SUSTAINABILITY REPORT

SINE 2020

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SINE 2020

Sustainability Report

Coordinator:

Institut Laue - Langevin (ILL)

NEUTRONS FOR SOCIETY

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SINE2020 was selected for funding under the European Commission 8th Framework programme Horizon2020 (INFRADEV-4-2015); there are two central strands to the programme: 'Joint Research Activities' and 'Networking'. The SINE2020 community already existed to a large extent, thanks to three former NMI3 grants (neutron/muon grants, under FP6 and twice under FP7). The four grants together have covered a timespan of about 15 years with a total budget of about 56.3 M€. The Horizon2020 framework programme is now coming to an end, as is, in its current form, the European funding for coordinated support or research & innovation in science with neutrons and muons.

Over its four-year period, SINE2020 has either initiated or pursued successful projects with demonstrable added value for Europe's neutron infrastructure and the science it produces. Most of these projects take the form of feasibility studies, adapted to the time-limited structure of the INFRASTRUCTURE calls. The emphasis on feasibility is now showing all its importance. The moment has come, a few months before the end of the funding, to evaluate the added value of the projects in terms of costs and benefits, and to reflect on their continuation, embedded in existing national and international neutron infrastructures.

If the projects now assessed as successful are not pursued from feasibility to execution, we could conclude that the effort and public resources expended have been spent in vain. Let us distinguish, however, between the Joint Research Activities (JRA) and Networking.

The JRAs have been organized around technical challenges: the experience gained is shared between facilities and remains accessible for future generations via publications and prototypes. Similarly, the projects in the Networking strand have invested the participants with know-how, which will be transmitted to future generations.

Networking, however, is not a short-term activity for which short-term funding can suffice. Nor is it cost-neutral for facilities, although a little investment, in resources for coordination for example, can go a long way and provide significant gains in efficiency for all facilities.

The neutron community has developed a high degree of coordination and cooperation on the technical level, and is considered to be an 'advanced community'. European funding has helped to set up task-specific groups with common interests; it has raised awareness of the need to share know-how and infrastructure. The next step is to reinforce long-term sustainability, with a coordinated strategy.

We hope that the content of this report provides support for this process, convincing decision-makers of the need to allocate resources for networking and projects. This will truly enhance the productivity of the progress made over the past 15 years in science with neutrons and muons in Europe.

In this sustainability report we describe the projects which have demonstrated benefits for the whole of the neutron community throughout the SINE2020 period.

INTRODUCTION

NETWORKING ACTIVITY

According to the definition of the European Commission, networking activities foster a culture of co-operation between the participants in the project, the scientific communities benefiting from the research infrastructures, industries and other stakeholders, and help develop a more efficient and attractive European Research Area.

Furthermore the H2020 work program details items like the following:

- reinforcing the partnership with industry,
- outreach and training courses for new users, and
- foresight studies for new instrumentation, methods, concepts and technologies.

SINE2020 covered exactly these three items with industry liaison (p.7), education with hands-on schools and e-learning tools (p.10), and by developing a network around the chemical deuteration of samples (p.12).

The three networking activities are now mature and seek the go-ahead of the respective decision making bodies.

The activities are presented by their objectives, their present status and their costs during SINE2020. Conclusions on sustained actions with future cost estimates, where applicable, are highlighted at the end of each project.

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INDUSTRIAL LIAISON

SINE2020 has devoted significant effort into establishing strategies for industrial collaboration and the coordination of industrial activities across the European neutron facilities. Details will be published in the last deliverable report [1]. *Here, we conclude on the levels of investment required to attract and retain industrial partners. On average, over the past 36 months of SINE2020 one industrial project per month has been set up. Sustainable industrial liaison depends on the efficiency of the neutron network; we propose the creation of regional hubs of liaison officers working closely with experts at neutron centres. The benefits should be judged not on the revenue generated, but on the impact on society of industrial collaboration and the accrued attractiveness of the Large Scale Facilities.*

The scope of this work package has been limited to the implementation of direct[1)] industrial access to European neutron facilities. To this end two Industrial Liaison Officers (ILOs) were employed full-time over the four-year period to attract industrial projects, preparing case studies with industrial partners and producing a robust business model [1]. They were assisted by local coordinators and scientists at different facilities. The activity did not include an evaluation of the financial income potentially available from industry for facilities. It focused rather on a reliable evaluation of the investment (human resources) required to attract industrial partners, perform measurements, and deliver the results.

Some of the existing long-term collaborations between facilities and companies, independent of the SINE2020 programme, were not considered. The following analysis is based on 35 industrial projects attracted in the first 36 months of the SINE2020 project.

Figure 1 shows the number of industrial projects carried out under SINE2020 at each facility, and the national origin of the projects (registered office of the industrial partner). The Liaison officers allocated the projects according to feasibility and beamtime availability at the facility.

75% of industrial projects were recruited in France, Germany, Denmark and Sweden, demonstrating on the one hand the proximity effect of ILOs (located in Grenoble and Hamburg) and the effectiveness of national hubs for attracting industrial partners. It should be said that northern European countries host and support several state-funded industrial programmes (LINX [2], Vinnova [3], Baltic TRAM, Science Link [4]), which provide a favourable environment for neutron activities, especially in the context of the upcoming ESS.

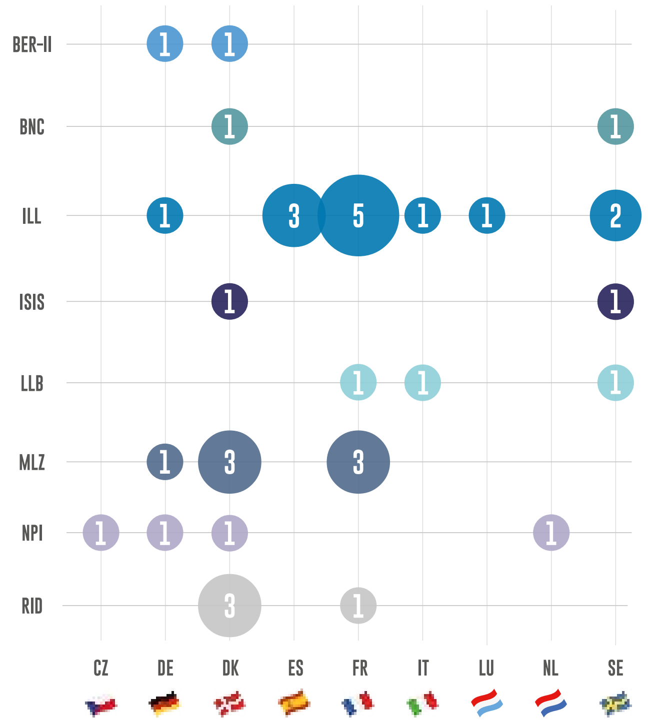

Fig.1: Industrial projects within SINE2020 performed at European neutron facilities, classified according to countries, where companies are seated. Status SINE2020 – January 2019.

AVERAGE INVESTMENT PER INDUSTRIAL PROJECT	
Campaigning, customer retention and networking per facility	*[PM/ year]*
Manpower scientific staff	0.25
Manpower ILO *	1
SUSTAINABLE NETWORK INVESTMENT	
General coordination of a future network	6

Table 1: Estimation of investment into staff. PM: Person months

* This is an average calculated from the SINE2020 feasibility studies and includes all activities, including outreach, coordination and facility networking.

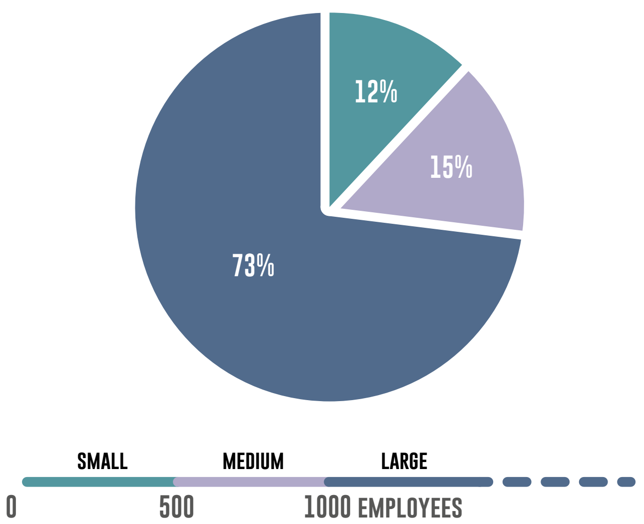

Fig.2: Distribution of industrial projects by size of industrial company. Status SINE2020 – January 2019

The size of the companies performing industrial projects at the neutron facilities (Fig. 2) reflects the classification of European companies by R&D expenditure [5]. It is clear that the larger companies (73%) have the appropriate R&D resources to perform research at LSFs[2] and thus remain the primary target group for LSFs. Smaller companies are certainly of interest, but may require supportive funding (such as joint PhD programmes with partners from academia, government research vouchers, etc.).

The industrial projects attracted by the scheme covered almost all the EU industrial sectors covered by the R&D Scoreboard of the European Commission [6]. Over the next few years the highest rise in R&D investment by European companies is expected to occur in the ICT, automobile and health sectors.

All three sectors are under-represented in the industrial projects and deserve special attention. In contrast, the industrial sector, combining metallurgy, mining, cutting tools and construction, occupies an important fraction of the total. The energy sector is not cited in [6], but is hidden in the 'transport' and 'other' sectors of the Scoreboard companies. Energy projects are explicitly included in the classification of neutron industrial projects, as they are considered to be a societal challenge.

The industrial projects are strongly diversified within each industrial sector. This demands adaptability skills of the ILOs and instrument scientists and the instrumentation available is not always adapted to industrial requirements. In addition, SINE2020's Industrial Advisory Board (IAB) has requested that facilities invest more in professional marketing and that they plan for a full scope of service to customers, in the interests of financial sustainability [7].

The work-load generated will have to be addressed by the limited number of scientists and ILOs at the neutron facilities. Consideration should therefore be given to ILOs cooperating in a business network and to stronger implementation of intermediary companies.

COSTS WITHIN SINE2020

The facilities spent an average of about 1 PM for an industrial project. This seems to be constant over time. However, it should be seen in the context of the resources spent to attract and retain industrial partners: the time required to establish first contact, perform feasibility studies, take the measurements and process the data, can vary from 1 to 24 months, with a median of about 10 months.

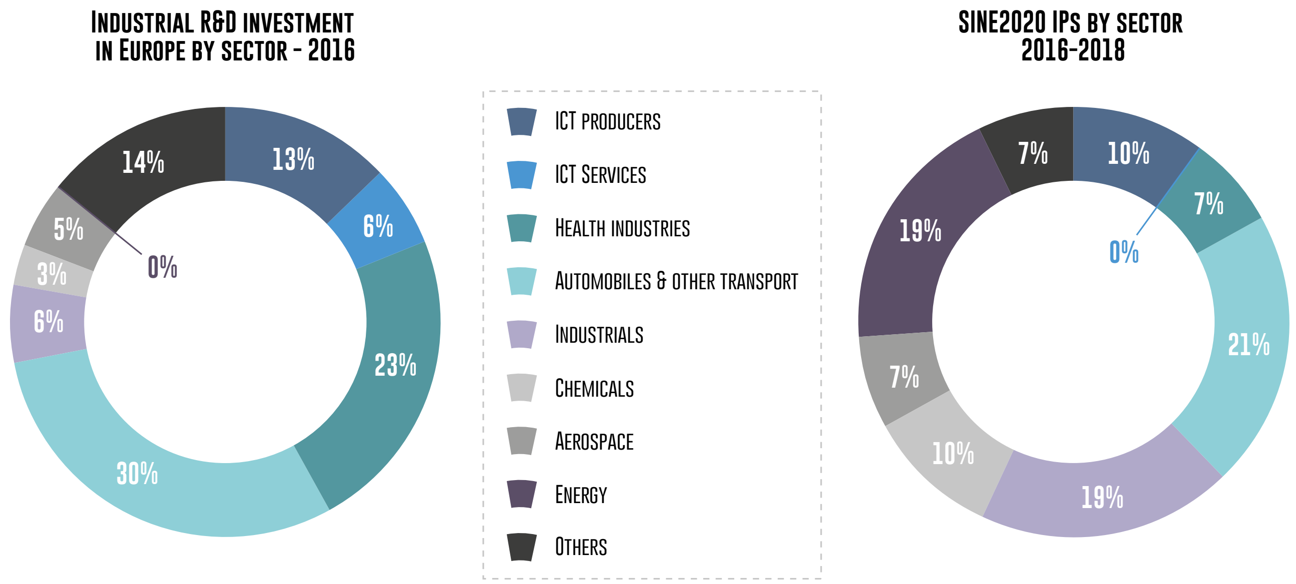

Fig.3:

Left: Distribution of industrial projects into different industrial sectors among the top 1000 R&D investing companies in EU [6].
Right: distribution of industrial projects in SINE2020 program in the first 36 months of the project.

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CONCLUSIONS

1 Under SINE2020, the cooperation with new industrial partners required 1.25 person-months (PM), on average, with 1 PM for the ILO and 0.25 PM for instrument scientists. These costs seem to be constant over time, indicating the level of investment of facilities needed for sustained industrial user programs.

2 The turnover of industrial liaison officers causes significant loss of experience and information. Industrial liaison needs solid foundations to maintain and increase momentum.

3 Efficiency gains and a rise in the number of industrial projects can be expected from the creation of a robust network of regional hubs close to or at the facilities and staffed with ILOs. Coordination effort between regional hubs is estimated 6 PM/year. This coordination should be taken further by integrating it into the recently initiated European Analytical Research Infrastructure Village (EARIV) [9] of neutron, synchrotron and laser facilities.

4 SINE2020 has focused specifically on direct industrial access. However, there is also a need to work with the many intermediaries capable of bringing neutron facilities and industrial partners together. This includes facilitating companies, research and technological organisations and university groups with specialist knowledge in specific domains.

5 In this scenario, the role of the ILO changes, shifting from technical consultations towards more coordination and liaison. The synergy effects between facilities is key to this endeavour and competition between facilities must be set aside. The pool of intermediaries will need to be strengthened in a common approach via outreach and training to enlarge the portfolio of proposed techniques.

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[9] https://www.eariv.eu.

[1] Direct collaboration is defined as collaboration between neutron facilities and industrial partners without a third party intermediary such as an academic partner.

[2] Large companies only represent 0.2% of the total enterprise population in the EU-28 non-financial business sector, but they employ 33% of the working population and generate 43.2% of the total added value [5]. Of these large EU companies, 577 figure on the 2018 EU Industrial R&D Investment Scoreboard, comprising the 2500 companies world-wide which invested over €25m in R&D in 2018 [6].

EDUCATION & TRAINING

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The benefits and costs of the European neutron facilities' educational programmes are based on introductory and specialised schools supported by SINE2020 Education & Training programme as well as e-learning activities. The figures are also based on information provided by the organisers of neutron schools [1]. Half of the schools are organised by universities or user associations where Neutron facilities contribute via teaching and hands-on practice. The other half is directly organised by the facilities.

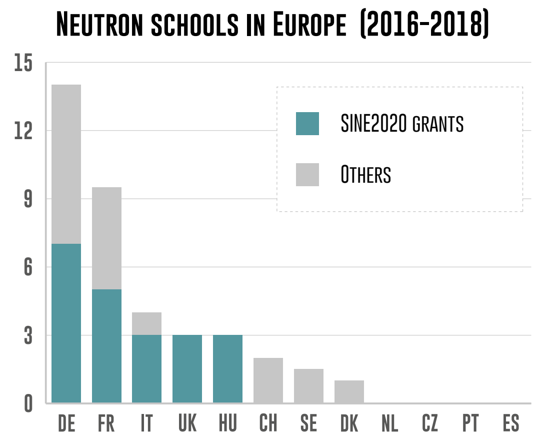
There are currently between 5469 [1] and 5777 active neutron users in Europe [2]. The loss per year due to retirement is estimated at about 2% [3], i.e. between 100 and 120 users per year.

Over the period 2016 – 2018, SINE2020 supported 21 schools which is an average of 7 neutron scattering schools per year, attracting about 300 participants a year overall.

As this represents about half of the forty neutron schools organised annually in Europe [4], we can suppose that the neutron schools attract about 600 participants per year in total. A detailed follow-up of the participants at the Italian neutron school shows that about ⅓ of them return to the facilities as users [5].

Extrapolated, this indicates about 200 new neutron users/year. To these numbers should be added the new users arriving from elsewhere (workshops or lectures), although it is likely that most academic groups with strong neutron scattering activities encourage their students to attend one of the domestic schools.

As shown in Figure 1, Germany and France have a relatively high number of neutron schools. Other countries with national sources (UK, F, H, CH) follow, with about 1 school/year. The ILL, as an international source, is counted separately. Italy is exceptional in that it runs 2 schools per year despite lacking a national source.



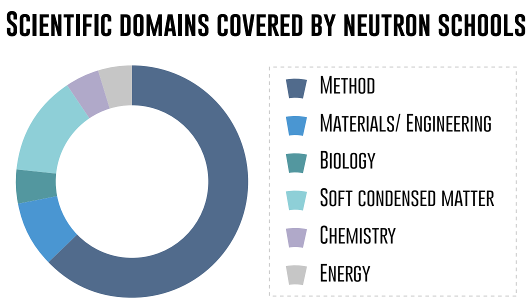


Fig. 1: The distribution according to hosting countries (top) and scientific domains (bottom) for about 40 schools organised in Europe in the period 2016 - 2018

Average investment for schools [per participant]	
Budget	1000 €
SINE2020 grant	200 €

Average investment for e-learning [per year]	
Present investment	[PM]
Manpower scientific, content	6
Manpower IT support	8
Future investment	[PM]
Manpower scientific, content	6
Manpower IT support	6

Benefit from schools

⅓ of school participants come back to a facility for an experiment.

Benefit from e-learning	
Number of users (April 2019)	1150
Number of new users/year (for last 3 years)	200
Number of visitors/month*	100
Number of WIKI users/month*	50-100

* web traffic screening over the last 36 months

Table 1: Estimation of investment into staff and resulting benefit from schools and e-learning. PM: Person months

The majority of neutron schools run general courses, providing an introduction to the theory and an overview of various techniques (labelled 'method' in Fig. 1). Schools focusing on specific scientific domains are a minority. Outreach could probably be improved by helping neutron schools to address various scientific topics or communities more specifically (e.g. as part of scientific workshops and conferences with specific lectures in the relevant fields), or with other techniques (x-rays, Raman, NMR, simulations) [6]. Almost all schools target PhDs and post-graduates. Undergraduate schools are rare, but the e-learning / training platform fills this gap with a content and style of presentation especially adapted for this target group [7].

The web platform offers the advantages of: 1) Interactive, self-regulated learning based on a wiki with exercises, hints and solutions; learning quizzes with built-in feedback; virtual experiment exercises supported by McStas simulations, all adapted to the web generation, and 2) Interactive monitoring of the on-line activity of the student, allowing for continuous adaptation of the content [8]. Regular screening of web traffic shows that students have used both the e-learning platform and the reading material at a level of about 100 visits/month over the last 36 months. The number of unique visitors rose considerably during European schools, e.g. visits to the wiki and exercises increased by an order of magnitude compared to average visitor levels. This suggests that it would be fruitful to further adapt the scientific content to the specialized neutron schools.

Costs within SINE2020

Average costs of schools based on statistics in SINE2020 are given in Table 1.

The e-learning platform has been developed and deployed throughout the NMI3-II project and provides complete content on neutron scattering techniques for a total cost of about €1.4m: NMI3 €0.6m and SINE2020 €0.8m.

CONCLUSIONS

1. The neutron schools are of utmost importance for maintaining the user community, at least at its present level.

2. There is no additional European funding for these schools after the end of SINE2020. The numbers show that the total costs are about €1000/student/school. SINE2020 provides about 20% of their total costs. This is very little, considering their importance for the neutron community and neutron science.

3. The content, location and frequency of neutron schools needs to be coordinated and promoted. This should be pursued after SINE2020. Appropriate monitoring of this activity is vital for the community. Larger facilities should consider investing in neutron schools in countries with weaker communities.

4. Neutron schools should bond with other experimental techniques, and specifically address particular scientific domains. This needs future investment in manpower developing content for these domains (estimated 3 PM / full day of course activity).

5. The e-learning platform provides a good supplementary learning environment which is accessible online at any time from anywhere. The investment period has ended. For sustained technical support and technical development further investment (6 PM/year) is needed to improve outreach to academia beyond the university groups already familiar with neutrons.

References

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DEUNET | THE EUROPEAN NETWORK FOR CHEMICAL DEUTERATION

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A new chemical deuteration network has been created to address a long-standing bottleneck in sample availability for neutron experiments in biology and soft condensed matter. SINE2020 provided resources that contributed to setting up the structure, initial activities and mission of DEUNET. It has grown into a successful example of synergy gain by sharing methods and infrastructures between large-scale facilities. The accumulated know-how resulting from joint R&D activities and transnational provision of samples provides a catalogue of deuterated materials to the user community and forms the basis for future development.

At the STFC Deuteration Facility, SINE2020 funding (24 PM) has allowed 18 deuteration projects to be launched for non-UK neutron users [1], as well as a new collaboration with FZJ on deuterated PEG surfactants and PDS.

At ILL, SINE2020 has financed 36 PM for the extraction and purification of deuterated lipids from cell cultures, in collaboration with the existing biodeuteration laboratory. These lipid biodeuteration and purification methods have also been introduced at the ESS, in collaboration with the Lund Protein Production Platform LP3 [2] and the ESS DEMAX biodeuteration service [3].

DEUNET ACHIEVEMENTS DURING SINE2020

1. ESTABLISHMENT OF A NEW CHEMICAL DEUTERATION LABORATORY AT ESS
2. ACCESS TO STFC DEUTERATION FACILITY FOR EUROPEAN USERS
3. DEVELOPMENT OF METHODS FOR LIPID DEUTERATION, AND SEPARATION FROM CELL CULTURES AT THE ILL
4. R&D IN THE ENZYMATIC & CHEMICAL SYNTHESIS OF CHIRAL BIOPOLYMERS AND LIPIDS AT FZJ + ESS

SINE2020 has provided support for the creation of DEUNET, a network for chemical deuteration, which has succeeded in fostering European collaboration between its participating facilities and in creating ties with its external members: international facilities (Australia and Japan), local infrastructures (LP3 at Lund University) and industry (Larodan Lipids, SE).

DEUNET provides a technical platform for scientific inter-facility exchange on state-of-the-art deuteration methods, and facilitates user access to a broad range of deuterated materials and expertise. The synergies between different types of expertise at the participating facilities considerably enhance the efficiency of development work in deuteration methods and the services available to the European user community.

For example, thanks to SINE2020 funding (Table 1), R&D in immobilized enzyme catalysis for the deuteration of chiral compounds at ESS (48 PM) enabled the synthesis of biodegradable biopolymers from L- and D- lactic acids at FZJ (18 PM).

Each laboratory operates within the framework of its home facility, and the coordination of DEUNET requires only a small investment. The key contribution of SINE2020 was to provide funding for staff to enable the joint platform to function.

The continuation of these activities depends on the resources for staff at the participating facilities, particularly at those which currently have no staff for chemical deuteration (ILL, FZJ).

The deuteration services offered today have limited human resources, restricting the number of experiments receiving optimal deuteration and hindering the application of neutron scattering to new materials. This is particularly important in scientific areas requiring either highly specialized and continuously changing materials (e.g. medicine) or multidisciplinary approaches (e.g. advanced nanotech and energy materials) that greatly benefit from neutron scattering.

FACILITY	ESS		STFC		ILL		FZJ	
CURRENTLY FUNDED (FTE)	2 scientists	2	4 scientists 1 technician 2 Post-Docs 3 PhD student	4 1 2 2	1 technician	0.2	-	-
REQUIRED (FTE)	3 scientists 1 technician 1 Post-Doc 1 PhD student	1 1 1 1	4 scientists 1 technician 2 Post-Docs 2 PhD students	3 1 1 2	1 scientist 1 technician 1 Post-Doc 1 PhD student	1 1 1 1	2 scientists 1 Post-Doc 1 PhD student	2 1 1
SINE2020 FUNDED (PM)	1 Post-Doc	48	1 Post-Doc	24	1 Post-Doc	36	1 Post-Doc	18

Table 1: Current and required staff for sustainable user service per year per chemical deuteration facility (at steady state operations, excluding biodeuteration/crystallization). FTE: Full time equivalent; PM: Person months

Typically, all deuteration laboratories have to support three modes of operation:

1) routine provision of deuterated compounds based on known techniques,

2) R&D on new compounds/techniques, and

3) management of the user access service.

In addition, all labs typically host PhD students and postdocs from externally funded scientific collaborations that require training and supervision. The management of DEUNET requires about 4 PM/year for network coordination and communication including maintenance and development of the DEUNET portal [4].

User workshops and outreach events provide excellent access to the user communities; they provide opportunities for dialogue and exchange and, thus, for the promotion of deuteration capabilities. Finance needs to be foreseen for these, as well as for regular meetings and staff exchanges, including in international facilities. Since the creation of DEUNET, international observers (ANSTO, Australia and JPARC, Japan) have provided valuable input, and scientists active in deuteration in the US (ORNL) have also expressed their interest.

DEUNET facilitates access to the full catalogue of deuterated compounds via the user programmes at the participating facilities. Its network portal and activities provide increased visibility to both academic and industrial users and partners via [4].

However, all DEUNET member laboratories need sustained funding of permanent technical and scientific staff in order to maintain the state of the art, and to profit from the synergy effects of the network. In the long-term, DEUNET offers the possibility to dissociate the location of synthesis completely from the location of the neutron experiments. To enable this, an agreement on inter-facility access to deuterated samples would need to be established, to take into account the different operating frameworks of the participating facilities.

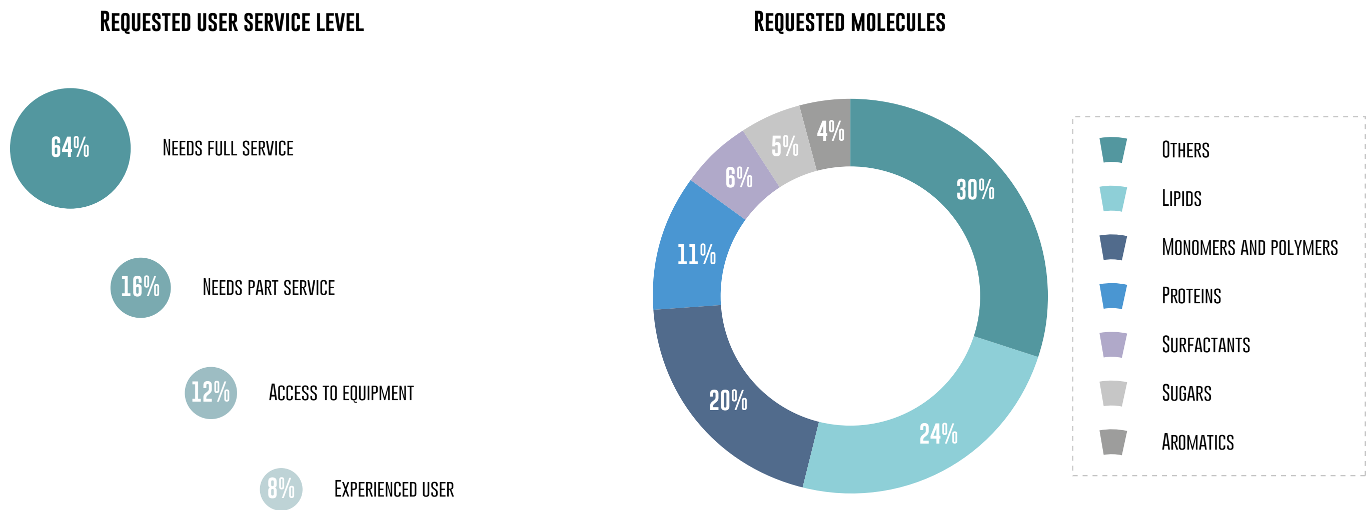

Fig. 1: Results of the DEUNET survey carried out in 2017 in conjunction with a joint DEUNET-STFC Deuteration user workshop. Left: a predominant fraction of users require a full synthesis and purification service by the facilities. Right: most frequently required molecules [5].

COSTS WITHIN SINE2020

The funding provided by SINE2020, and the current and future staffing requirements for the participating deuteration laboratories at steady state service are summarised in Table 1. As each facility provides a different range of services, the current staffing levels and future requirements differ. This is particularly important for those facilities (ILL and FZJ) who do not yet have funded staff to provide a user service at the moment, and whose ability to provide deuterated samples and participation in a sustainable DEUNET are entirely dependent on continued funding.

The support and funding from each facility are essential but will ideally be complemented by continued EU and national grant funding in collaboration with partners and users to develop solutions to specific challenges. In these cases, facility commitment to co-funding requirements is a pre-requisite.

Synergy effects with biological and chemical deuteration

Experience from facilities with both chemical and biological deuteration capabilities (ANSTO, ESS, ILL, STFC) and macromolecular crystallization facilities (ESS, ILL) has shown that there are many synergies to be gained from close collaboration at all stages of the sample deuteration process. This is particularly true in the overlap cases where the target molecules may be deuterated either chemically or biologically, or where deuterated reagents are needed for protein crystallization or reconstitution. Ideally, therefore, DEUNET should acquire biodeuteration and macromolecular crystallization facilities

CONCLUSIONS

1 DEUNET facilitates access to the full catalogue of deuterated compounds via the user programmes at the participating facilities. Its network portal and activities provide increased visibility to both academic and industrial users and partners [4].

2 All DEUNET member laboratories need sustained funding of permanent technical and scientific staff in order to maintain the state of the art, and to profit from the synergy effects of the network (see Table 1).

3 Long-term, DEUNET offers the possibility to dissociate the location of synthesis completely from the location of the neutron experiments. To enable this, an agreement on inter-facility access to deuterated samples would need to be established, to take into account the different operating frameworks of the participating facilities.

4 Inclusion of biodeuteration/macromolecular crystallisation facilities in DEUNET should be considered.

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JOINT RESEARCH ACTIVITIES

The success of the Joint Research Activities (JRAs) equally rely on the networks of experts in various neutron technological fields. Nevertheless, for this section these existing networks are considered as established and emphasis lies on the technological progress in various fields during SINE2020.

According to the expectations of the European Commission, JRAs are to be innovative and to explore new fundamental technologies or techniques underpinning the efficient and joint use of the participating research infrastructures. They should involve, whenever appropriate, industries and SMEs to promote innovation and knowledge sharing through co-creation of needed technical solutions. In order to improve, in quality and/or quantity, the services provided by the infrastructures, the joint research activities address:

- higher performance methodologies and protocols, higher performance instrumentation, including the testing of components, subsystems, materials, techniques and dedicated software, taking into due account resource efficiency and environmental (including climate-related) impacts;
- integration of installations and infrastructures into virtual facilities;
- innovative solutions for data or sample collection, management, curation, annotation, and deposition; and
- creation of specific services for supporting research addressing large research challenges.

The SINE2020 consortium fulfilled these expectations, as demonstrated on various selected projects in the following. From a project point of view, timeline and available budget for JRA grants typically match the scope of feasibility studies and the demonstration of principle through prototyping. Most of the chosen examples have passed this step with success and are ready for application, if decision makers agree on the relevance of the projects for the neutron community, and, if they are ready to invest.

The projects are therefore presented by their objectives, their present status and their costs during SINE2020. Conclusions on sustained actions with future costs estimates, where applicable, are highlighted at the end of each project.

Common projects between various facilities naturally bring along a standardization of techniques and various standards have been set within SINE2020. Due to their added value for the neutron community as a whole, we start this part of the sustainability report with standardizations in three different areas: sample environment communication protocol, scientific data analysis software standards and Monte Carlo simulation particle list.

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COMMON STANDARDS

EXAMPLES FROM SAMPLE ENVIRONMENT AND SOFTWARE DEVELOPMENT

Within different Joint Research Activities (JRAs) there have been efforts to reduce the technical hurdles for efficient collaboration between different partners and facilities. We present three projects below on the development of common standards: the Sample Environment Communication Protocol (SECoP), Data Analysis Software standards, and Monte Carlo Particle Lists (MCPL). These have proven their viability as a framework for future development, potentially even beyond the classical neutron and muon community, e.g. as part of specifications for industrial partners or in particle physics.

THE SAMPLE ENVIRONMENT COMMUNICATION PROTOCOL - SECOP

SECoP addresses the portability of sample environment tools between different neutron (and x-ray) facilities, on a plug-and-play basis. Neutron facilities would benefit from the exchangeability of complex (and expensive) sample environment equipment, e.g. via reduced instrument down-times, caused by the non-availability of sample environment requirements.

The crucial technical hurdle has been to improve communication between the different hardware and software components, whilst ensuring low complexity on the client side (instrument responsibles, users) and low development costs on the facility side. Supported by SINE2020, the SECoP development team targeted Inclusive, Simple and Self-Explanatory solutions [1]. Facilities should be able to use the protocol without, for example, having to rewrite drivers or reorganise hardware. It should be easy to integrate and use and it should make the environment-control software more easily configurable by adding meta data to the experimental data flow.

During development, the protocol was constantly tested for feasibility. Different test implementations were written and continually adapted at different neutron facilities, such as Helmholtz-Zentrum Berlin (HZB), the European Spallation Source (ESS), the Heinz Meier-Leibnitz Zentrum (MLZ) and the Paul Scherrer Institut (PSI), with a special focus on the interoperability of the different SECoP solutions. Version 1 of the *Sample Environment Communication Protocol to facilitate communication between instrument control workstations and sample environment equipment* is now publicly available [1].

COSTS WITHIN SINE2020

SINE2020 has helped to bring SECoP into life with a total of 60 PM shared among different facilities under the lead of HZB.

GUIDELINES AND STANDARDS FOR SCIENTIFIC ANALYSIS SOFTWARE

The development of good data treatment software depends on a creative environment involving facility computing departments, instrument scientists and dedicated users, for they all share an interest in the quality of scientific tools. As service facilities with a commitment to users, user facilities have different constraints as regards software development than university research groups for example. Their software needs to be maintainable, sustainable, extensible, reliable and stable [2] in order to be operational across bespoke beamlines and large facility user programs. As the available manpower is limited, software should be shared across facilities. For this, the user community needs to be involved and there must be efficient coordination between the developer teams. Software must become interoperable. Several software groups have therefore agreed on a set of common guidelines and standards [2], which will provide a development framework for existing and future data treatment packages, including the development of software for the ESS [3-8] (see also *Data Analysis and Atomistic Modeling Software* chapter, p.28, for details).

COSTS WITHIN SINE2020

The establishment of the guidelines required about 1 PM with input from several facilities.

MONTE CARLO PARTICLE LISTS - MCPL

Neutron instrument simulation packages based on Monte Carlo techniques are indispensable during the design phase of any new component exposed to a neutron beam. Several packages have been designed for broader use [7,9,10], but there is a plenitude of programs tailored on specific, individual needs. Monte Carlo methods are also used to simulate and optimise neutron sources and shielding [11] as well as in the design and optimisation of detectors [12-13]. All these MC packages generate particles or rays with an initial state of parameters (position, time coordinates, momentum vectors, time and possibly statistical weight/intensity, etc.). These particle lists 'interact' with the components of interest, thereby altering their states.

There would be efficiency gains if the particle lists were stored in hard memory, to be able to continue previous simulations, to test similar components in other simulation packages, or to reduce simulation times by focusing on sub-assemblies. The possibility of starting a simulation in software A and continuing or completing it in software B would also open up new routes, both to increased realism and also to new applications not initially targeted.

Monte Carlo Particle Lists (MCPL) provide a compact but flexible on-disk binary format for particle state information, portable, well-defined and accommodating a wide range of use-cases, with close to optimal storage requirements [14]. The code used to access the files should be small, efficient and easily integrated into existing codes and build systems. MCPL updates are available through GitHub on the project website [15].

COSTS WITHIN SINE2020

The core MCPL library was developed with synergy between the EU project BrightnESS [16] and SINE2020. T. Kittelmann (ESS) devoted 12 PM from BrightnESS, whilst approximately 6-8 PM of SINE2020 resources were used to develop MCPL-related MCNP, McStas and RESTRAX-related code. About 12 PM were devoted to the application of MCPL for core SINE2020-WP8 activities. In addition, we estimate that HZB provided 1 PM for VITESS-related MCPL code.

CONCLUSIONS

1. Enhanced collaboration between facilities naturally needs standardisation of shared techniques.
2. Common facility standards facilitate negotiations with industrial suppliers.
3. The implementation of standards and protocols, once developed, is of minimal recourse to manpower.
4. The SECoP protocol for sharing common sample environment, for example, needs about 3 PM/facility to enter its final implementation phase at different facilities.
5. Maintenance of common standards requires little investment and is of the order of 0.5 PM/year/facility.

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NEW DIRECTIONS FOR MONTE CARLO SIMULATIONS

Simulations of instruments or components based on Monte Carlo algorithms have moved up a level, with promising future impact. While they still focus on the optimisation of optical components for perfect beam shapes and optimum count-rates, interest is shifting to the samples themselves; calculations evaluate expected signals with respect to (calculated) instrumental background. Despite an unlimited number of possible sources, a systematic study of background scattering from already known sources can give considerable insight into, for example, scattering geometries or materials in the sample environment. In this respect, the common MCPL standard (see also Common Standards, p.16) facilitates dataflow between codes for neutron transport simulations [1-3] *and particle transport codes* [4], *the latter highlighting radiation and shielding aspects. In the following, we present two simulation projects which were carried out within the period of SINE2020.*

EFFICIENT CRYOSTATS FOR UNIQUE INSTRUMENTS

Sample containers, cryostat calorimeters and tails belong to the intensively used components closest to the samples and therefore most difficult to screen for background. Two new McStas components developed by ICMA calculate neutron pathways through these typically textured metals, taking elastic and inelastic scattering into account, including multiple scattering [5]. Inelastic scattering, dealing with single- and multi-phonon scattering, is covered by the phonon-incoherent approximation, using an effective Density of States as input [6]. Complex microstructures of the polycrystalline metal structures (such as the preferential orientation of grains or texture) are implemented by locally combining a new form of the scattering cross-section suitable for smooth textures (based on the generalized Fourier expansion of the Orientation Distribution Function [7]) and three limiting cases of scattering conditions: randomly oriented polycrystals (powders), mosaic single crystals and 2D disordered crystallites (as for highly oriented pyrolytic graphite HOPG).

The new McStas components were applied to redesign the calorimeter of the cryostat used on the IN5 time-of-flight spectrometer at ILL. Excellent machining skills were required to reduce wall thickness down to 200 µm, as managed by the ISIS sample environment team.

Comparative measurements at IN5 showed that the signal to background could be improved by a factor of three [9]. In addition, a new type of sample can for powder diffractometers has been developed. This null-matrix vanadium container reduces background by about one third and is now being adopted by different facilities [8].

COSTS WITHIN SINE2020

The development of the new component demanded 34 PM within the SINE2020 framework. Several cryostats are being modified at the ILL by applying the techniques developed during the project.

SHIELDING OPTIMIZATION OF SUPER-MIRROR GUIDES

The proper evaluation of guide shielding in particle transport codes such as MCNP [4] is challenging as guide geometries with inherent long distances from the neutron source prevent efficient calculations in the particle transport codes, and physical aspects of super-mirror reflection were not implemented at all. Lacking proper evaluation tools, real shielding components could suffer either from costly over-dimensioning, or might need equally costly and time-consuming rework to cover insufficiencies. Prior to this work super-mirror algorithms, tested in McStas, were implemented in the latest MCNP release [9]. Up to now however, the combination of reflective supermirrors and variance reduction methods, such as the so-called DXTran sphere method in MNCP was not available, which severely limited the quality of statistics, when transporting particles through the sample position. The most recent developments by ESS-Bilbao solve this issue and a new algorithm is available in MCNP: the deterministic transport method. Hence it has become possible to achieve satisfying event numbers in the detectors, even for complex guide geometries [10]. The improved code was finally used to generate the neutron distribution along the 150 m guide of the future back-scattering instrument MIRACLES at ESS. The agreement when comparing the new algorithm to an earlier MCNPX implementation of supermirrors without variance reduction, is very good: less than 6% throughout the guide, when using material cross-sections that may be different between the versions, and within 0.013%, when a model void of materials is used.

Applied mesh sizes have a resolution of 10x10x10 cm^3 throughout the system. The particle distribution around e.g. neutron choppers were evaluated and shielding optimized. Future development, led by ESS-Bilbao, foresees full transport simulation including gamma ray generation, among others. Further, the inclusion of other variance reduction schemes and strategies from McStas and RESTRAX are foreseen.

COSTS WITHIN SINE2020

The implementation of the McStas algorithm and adaption of the source code needed approximately 12 PM within the SINE2020 framework, and a similar magnitude of contribution from outside SINE2020.

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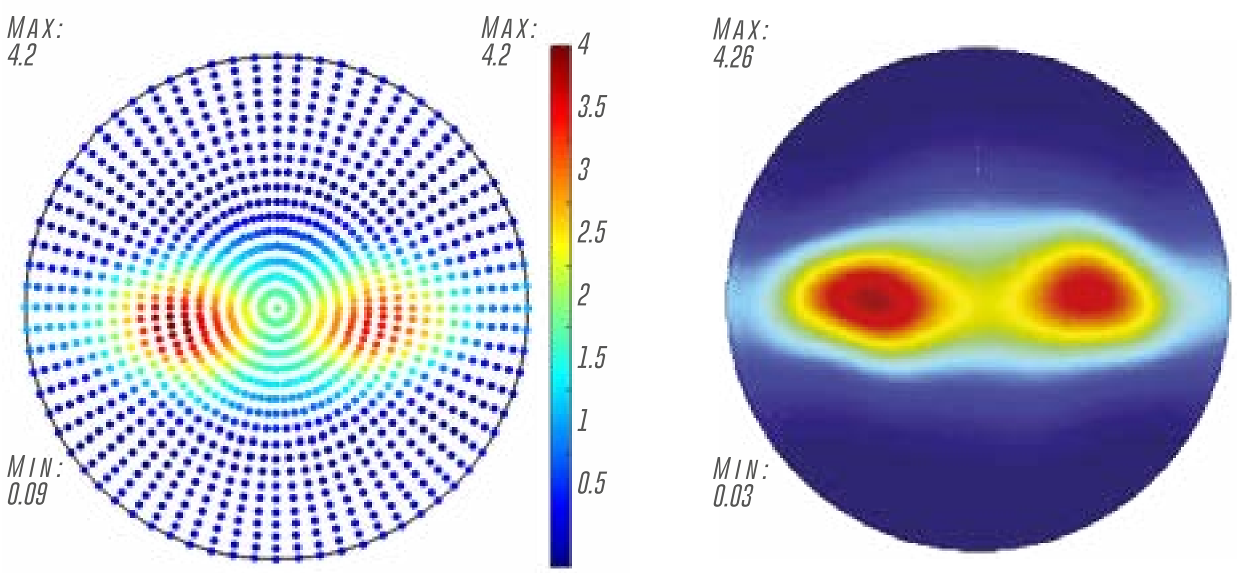

Fig. 1: Pole figure of the (0002) crystal planes of a Zircaloy-4 plate. *Left:* computed by Monte Carlo simulations with McStas, with the new component Texture.comp developed in the context of the SINE2020 project. *Right*: experimental result from the publication F. Malamud et al.[11].

CONCLUSIONS

1 Sophisticated Monte Carlo algorithms are a prerequisite for future signal to noise optimisation of neutron instruments and sample environment and need adequate staffing for every new project.

2 The maintenance costs of software and IT are about 6 PM per simulation package (McStas [1], Restrax [2], Vitess [3]). At present, these costs are shouldered by universities and need support of facilities in the interest of the facilities.

3 On top of maintenance costs, development costs of the order 24PM per project should be considered for new instrumentation projects. Such costs are quickly compensated by the gain in neutron statistics and beam time as shown on the example of a cryostat modification on IN5.

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LARGE CRYSTAL GROWTH

FOR NEUTRON MACROMOLECULAR CRYSTALLOGRAPHY

TEXT CONTRIBUTORS: Ashley Jordan, Trevor Forsyth - ILL (FR) | Marialucia Longo, Tobias Schrader - JCNS (DE)

Neutron macromolecular crystallography (NMX) is steadily emerging as a powerful technique that provides crucial insights in structural biology. In the recent past, considerable progress has been made in the development of instrumentation at central facilities throughout the world, and for sample preparation methods (notably biological deuteration approaches) which optimize the efficacy of NMX; this area is also being prioritized as part of upgrade plans at existing and future neutron sources such as ESS. However, for the foreseeable future, the single biggest bottleneck to the wider exploitation of this method remains the availability of large crystals with volumes of 0.1 mm³ or more. During the SINE2020 project, ILL, JCNS and ESS tested various systematic approaches that seek to address this issue. Two of the strategies are summarized below and constitute areas that should be prioritised in terms of sustainability beyond SINE2020.

LARGE CRYSTAL GROWTH AND MICROCRYSTAL ALIGNMENT BY HIGH MAGNETIC FIELDS

It has been shown that high magnetic fields (e.g. 17T) can be used to augment the growth of large crystals and induce the alignment of microcrystals that can subsequently be immobilized in hydrogels. As part of a SINE2020 project that links the Grenoble Partnership for Structural Biology (PSB) with Birmingham University (UK), JCNS (Germany), and Lund University (Sweden), Dr A. Jordan (ILL) and collaborators have extended this approach, further demonstrating the potential for the growth of larger crystals in magnetic fields, and carrying out monochromatic neutron single crystal analyses on such crystals.

Larger single crystals

The exploitation of the ability to produce larger single crystals in this way needs little clarification other than to speculate why it has not been more widely applied in the past in connection with NMX work. The main reason is almost certainly the simple fact that routine and continuous access to such field strengths over the extended periods associated with crystal growth is not at all easy, and furthermore that the costs of a dedicated system are not insignificant. However, as is often the case for sample environment needs, these initial investment costs are relatively small by comparison with the accumulated costs of neutron beam time associated with the research measurements.

Microcrystal alignment in hydrogels

The microcrystal alignment approach, while less known and less characterized, has also been shown to have huge potential. In many crystal symmetries, the net effect is the alignment of thousands of microcrystals along one of the principal axes, with random rotation of the crystallites about this axis. The net result is the cylindrical averaging of the data in the same way as would occur for a crystalline fibre or for a single crystal if was rotated about this axis during data collection. The fixation of samples that are ordered in this way can be achieved through the preparation of samples in hydrogels that are liquid at protein-tolerable temperatures and which then serve to immobilize the aligned crystallites when the temperature is reduced.

KEY POINTS

1 The formation of microcrystalline "slurries" in protein crystallization happens very frequently and is typically regarded as a nuisance in crystallogenesis work aimed at the production of larger single crystals. Any method that successfully exploits the alignment approach in a widespread way opens up NMX to a hugely increased range of problems, as indicated in Figure 1.

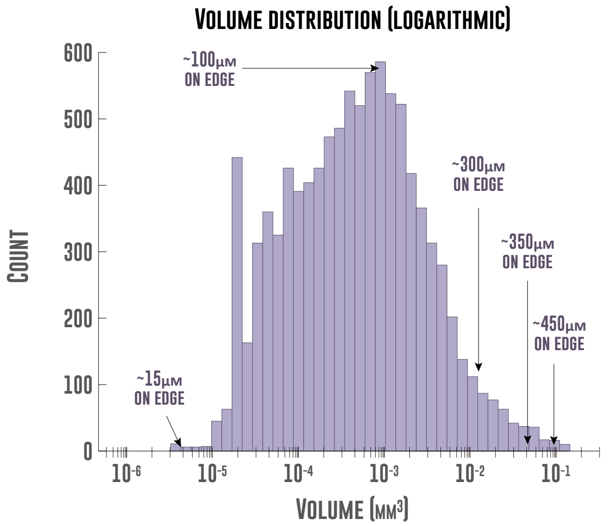


Fig.1: Histogram showing crystal volumes measured over a year at ESRF. Microcrystal "showers" occur over the entire range of systems.

2 While cylindrical averaging does incur some loss of information, the extent of this is far less than might be expected – especially when it is recognised that the reflections that overlap systematically as a result of the crystal symmetry are, depending on the specific space group, very often equal in intensity.

3 A cylindrically averaged "fibre" dataset (which naively can be thought of as two-dimensional) can be collected much more rapidly than a full three-dimensional dataset, offering the prospect of very serious gains in terms of valuable neutron beam time.

4 Phasing data extracted from cylindrically averaged neutron data is very unlikely to be a problem, given the fact that for essentially all neutron related problems, X-ray structural data are available.

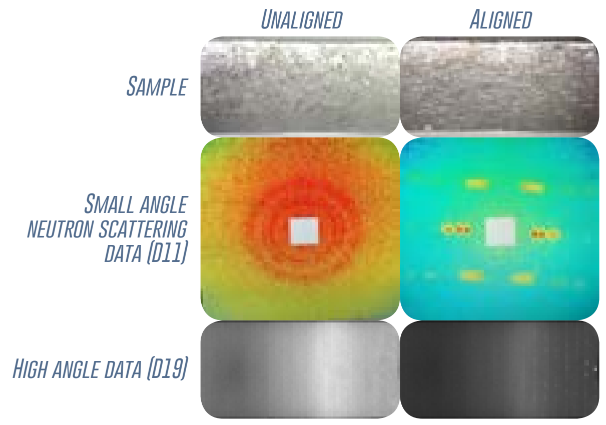
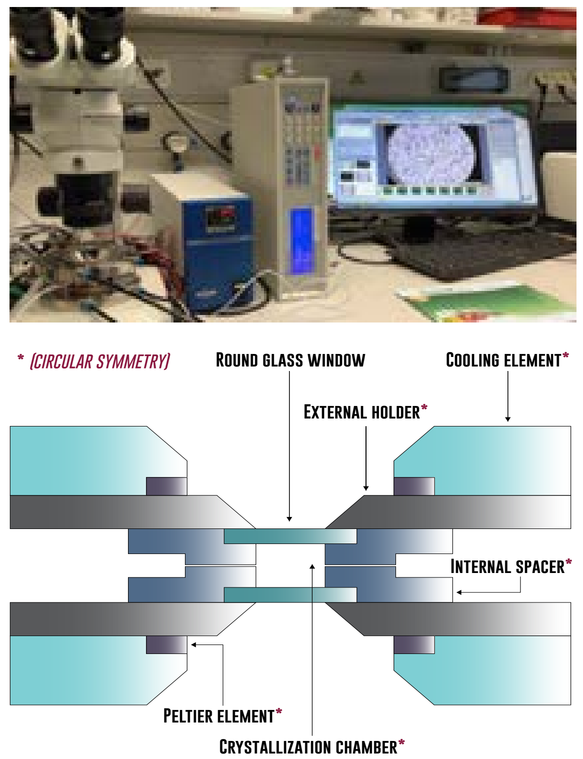


Fig.2 (above): Pictures showing microcrystal alignment and consequences for low and high-angle diffraction.



COSTS WITHIN SINE2020

SINE2020 supported the studies of growth and alignment of crystals in an external field with 24 PM (Post-Doc). The high-field magnet was supplied by Birmingham University.

A NEW CRYSTALLIZATION APPARATUS FOR LARGE PROTEIN CRYSTAL GROWTH

Forschungszentrum Jülich have developed a crystallization apparatus for large protein crystal growth. The main purpose was to make this apparatus available to the neutron crystallography community, in particular to the users of the instrument BIODIFF at FRM II. This apparatus is intended to improve their crystallization conditions and obtain bigger crystals. Indeed, this apparatus is able to control and change different crystallization parameters simultaneously such as the temperature, the precipitant and the protein concentration.

In addition, the choice of crystallization method (either batch or vapour diffusion technique) is opened up by changing the internal space of the apparatus. These elements are 3D printed in collaboration with the engineers at the Forschungszentrum Jülich. They define the crystallization chamber together with two flat glass windows and two o-rings. The temperature is controlled by means of two round Peltier elements. These are in thermal contact with the crystallization chamber by means of two external holders, which keep the system sealed, and two round cooling units. The whole design is based on a circular symmetry in order to allow a uniform and isotropic transmission of the heat into or out of the crystallization chamber. A first test of the crystallization apparatus has been performed using lysozyme as a model system, which has the advantage that the phase diagram is well known and crystals form readily and fairly reliably. The crystallization apparatus will be tested with other systems in the future.

Fig.3 (left): *Top*: Experimental set-up of the crystallization apparatus at the Biolaboratory (JCNS, Garching). The crystallization apparatus is located under a stereomicroscope, which allows us to monitor the evolution of the crystallization. *Bottom*: Schematic view of the crystallization apparatus (batch condition). The picture shows a vertical cut of the main components of the crystallization device.

CONCLUSIONS

1 The single biggest bottleneck to the wider exploitation of neutron macromolecular crystallography remains the availability of large crystals with volumes of 0.1 mm³. The tremendous potential for his is demonstrated in Fig.1.

2 Exploring crystal growth conditions requires systematic approaches, and thus profits from the coordination of specialised laboratories at the different facilities.

3 The alignment of microcrystals in strong external magnetic fields turned out to be a highly promising alternative. The feasibility has been successfully demonstrated and needs further investment on the level of 48 PM and 0.5 M€ into a high-field (18T) closed-cycle magnet adapted for sample visualisation, time-lapse photography, optical polarisation and sample rotation control.

SUCCESSFUL PROTOTYPES IN SAMPLE ENVIRONMENT

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The continuous development of the neutron sample environment is not only vital for scientific progress but is one of the key strengths of neutron scattering. The International Society for Sample Environment (ISSE) brings together the sample environment groups of 20 large-scale facilities and 12 companies from within and outside Europe, with the aim of ensuring the innovative, successful and cost-effective use of beam time at existing and future large-scale facilities [1]. *SINE2020 has benefited from the working spirit of this firmly established network, as demonstrated by the development of the three prototypes presented below. These projects are examples of how it is possible to push the limits of science and gain in efficiency with little investment.*

A HIGH PRESSURE, LOW BACKGROUND CELL FOR MUON-SPIN EXPERIMENTS

Pressure cells reaching the scientifically interesting GPa regime for sample volumes adapted to muon and neutron scattering (of the order of 100 mm^3) is an engineering challenge. As well as being able to resist strong mechanical stress, cell materials must be non-magnetic, produce low background and have minimal temperature- and field-dependent relaxation rates. By establishing a strong collaboration with high-pressure experts within the framework of SINE2020, PSI has been able to successfully design, fabricate and commission a new type of piston cell for µSR measurements reaching 2.6 GPa for a sample volume with an inner diameter of 6 mm and a height of 12 mm [2].

The muon capture efficiency and low background were achieved by optimising the thicknesses of the double wall materials: hardened CuBe2 and MP35N (Ni-Co-Cr-Mo-C alloy). The former has lower relaxation rates, especially at low temperatures, but had to be confined in an outer sleeve of MP35N capable of resisting higher tensile strain. The thicknesses of both cylinders were optimised by finite element calculations for the maximum applicable stress, as well as by detailed simulations for the stopping profile of muons inside the cell materials. The diameters are now optimised so that, for the selected incoming muon energy of 44 meV, most muons are stopped within the sample and inner cylinder area and only a minor fraction are stopped at the outer cylinder of the cell.

The cell has been successfully tested on the GPD (General Purpose Decay) instrument at PSI for a study on the binary helimagnet CrAs, gradually suppressing bulk magnetism in favour of a superconducting phase in the pressure regime $0.35 < p < 0.7$ GPa below a temperature $T_c \approx 1.2$K [2,3]. The adaption of the cell to neutron scattering requirements is currently being studied. Based on a series of measurements performed at ISIS, TA6V (titanium alloy) and hardened CuBe2 have been chosen to build the neutron cell. Calculations are ongoing to optimise thicknesses and an in-situ pressure measurement technique is being tested for ensuring reliable measurements.

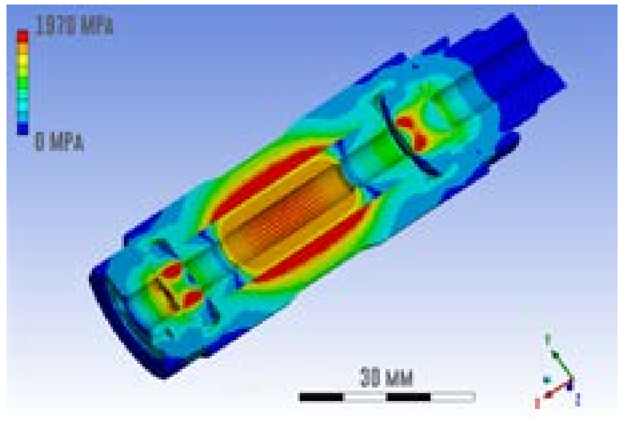

Fig.1: Calculated stress distribution in the high-pressure (2.6 GPa), low background, double-wall cell developed for muon spin resonance experiments. The thicknesses and materials were optimised in non-linear regime to increase the maximum pressure by 25% whilst maintaining the background to a minimum.

COSTS WITHIN SINE2020

The cell calculations, the acquisition of the know-how necessary to prepare the cells (fretting, etc.) and the numerous tests conducted required a total of 48 PM.

FAST COOLING FURNACES

The modification of a cooling procedure in standard furnaces is another illustration of how efficiency can be achieved through facility collaboration. A comparison of the types of furnaces and the associated usage protocols at the different facilities showed that a majority of experiments are conducted with an ILL-designed furnace supplied by AS Scientific Ltd (UK), with cooling times of ~6.5h. This cooling time is of the order of the experimental time on most diffractometers, thus causing severe downtimes on these instruments.

After a systematic comparison of the cooling efficiencies of exchange gases such as argon, helium and nitrogen in identical conditions, it was found that a technically rather simple modification to the ILL-style furnace leads to impressive gain factors of 4 - 5 [4]. This is achieved by isolating the vacuum system and inserting helium gas into the furnace at a controlled flow rate. After integrating the modified version into the experimental programmes, regular observations over the course of one year have not identified any abnormal aging effects on components or heat shielding elements. The control system is currently being extended from the fastest cooling procedure to controlled cooling procedures.

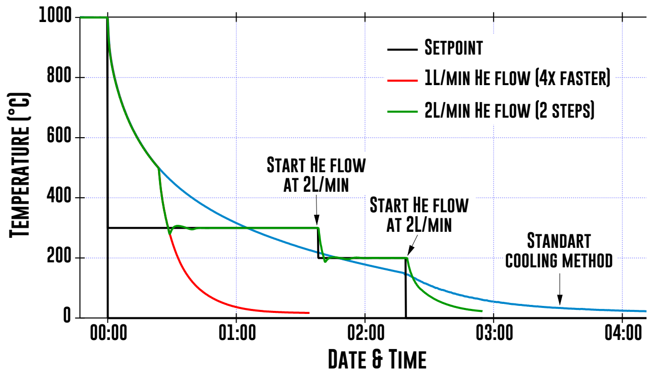

Fig.2: Fast cooling mode performances: the blue curve shows the standard temperature decrease of a sample placed in the vacuum space of an ILL-type furnace. The other curves are obtained by circulating He gas below 1000°C to divide the cool-down time by a factor 4 (in red) or by steps to perform additional measurements (in green). Applied at ISIS, this method saved 22% beam time.

COSTS WITHIN SINE2020

Systematic studies of cooling times as a function of various parameters required a total of about 15 PM shared among the facilities. To automate cooling, ISIS and the ILL have upgraded the design of their controllers with new electronics, cables, He supply, turbo pump, etc. (total of 30 PM).

ORIENTING SAMPLES AT ULTRA-LOW TEMPERATURES

The cooling and thermalization of samples inside dilution fridges take up a significant proportion of beam time. In addition, mechanical constraints for complex sample environments, such as cryomagnets and spherical neutron polarimetry, require precisely oriented samples and do not allow alignment corrections to be made using goniometers mounted below the sample environment. These constraints can lead to downtimes of orders of days, if samples have not been correctly oriented within the required precision of the instruments. Miniature motorised goniometer heads adapted to very low temperatures (≈40 mK) could therefore vastly improve experimental conditions. These goniometers must be rigid to be able to resist strong forces on magnetic samples inside cryomagnets, but must also fit into quite narrow circumferences (Ø36 mm from the survey conducted at the beginning of the project). Encoder readout is mandatory, with no heat transfer to the samples either by encoder readout or by motor movements at such low temperatures. PSI has developed and tested various prototypes and finally proposed with the ILL a modified version of a commercial product. A prototype two-stage miniaturised goniometer head is currently being assembled in collaboration with the company Attocube [5] and will soon be tested at PSI and the ILL.

COSTS WITHIN SINE2020

Feasibility studies, design work, fabrication and testing of two different kinds of goniometer head required a total of 24 PM. The design and construction of the prototype required about 6 PM and will need 4 PM for commissioning.

CONCLUSIONS

1 The sample environment network is one of the most advanced and interactive networks within the neutron and muon commnuity.

2 Cooperation favours technological development at facilities, to gain efficiency and push the limits of science, with moderate investment, e.g. for cryo-furnaces: 15 PM for reducing cooling times by a factor 4-5, or for gonio-heads at ultra-low temperatures: 34 PM of development costs against a gain up to days per experiment for setup.

3 Projects have passed feasibility studies and developed prototypes but await investment at various facilities to refurbish the equipment and fully profit from this investment:

- It is planned to produce a series of clamp cells optimised for different neutron techniques and to deploy in-situ pressure measurement techniques (about 200 k€ investment and 49 PM)
- Work is still needed to upgrade each furnace (about 3 k€/furnace investment) and all temperature regulators (about 7 k€/rack). At the ILL, the upgrade of 25 furnaces and 7 racks will cost ~124 k€ and require 18 PM
- The final goniometer head will be made commercially available with costs ~9 k€/stage + 9k€ of electronics..

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SPECIAL HEAVY CONCRETES FOR FAST NEUTRON SHIELDING

Finding an alternative neutron shielding material for heavy concrete to gain higher precision and lower costs.

Although heavy concrete has excellent shielding characteristics, it has the disadvantage of considerable shrinking rates (~0.25%); this limits its use for shielding components demanding high precision. In collaboration with industrial suppliers (Rampf of Germany and AlphaBeton of Switzerland), PSI has tested alternative shielding materials, comparing their performance with different recipes of heavy concrete, in terms of absorption of epithermal and fast neutrons.

The shrinking rates of mineral cast - a mixture of quartz, sand and hydrogen containing epoxy - are at least one magnitude lower, and its costs are comparable to standard concrete, i.e. at least five times less than heavy concrete. In addition, the mineral cast composition was modified by adding boron-carbide powder to avoid activation and improve thermal shielding behaviour.

The neutron transmission of different cast and heavy concrete compositions for neutron energies up to MeVs was measured at the ICON and BOA beam-lines at PSI. A special method of detection based on Bonner sphere detectors was also developed to ensure neutron sensitivity over the whole spectrum. Results show that the neutron absorption of mineral cast composites and heavy concrete are comparable, and further improvement on the mineral cast is possible by adapting the epoxy content.

COSTS WITHIN SINE2020

Both developments - mineral cast shielding and the use of Bonner sphere neutron detection - required around 36 PM (30 PM for scientists and 6 PM for technicians), out of these 9 PM have been financed by SINE2020. The costs of the detector were 150 k€.

CONCLUSIONS

1. Development of alternative neutron shielding materials based on cast is an excellent example of innovation at neutron facilities. The feasibility studies have been successfully done within SINE2020 and various materials tested in collaboration with industrial partners.

2. Further improvement on the mineral cast is possible by adapting the epoxy content.

3. New cast products have been on the market since March 2019. PSI acts as the reference facility for the new material.

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DETECTOR DEVELOPMENT

The dramatic shortage of ^{3}He a decade ago severely influenced the development programs of detectors at all major neutron facilities [1] and intensified cooperation in research and development between them. Recent years show a slight relaxation on the ^{3}He market. During SINE2020 emphasis has therefore shifted towards neutron detectors with high rate capability (several kHz/mm^2), improved spatial resolution (1-3 mm with a perspective into the sub-mm regime) and increased time resolution (better than 100µs, as specified at the start of SINE2020), which replies to a high need in new instrumentation, such as reflectometers at the ESS. Out of several promising ongoing projects [2] three different technical solutions are presented below.

RESISTIVE PLATE CHAMBERS AS HIGH RESOLUTION NEUTRON DETECTORS

Within SINE2020 the LIP group, in collaboration with the TUM-FRMII and ESS groups, has refined the concept of a novel type of position-sensitive neutron detector based on resistive plate chambers (RPC) with ^{10}B layers (^{10}B-RPCs) as neutron converters and successfully demonstrated the feasibility of this detection technology.

One of the challenges was a relatively low neutron detection efficiency of an RPC detector with a single converter layer. Typically, the converter has a thickness of the order of one µm, leading to a detection efficiency of about 5%, quite low compared to almost 100% of ^{3}He proportional counters.

The work performed by the LIP group has shown that this limitation can be overcome by designing the detector in a multilayer or inclined architecture (the latter proposed by ILL [3]), allowing to reach an efficiency above 50% for thermal neutrons [4]. It has been demonstrated that spatial resolution in the sub-millimeter regime is indeed possible by reducing the gas-gap width of the RPCs in the stack to ≈ 0.35 mm.

The advantages of this type of detector are manifold. Thin-gap ^{10}B-RPCs show sub-millimeter spatial resolution and there is a strong potential to approach resolutions of about 100 µm, together with improved detection efficiency. Another attractive feature of these detectors is fast timing, which should allow measurements of the neutron time-of-flight (TOF) with nanosecond resolution. Additionally, RPC based detection technology allows high

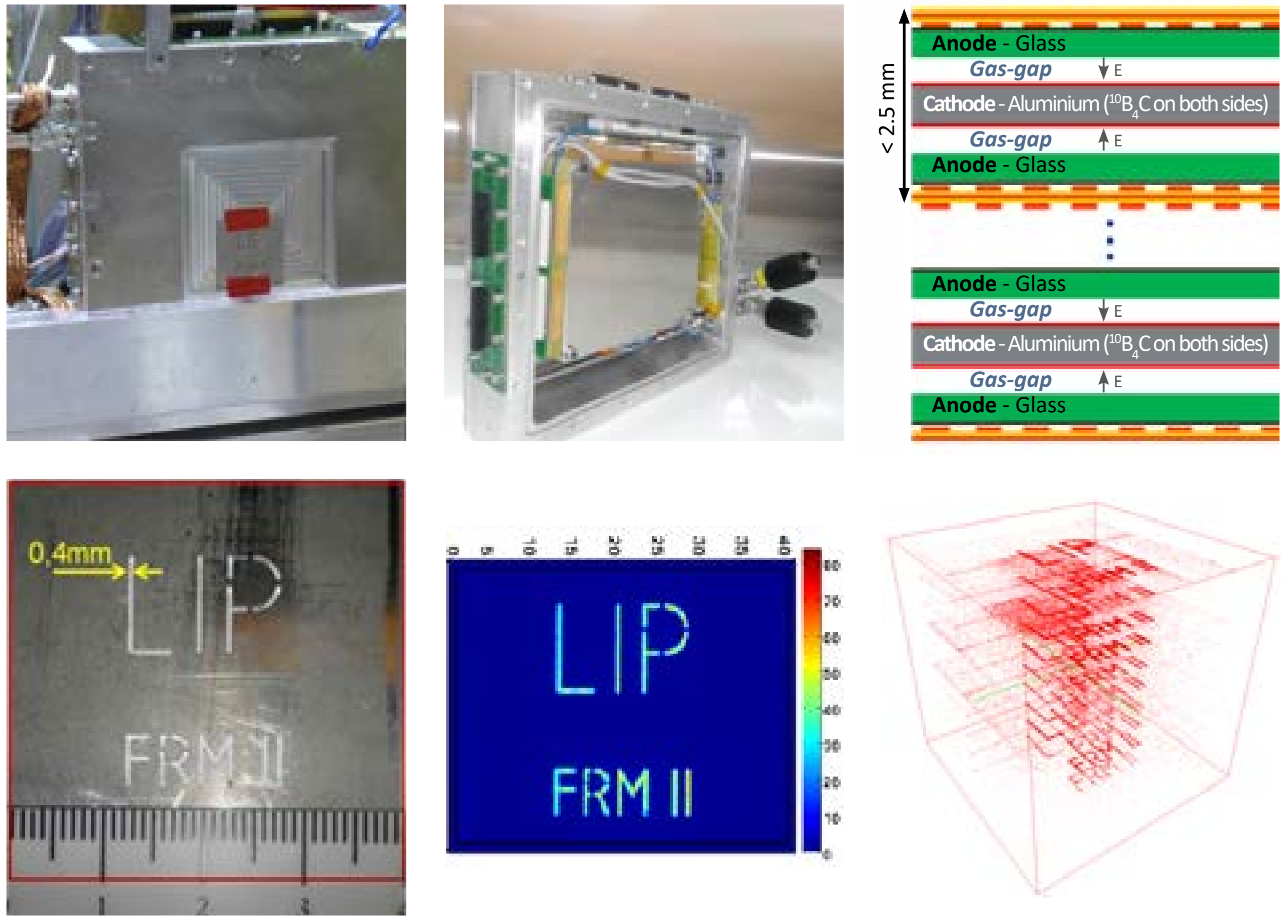


Fig.1: Boron-10 Resistive plate chamber (^{10}B-RPC) as position sensitive neutron detector (PSND). *Top left and middle*: views of the detector housing. Top right: schematic view of the multilayer architecture with 2 RPCs units. Bottom right: 1mm thick Cd mask used for neutron tests at FRM-II. *Bottom middle and right*: real space 2D and 3D maps of neutron events registered with a 10 double gap ^{10}B-RPC detector.

modularity of the design and robustness, is highly scalable and very cost-effective, as is demonstrated by its application in large-area (>100 m^2) detectors for High Energy and Astroparticle physics.

All this renders RPC-based neutron detectors a promising technology. Nevertheless, there are challenges which still have to be addressed, the increase of the counting rate capability of RPC-based detectors a key one.

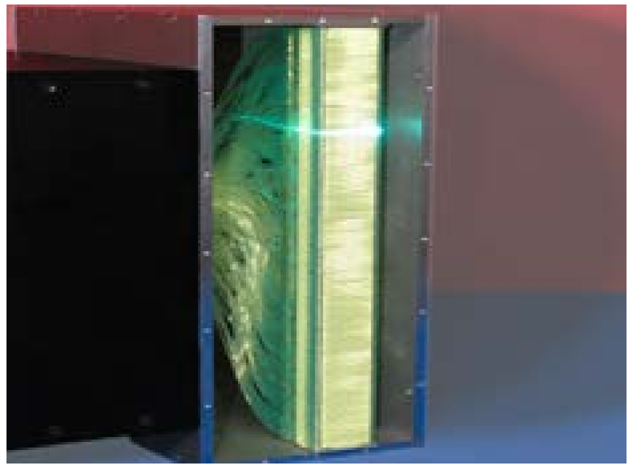
COSTS WITHIN SINE2020: See Table 1

NOVEL ^{3}HE DETECTOR

For SINE2020 the ILL detector group investigated a novel resistive cathode layout to improve the performance of the so-called microstrip gas chamber (MSGC) detector. MSGCs were initially conceived in the 1980's at the ILL for one-dimensional (1D) ^{3}He Position Sensitive Detectors (PSD). One intrinsic advantage of the MSGC technique comes from its high counting rate capability. Within the SINE2020 project the initial device idea was extended to two-dimensional (2D) PSD with about 1mm^2 resolution with a 2D readout system, where both ends of the cathode strip are connected to an amplifier to measure the position along the strip by charge division. A 2D MSGC was constructed, calibrated and tested on a neutron beam line. Good quality images were obtained at moderate counting rate, although the maximum counting rates did not reach our expectation because of ion feedback in the conversion gap.

Building on this experience, the second part of the SINE2020 period focused on trench multiwire proportional gas chambers (MWPC). These have a compact geometry, favorable to reduce the density of ions in the amplification zone, and to be operated at low gain and high electric field to reduce the ion feedback. Its cathode is made of metallic blades containing teeth machined with high precision, so that, when stacked together, these blades make trenches into which the anode wires are mounted. This detector has a very compact anode-cathode structure like MSGCs, and is operated at low gain like a standard MWPC. A 1 mm resolution trench-MWPC prototype, with a sensitive area of 6 cm x 6 cm, has been developed and successfully tested at the end of SINE2020. Experimental results confirm the potential of this technique for high counting rate applications.

Fig.3: Prototype of a ZnS:Ag/^{6}LiF scintillation detector with wavelength shifting (WLS) fiber readout developed by STFC. This is a single segment with 256 pixels (each 1x30 mm^2).



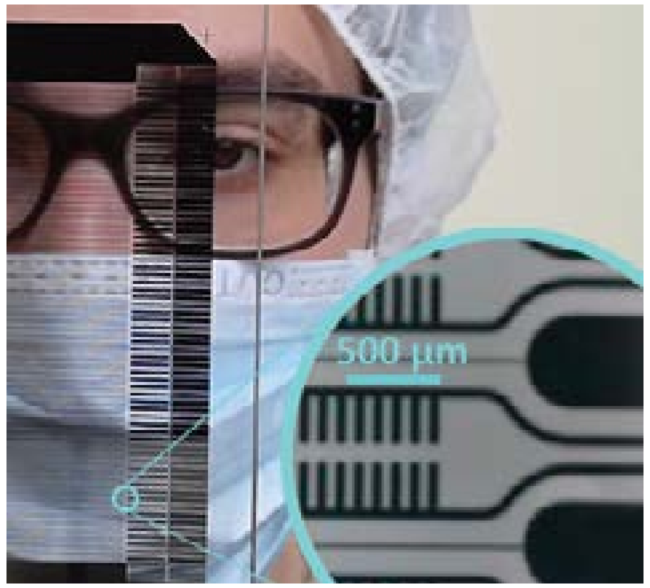


Fig.2: Electrodes etched on a glass substrate for a microstrip gas chamber (MSGC) detector tested during SINE2020. The insert shows a detail of the half-cathode (in black) with the teeth-like extensions.

Based on this design, a new 2D detector could be developed with a sensitive area enlarged to 20 cm x 20 cm. This detector would have the same position resolution as the MILAND detector developed in the NMI framework (FP6/JRA2) [6], and would outmatch MILAND's local counting rate by a factor of 3. This new detector would be directly usable on a reflectometer instrument. The technical risk in this project would be limited, building on the obtained know-how in FP6/JRA2 [6], and on the experience with the trench-MWPC prototype developed in SINE2020, as well as in the XtremeD project at the ILL.

COSTS WITHIN SINE2020: See Table 1

ZnS DETECTORS WITH WAVELENGTH SHIFTING FIBRE READOUT

In SINE2020 ISIS developed a ZnS scintillation detector concept with wavelength shifting (WLS) fibre readout for reflectometry applications. ZnS scintillation detector systems with WLS readout are already in use at ISIS, the SNS and J-PARC and have been developed within FP7 NMI3-II for large area detectors. However, despite the high light output and the excellent neutron gamma discrimination that can be achieved with this scintillator, its afterglow limits the detector rate capability to ~ 20 kHz per photomultiplier tube (PMT) pixel. For high rate applications this is a severe problem.

To alleviate the rate limitation problem ISIS has developed a segmented detector system, where a 64 channel multi-anode PMT is used to code the pixels in each detector segment, [7]. The position resolution of the detector is 0.5 mm in the direction of the reflected beam and the width of the segment in the other direction. The detector rate capability is enhanced by the number of segments in the detector and can be 10 or more. Moreover, the fibre optic code has been chosen to concentrate more PMT pixels in the high count rate region of the detector. In this region a count rate capability of 1 kHz/mm^2 has been achieved.

Facility	Technology developed in SINE2020	Applications	Improvement	Solutions	Development costs SINE2020	Investment costs
LIP	Neutron sensitive multilayer RPC	Reflectometry + wide range of other applications	Rate	optimise converter thickness, optimise electrode conductivity, increase electronics sensitivity	154 k€ incl. 19 PM	220 k€ incl. 24 PM
ILL	2d MSGC	Reflectometry SXD	Rate	-	215 k€ incl. 36 PM	-
	1 mm resolution Trench MWPC	Reflectometry SXD	Area	Develop for 20 cm x 20 cm area		350 k€ incl. 36 PM
STFC	Segmented ZnS detector with WLS fibre and MaPMT readout	Reflectometry	Rate	256 channel PMT Improved signal processing	200 k€ incl. 56 PM	200 k€ incl. 36 PM
PSI	ZnS Scintillation detector with WLS fibre and SiPM readout	Reflectometry Diffraction	Position resolution / Rate	Crossed fibre / pixelated detector	110 k€ incl. 8 PM	340 k€ incl. 24 PM
FZJ	GS20 Scintillation detector with Anger camera readout	Reflectometry SXD	Rate	Signal transfer/processing	166 k€ incl. 18 PM	200 k€ incl. 20 PM

Table 1: Summary of detector techniques developed in SINE2020 and possible exploitation.

A count rate capability of 1 kHz/mm^2 is now deemed to be insufficient for some reflectometer requirements and we envisage a further development based on a 256 channel multi-anode PMT. This is expected to deliver more than a factor of four increase in detector rate capability, since the extra PMT pixels can be used to preferentially segment the high data rate region of the detector.

In addition the signal processing of the PMT signals could be improved. There is already some evidence at ISIS that this is possible, while at PSI, significantly higher rates have been reported for new signal processing algorithms developed for ZnS detectors with WLS fibres and SiPMs.

COSTS WITHIN SINE2020: See Table 1

CONCLUSIONS

1 Detector laboratories located at various European facilities have specific and complementary expertise. This complementarity offers comparison of various technical solutions, once a common goal has been defined within a commmon framework, such as development of large area detectors for next generation reflectometers in SINE2020.

2 The cost benefit of any detector enhancement is huge. With beam time valued at 20 k€/ instrument/ day, operating an instrument for 150 days a year for 10 years equates to 30 M€. Anything that increases the data quality or the throughput of an instrument is of benefit to neutron scattering science. This applies to all three projects.

3 EU funds allow for the development of propotypes. Various technical solutions are presented in Table 1. The technical challenges (Improvement) and their solutions (Solutions) during this period have been identified. Measurements using propotypes demonstrated the feasibility, but additional investment is needed for finalising.

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DATA ANALYSIS & ATOMISTIC MODELLING SOFTWARE

Data reduction and analysis is the pivotal step in the chain of actions between proposal submission and final publication. Expectations from the user community towards user facilities are extremely varied, which has prompted a common structured approach towards software development and maintenance [1].

One of the main objectives of the software development activities under SINE2020 was to ensure that mission-critical software packages that are used regularly in the neutron and muon scattering domains are developed in a maintainable manner. Another objective was to minimise single points of failure in the software development and maintenance workflow, thus ensuring that the neutron community has access to the software tools it needs for data treatment and analysis.

In terms of efficiency, despite increasing amounts of data, data reduction and visualisation should be quasi-instantaneous, allowing interactivity during the experiment in order to avoid downtime on the instruments and provide users with as much pre-treated data as the scientific analysis process allows during and shortly after experiments.

The European neutron community has about 5500 active members [2], with a similar number of experiments performed per year across all European facilities [3]. Depending on the various instruments and science categories, a host of software packages exist with user groups of the order of between 100 (e.g. TAS, QENS) and 1000 (e.g. SANS, powder diffraction [3]).

The balance between quality, based on jointly agreed standards [1], and the inherent plurality, inevitably leads to considerations at every facility about the resources available and how to coordinate tasks efficiently between them, while supporting an active user community.

Within the SINE2020 framework, the existing analysis software packages of three instrument groups (SANS, Reflectometry and Imaging) have been identified and their functionalities extended so that they now comply with the newly defined common standards [1] in order to facilitate interoperability, extensibility, maintainability and sustainability.

Together the three instrument categories cover about 40% of scattering experiments [2], thus have high data and user throughput and feature among the first generation of ESS instruments. Moreover, the QENS community has agreed on the creation of an interoperable fitting model library with a dedicated graphical user interface (GUI) for fitting within the data reduction software MANTID [4,5]. More details on the analysis software packages are given in Table 1.

	BornAgain	MuhRec	SasView	QENS
Project start	2012	2011	2006	2012
Download	www.bornagainproject.org/download/	www.imagingscience.ch/downloadsection/	www.sasview.org	-
Code repository	github.com/scgmlz/BornAgain	github.com/neutronimaging	github.com/SasView/	github.com/QENSlibrary for model library. *QENS GUI is part of the Mantid distribution*
Main coordinator within SINE2020	JCNS	PSI	ESS	ISIS
Development costs during SINE2020 (PM/Y)	36	18	42	8
SINE2020 support (PM)	42	21	41	32
Maintenance > 2019 (PM/Y)	24	24	24	12

Table 1: Overview of data analysis software supported during the SINE2020 period. For details, see [8].

	MuESR	MDANSE	AbINS (Mantid)
Download		mdanse.org/ downloads	download.mantidproject.org
Code repository	github.com/bonfus/MuESR for library and github.com/mantidproject/scriptrepository/tree/master/muon/MuESR for Mantid plugin	code.ill.fr/scientific-software/mdanse	github.com/mantidproject
Main coordinator within SINE2020	UNIPR	ILL	ISIS
Development costs during SINE2020 (PM/Y)	5	5	7
SINE2020 support (PM)	18	18	3
Maintenance > 2019 (PM/Y)	6	6	6

Table 2: Overview of atomic modelling software supported during the SINE2020 period. For details, see [8].

Atomistic modelling has become the key for meaningful and efficient scientific output, in particular on the inelastic neutron instrument suites. The interpretation of experimental data needs direct comparison with the results produced by atomistic modelling software, ideally in an interactive way during the experiments.

These packages must combine results from general scientific software on structures and dynamics with specific neutron and muon aspects of interaction probabilities and instrument resolution. Several atomic simulation techniques have been addressed during the SINE2020 funding period.

In muon spectroscopy, the MuESR programme for local magnetic-field calculations has been extended and interfaced with MANTID, so that it is now possible to run it by command line. In addition, DFT methods for predicting the muon site of implantation have been reviewed [6].

The neutron scattering community focused on the calculation of inelastic neutron scattering spectra using two programmes: MDANSE based on molecular dynamics simulations, and the plug-in algorithm abINS in MANTID based on DFT lattice dynamics simulations. More details on the atomistic modelling software packages are given in Table 2.

COSTS WITHIN SINE2020

The development costs for the various software packages within SINE2020 are summarised in Tables 1 and 2, rows: 'Development costs during SINE2020' and 'SINE2020 support'.

CONCLUSIONS

1 Facilities agreed on providing user software with predefined standards (see 'Common Standards',p.16), which implies close collaboration among computing groups at different facilities in the future.

2 A better understanding has been obtained of the amount of resources needed to make software pacakges sustainable, which helps facilities to determine maintenance costs and set ambitious targets. An estimation for the packages developed during SINE2020 is given in Tables 1 and 2, last row.

3 The landscape of user software in Europe has been corroborated. A large fraction of facility supported analysis software pacakges benefits from common standards and joint computing efforts.

4 Despite the initiated efforts to create synergies between the neutron facilities, computing resources will need to increase in the near future to ensure that neutron scattering remains attractive and competitive for the user community. For the selected software packages, manpower will shift from development to maintenance and improvement. According to literature, these tasks typically absorb an average 60% of software costs [7]. Given the successful development within SINE2020, future manpower needs should be considered (Table 1 and 2).

5 Users will also need increased assistance with advanced analysis and modelling software,e.g. based on materials and molecular modelling and simulations, multi-modal data (combining data from different instruments and techniques) and machine-learning techniques.

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FINAL REMARKS

SINE2020 has received 10.8 M€ from the European Commission under INFRADEV-01-2014 and a direct contribution of 1.2 M€ from the Swiss government to the Swiss beneficiary. By the end of the project it will have delivered 112 deliverables and 10 milestones. Approximately 120 experts from 18 different institutions, unifying neutron and muon facilities as well universities and other academic organisations, participated in networks and Joint Research Activities in the period from 2015 to 2019.

All participants demonstrated a high degree of commitment and delivered high quality work within the announced timelines.

SINE2020 builds on expertise established in the three previous grants NMI3, NMI3-I and NMI3-II since 2004. Thanks to this long lasting partnership, the neutron and muon community is today an 'advanced community'.

The new, and the already established, networks have demonstrated their added value for the European neutron and muon communities. Whereas networks like education and training need little investment for levering important gains for the communities, other network gains like those from industrial liaison and DEUNET are directly proportional to future investment. The gains are outlined in the conclusion of the respective section of this report.

Joint Research Activities equally rely on previously established networks. The association for sample environment is one example, which might be followed by other technical sectors. Most technical developments reached the level of demonstrating feasibility. Among them several are ready for fabrication and use at the facilities with investment. Again the gains are listed in the conclusion of each relevant section.

With the end of the SINE2020 project, we are also close to the end of the Horizon2020 framework program. The funding schemes in the new Horizon Europe program are still to be defined. Up until now, all described networks have been relying on European support. Nevertheless as an 'advanced community' the networks are expected to be less dependent on EU funding.

The financial support is the major driving force for any proposal preparation and collaboration. Although the financial contribution through European grants is of the order of a percent or less of the overall facility budgets, it provides the framework for collaboration and synergy effects between the various European institutions. These collaborations need to continue for the general interest of the future neutron and muon community in Europe.

The main risk is the disintegration of the established networks, rather than the eventual lack of financial support. It is indeed the stringent, and therefore securing, organizational and legal framework of the European grant that keeps the momentum for respecting timelines and deliverables. We sincerely hope that the newly created League of advanced European Neutron Sources (LENS) will help to create the favourable environment required to sustain collaboration in the future.

Martin Boehm and Miriam Förster

Coordinator and Manager of SINE2020

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