of states) using the input from most popular DFT packages. Initial work in this direction has already been started independently at the ILL by Emmanuel Farhi and a likely possibility would be to recruit a developer in 2017 using SINE2020 funding to help him complete this work in collaboration with the other facilities.

UNIPR: UNIPR works solely on muon spectroscopy in collaboration with ISIS. A PhD student (Ifeanyi John Onuorah) has been recruited and works under the supervision of Prof. Roberto De Renzi and Dr. Pietro Bonfá (now at CINECO). Current ongoing activities related to muons are: subroutine development for site refinement in the code muESR, ensuring adherence to guidelines, development of methods for visualization of results using the Mantid framework, development and evaluation of DFT methods as a predictive tool for muon spectroscopy.

ISIS:

ESS: ESS organized the above mentioned mini-codecamp and has independently from SINE2020 also obtained funding from the Swedish Research Council for two post doc projects and from Chalmers University of Technology for a third post doc project to work on atomistic modelling projects with Swedish Universities and also with ISIS in case of the projects funded from the Swedish Research Council. These activities will be linked to SINE2020 when appropriate in order to avoid duplicate work and converge towards having community driven, maintainable, and sustainable solutions in place.

Dissemination and communication activities:

- Workshop I (PSI, 4-5 April 2016) organized as part of WP10. http://indico.psi.ch/conferenceDisplay.py?confId=4313). 26 participants.
- Workshop II (ILL, FR, April 24-25, 2017) organized as part of WP10. https://indico.ill.fr/indico/event/77/. 58 registered participants including from research

institutions external to SINE2020 (i.e. EMBL; ESRF; CINECA; Spallation Neutron Source, Oak Ridge National Laboratory, University of Bath; and Petersburg Nuclear Physics Institute).

- T.H. Rod, A. Kaestner, E. Rantsiou, R. De Renzi, F. Ott, M. A. Gonzalez, J. Wuttke, A. Markvardsen, T. Perring, S. Cottrell and M. Strobl. *Pan-European cooperation on data treatment software in SINE2020*. Oral presentation at ICANS XXII (Oxford, UK, 27–31 March 2017).
- W. Potrzebowski, P. Rozyczko, T. Nielsen, A. Jackson and T. H. Rod. *SasView for small angle scattering data analysis within SINE2020 project.* Poster presentation P1.35 at ICANS XXII (Oxford, UK, 27–31 March 2017).
- W. Potrzebowski. Tutorial at VI SasView Code Camp (ILL, April 4th - 11th). http://trac.sasview.org/wiki/DxevIntroTutorial.
- W. Potrzebowski and P. Rozyczko. Parcipitation and contributions to SasView Code Camp IV, V, and VI.
- I.J. Onuorah, R. De Renzi, and J.J. Mortensen. Tutorial on homepage for GPAW DFT code: https://wiki.fysik.dtu.dk/gpaw/tutorials/muonsites/mnsi.html.
- SasView v4 (https://github.com/SasView/sasview/releases/tag/v4.1.0)
- W. Potrzebowski, P. Rozyczko, T.R. Nielsen, A. Jackson, T.H. Rod. *ESS View on SasView*. Poster presentation at the 8th DanScatt meeting (26-27 May, 2016, Copenhagen, Denmark).
- W. Potrzebowski, P. Rozyczko, T.R. Nielsen, A. Jackson, T.H. Rod. *ESS View on SasView*. Oral presentation at NOBUGS 2017 (Copenhagen, Denmark, 16-19 October, 2016).
- F. Montesino Pouzols, A. Markvardsen, R. Tochenov, N. Draper, T. Rees, N. Gould, J. Hogg, J. Scott. *Comparing local minimizers for fitting neutron and muon data with the Mantid framework*. Poster presentation at NOBUGS 2017 (Copenhagen, Denmark, 16-19 October, 2016).
- http://arxiv.org/pdf/1604.03281.pdf
- http://arxiv.org/pdf/1602.01756.pdf
- http://arxiv.org/pdf/1603.03367.pdf

1.3 Impact

The tasks of all work packages have clearly defined objectives with impact beyond the time horizon of the SINE2020 project. Instrumentation at the ESS will be powerful, and partly new to the user community. Having the right environment to perform the experiments, in terms of sample environment, support laboratories or data reduction and treatment, is key. As mentioned in 2.1 of the DoA SINE2020 addresses the challenge of providing a common infrastructure across Europe that will facilitate the integration of ESS and the efficient use of ESS from day one.

The benefits of the suggested technical and educational improvements will directly impact on the scientific quality of experiments and successive publications at the ESS and other neutron large scale facilities in Europe. The scientific output of neutron related experimental investigations has contributed to societal relevant sectors such as energy, environment, healthcare, information technology or cultural heritage over the past decades (see e.g. Report of the *Neutron Landscape Group* on '*Neutron scattering facilities in Europe – Present status and future perspectives*' presented to the *ESFRI Physical Sciences and Engineering Strategy Working Group*, June 2016). The commitment of all SINE2020 partners to their respective tasks demonstrates the on-going, decade proved, capacity for innovation in the neutron sector and capacity for adapting neutron science to the current societal challenges.

We underline the expected impact of SINE2020 by highlighting several actions from the SINE2020 consortium, started in the first period.

- As mentioned in 2.2 of the DoA the user-oriented project SINE2020, based on a large extent on outreach to new users, including industry, and developing appropriate services, impact depends on the effective dissemination of the project activities and results. To this end the project the **internet portal SINE2020.eu** has been set-up, **receiving currently about 1000 visits/month**. Our information officer at TUM maintains the SINE2020 webpage in parallel with the neutron.org webpage, which is the sustainable version, accessible to the user community after the end of the SINE2020 project. The neutron.org website went live in July 2013 and counts now with around 2000 visitors/month. Social media accounts for about 12% of the website visits.
- Different **platforms** have been put in place and maintained in the SINE2020 project. These platforms play an important role for the outreach and sustainability of results obtained by the cooperation of our partners: The **e-neutrons platform** is the world leading e-learning platform for neutron scattering. By providing online and free education on neutron scattering with active learning modules based on synergetic combination of neutron scattering theory with virtual experiment simulations on a broad range of scientific topics, we expect to expand the neutron scattering user base significantly, equip the new users to perform experiments at ESS and elsewhere beyond the state of the art. A significant fraction of the materials that will be synthesized within the **DEUNET platform** have industrial applications or recognized innovation potential. Detailed neutron scattering studies enabled by chemical deuteration are of crucial importance for understanding the function and improving the efficiency of new materials and technologies. Our joint effort for developing new lipid extraction methods, new polymer synthesis and enzyme-technologies for the synthesis of complex small molecules, particularly chiral compounds, will considerably enlarge the experimental possibilities by providing neutron users with deuterated compounds that have been inaccessible until now. The DEUNET network **will ensure the provision and development of expertise** on a broad range of

deuterated materials for the European science community beyond the frame of the present SINE2020 project and guarantees sustainability in a rapidly developing field where there is a trend towards increased soft matter experiments at all neutron scattering facilities.

- During the first period our Industry Consultancy group elaborated a **strategy for addressing industrial partners** and analysed needs and possible outcome in joint research activities. Future effort will be spent on adapting characterisation methods and training in order to further improve the service provided by neutron centres with the aim of presenting the **business model for industrial liaison** at due date M46.
- Due to developments of WP5 (Deuteration) biologically relevant unsaturated lipid membranes in many different types will be used in neutron experiments related to cell membrane and **membrane protein function in health and disease** (D5.9, D5.10). The synthesis of lactic acid enantiomers will enable the synthesis of tailored polylactic acid polymers for user experiments investigating the dependence of polymer microstructure, physical properties and dynamics on the chemical structure, which will provide **new understanding on the properties of this important class of biodegradable plastics with biomedical and technological applications** (D5.11).
- The sample environment (WP7) is essential for the future performance of experiments and scientific quality. We anticipate impressive gain factors, typically x2 to x5 in background reduction, greater than x5 in cool-down time in furnaces, and 50% in max pressure of clamped cells. It is too early to estimate those related with the transparency of anvils and the transmission of pressure cells. Two per-reviewed manuscripts have already been published (*High Pressure Research* **36** (2016) 73, *High Pressure Research* **36** (2016) 140) and partners are going to present their work (posters and oral presentations) at forthcoming workshops / conferences.
- The new detector technologies of WP9 are an essential requirement for both new and existing neutron and muon facilities. As one example out of all the developments of WP9 we highlight the work on developing resistive plate chambers (RPCs) for high resolution position sensitive neutron detectors. RCPs have been used extensively as large area position sensitive detectors in High Energy Physics, but have had little impact to date on the neutron scattering community. Neutron sensitivity has been achieved by coating the aluminum electrode of each device with a layer of $^{10}B_4C$. Detector characteristics have been measured including a neutron detection efficiency of 12.5% at 4.7 Å and a very impressive spatial resolution of better than 0.25 mm FWHM.
- The implementation of state-of-the-art software tools and virtual experiments is a strategic pillar for the user community and the future scientific impact. The fluid information/data flow from data acquisition to data treatment and ready-to-publish data is at the heart of WP10. Based on the guidelines defined in D10.1 data reduction and data treatment software tools are developed for the so-called Phase I and Phase II neutron instruments at ESS, comprising imaging, reflectometry and SANS (Phase I) and QENS and INS (Phase II), respectively. Starting from five selected software packages, functionalities are added for graphical user interfaces, algorithms are optimized and fitting models extended with due dates M30 (D10.3 to D10.5) and M42 (D10.6).