Executive Summary:
Neutron scattering and muon spectroscopy are two of the most powerful probes for the investigation of materials, from the subatomic to the mesoscopic scale. Neutrons and muons have unique properties, which make them indispensable probes for achieving a complete picture of the structure and dynamics of matter. They are sometimes in close competition to other probes like synchrotron radiation or NMR, but most often they are complementary. Microscopic structure and dynamics are key to the technological and functional performance of materials. Neutron and muon studies are, therefore, of relevance to all areas of modern society. The knowledge obtained from neutron scattering and muon spectroscopy is published in the most prestigious scientific journals. These papers draw attention from a wide scientific community, as demonstrated by the numbers of citations. The scientific knowledge generated is often fed in the long term into innovation processes, thus closing the knowledge cycle.
Europe has an exceptionally strong tradition in providing world-class research infrastructures in the fields of neutron scattering and muon spectroscopy. These infrastructures serve the scientific needs of a broad user community - 9000 individual researchers - ranging from fundamental physics to materials science, engineering, life sciences and cultural heritage (see http://pan-data.eu/Users2012-Results). Many of the technical services provided are unique, hence creating a highly mobile user community, coming from all around the world.

Neutron and muon research infrastructures are evolving rapidly. The last few years have seen a strong increase in the capacity and quality of the research infrastructures in this area. Despite considerable international effort, Europe still retains the lead both in terms of the quality of the infrastructures and the scientific output. All major facilities, like the European Intergovernmental Research Infrastructure, ILL, in France and the British, German, French, Dutch and Swiss national sources, are continuously engaged in ambitious upgrades of their instruments. Due to these combined efforts, Europe’s competitiveness in the field will be maintained over the coming years despite the launch of strong, third generation sources in the USA (SNS) and Japan (J-SNS).

The technological difficulties of providing high-brilliance neutron and muon beams lead to a requirement for very large experimental installations. International competitiveness, at a sustainable cost, therefore demands strong coordination of their development and use on a European level. NMI3 aims to facilitate this coordination with the Integrating Activities scheme as means of leverage. NMI3 comprises all major European neutron and muon providers. Transnational access helps structuring the user community and optimises the use of the existing infrastructures. Joint research activities help to foster a coordinated and cost effective development of the facilities. Explicit networking actions create stronger links between the facilities such that users experience a more coherent and thus easier to use, research infrastructure. The overall management ensures that strategic decisions are taken from a European perspective, playing to the respective strengths of the individual facilities. NMI3 networking activities try to establish a greater degree of coherence in instrument simulation and data analysis.

Project Context and Objectives:
Despite the shortened period for transnational access (only 24 months), the facilities demonstrate considerable activity with non-national users. A large number of publications have resulted from experiments and also the joint research activities. Concerning the joint research activities, further important break-throughs have been achieved in various areas:
The work performed in Neutron optics has demonstrated the use of innovative concepts and devices. During the late 80’s and early 90’s, tremendous improvements were made in the production of neutron mirrors. New coatings allow building guide systems with an increased neutron flux of a factor 3 to 4. More recently these improved supermirrors have been implemented into optical devices: trumpet guides, ballistic guides, polarizing benders etc. and have allowed improvements to existing spectrometers. Our challenge has therefore been to increase the luminosity of the neutron spectrometers even further. We aimed to show that neutron optics technology and components, which are presently available, enable new spectrometers to be designed which can be at least 10 times brighter than existing ones. The principles that have been demonstrated could easily be implemented across facilities. The outcome will be a more efficient use of the existing neutron sources. This would benefit neutron users directly in the short term.

The work was focussed on 3 main objectives:
1) High flux reflectometry,
2) High flux SANS and
3) Focussing of thermal neutrons.
Each thematic task gathered instrument scientists, experts in their fields (reflectometry, SANS, diffraction or imaging) and having a direct interest in improving their spectrometers. Most of the proposed developments will be implemented on existing spectrometers in the short term. Most of the optics developments have required advanced numerical simulations. Monte-Carlo simulation programs have been upgraded or rewritten to include new advanced components and optimization tools. This will also benefit the widest community.

Similarly exciting and useful results have been obtained in the other JRAs:

The developments arising from the deuteration JRA within NMI3 are resulting in clear changes that are affecting the efficiency, volume and scope of biological neutron scattering at centres throughout Europe. The need for this was very clear given increasing trends towards interdisciplinary and integrated approaches for the study of biological systems. Neutron scattering has a unique and important role to play if the right types of sample can be made available. Deuteration is essential to this: the ability to label complex/interacting systems offers approaches that are simply not possible using other methods. This project focused on widening the access of neutron scattering methods to biologists throughout the EU, both by extending the range of problems that can be tackled, and by reducing the cost impact of sample preparation. It has exploited an obvious synergy with the NMR community, which also has important needs for isotope labelling and within which there is increasing use of neutron scattering. More specifically, the main objectives were the optimisation of deuterated biomass production, development of deuterated protein production using Pichia pastoris, segmental labelling of specific parts of proteins, methods for the low-cost production of deuterated glycerol, methods for the optimisation of membrane protein production and deuterated lipid production.

Polarized neutrons are particles with preferential direction of their spin (magnetic moment). They can be considered as a kind of elementary magnetsthat change their direction when interacting with a magnetic field in the sample. Their relative orientation can be measured very precisely using neutron polarimeters. On the other hand, the precession of the magnetic field direction allows a “Larmor clock”, with rotation speed depending only on the magnitude of the magnetic field, to be attached to every neutron. Such Larmor labelling opens the door to “novel” neutron scattering techniques. In the past, neutron polarization analysis experiments were considered as delicate, complicated to understand and often limiting the flux too much. Decisive progress has been made in instrumentation for and understanding of polarized neutron scattering, allowing investigation of the nature of magnetism and magnetic phenomena in solids. Developments made in the current project are obviously extending the power of polarized neutron scattering and showing the way forwards. Cooperative efforts have been concentrated both on the use of polarized neutrons as an elementary magnetic probe in condensed matter investigations and the application of the Larmor precession (LP) technique for development of a new generation of LP-based neutron scattering instruments. This allowed further improvements in wide-angle polarization analysis. It will also influence the next generation of neutron scattering instruments using polarized neutrons (e.g. high-resolution spectrometers, diffractometers and reflectometers). New approaches using polarized neutrons, such as measurements of triplet correlation functions and development of an ultra-flexible neutron magnetic resonator have been successfully explored and prototypes built.

An extensive dissemination of results has been achieved by the training program within the polarized neutron schools, by a number of dedicated workshops and by mutual contacts between the partners. Muon spectroscopy provides a uniquely sensitive probe for measurements in the gas phase of direct...
Muon spectroscopy provides a uniquely sensitive probe for measurements in the gas phase of direct relevance to the study of combustion processes and atmospheric chemistry. To stimulate this area of research, gas pressure cells have been commissioned for the ISIS high-field spectrometer and are now available to the users. Novel detector technologies have been developed and used to prototype a high performance array for the new PSI high-field spectrometer. Excellent performance has been achieved, establishing avalanche photo diode detectors as an important new technology for muon spectroscopy. New experimental methods have been investigated, with high power radio-frequency pulse sequences being developed to extend the scope of the technique.

Spin polarised muons are an important probe of materials at the atomic level. Applications of the muon technique (μSR) are remarkably diverse, encompassing studies of magnetism, superconductivity, and spin and charge transport, while providing a highly sensitive hydrogen analogue to probe semiconductors and proton conductors. Researchers frequently use μSR in tandem with techniques such as neutron scattering and magnetic resonance; the techniques provide complementary information and it is only through a combination of measurements that detailed understanding of a system can be obtained.

A significant aim has been the development of technologies required for μSR spectroscopy in high magnetic fields. The importance and success of this work is evidenced by recent grant awards to both facilities.

The Sample Environment JRA is a far-reaching collaboration, providing a diverse range of new technologies enabling users to expand their exploitation of neutron facilities. The new sample environments will open up new territories for hydrostatic pressure, temperature and advanced gas adsorption facilities, pushing the boundaries of in-situ experimentation. Significant progress has been made in overcoming the technical challenges associated with these advances in sample environment, which has been greatly aided by the continuous, and increasingly extensive sharing of knowledge and experience between facility technical groups. Synergies have been created in three areas – high pressure gas cells, high temperature furnaces and gas adsorption. As a common goal they aimed for an increase of capabilities and thus improvement of the scientific use of each facility. Prior to this project, equipment was either not commercially available or not suited to the restrictive conditions of the experimental area of a neutron beam line.

The design of a standard sample stick was a collaborative spin-off, which will ease the transition of users from one facility to another. This JRA provided a breathtaking array of new sample environment equipment (e.g. hydrogen-safe, neutron-compatible, high pressure cell and gas adsorption measurements under extreme conditions) and experience in much desired but technically very challenging areas, opening up new realms of scientific exploration.

The detector JRA is a lively collaboration exploring a new neutron detector technology based on Gaseous Scintillation Proportional Counters allowing very fast and efficient neutron detection with high spatial resolution. This new technology takes advantage of combining the benefits of two different techniques commonly used in neutron detection: the currently unmatched performance of 3He gas as absorbing material in terms of detection efficiency and an optimal signal to noise ratio and the high count rate capability of scintillation detectors. Investigating the new detection process and developing adequate readout electronics were the main tasks within this JRA project, which aimed to demonstrate the feasibility of this new kind of detector with a 20 x 20 cm2 active area, capable of achieving a 0.5 mm position resolution and a 1 MHz count rate capability. Considerable understanding of the physical processes underlying this new technology has been gained and resulted in the development of the simulation package ANTs, which allows a detailed study of the performance of realistic detector designs. In the course of the project several prototype detectors, including related readout electronics, were developed.
course of the project several prototype detectors, including related readout electronics, were developed and finally resulted in the construction of a large area GSPC with Anger Camera readout. In a first successful test, the device could achieve a spatial resolution of 0.6mm close to the physical limit.

The efficient project management and very successful networking activity have contributed to the integration of the neutron facilities. As an example NMI3 is actively involved in building strategies for an efficient e-learning platform. The revamped NMI3 website is recognized as an outstanding information hub in the worldwide community. American and Australian Neutron Organizations are in frequent contact with our dissemination manager and we will soon achieve a worldwide neutron portal. In terms of training of young researchers, NMI3 supported 32 individual Neutron and Muon schools (in total 70 awards) for 450 unique students (mainly at PhD level) during the whole period. Furthermore, two data related networking activities have been coordinated, leading to a very young and dynamic group on Monte-Carlo-Simulations and related software developments. The network on data analysis standards has been initiated and is part of the next project NMI3-II.

Project Results:

Neutron Optics (WP17)
[This workpackage report is strongly linked to figures and graphs, for a better understanding please refer to the pdf version containing figures.]

One of the main objectives was to investigate the possibility of increasing the efficiency of neutron reflectivity experiments by improving the use of the neutrons. Several routes were proposed so as to be able to use a very large part of the total flux available in the neutrons guides.

Task 17.2 High flux reflectometry using focusing optics

The first route aimed at using reflective optics. The initial project was based on the REFOCUS concept. This concept has been upgraded so as to simplify its implementation. A new scheme allows to split the monochromatization and focusing functions which provides more flexibility to the design together with a much easier implementation. The new design is called SELENE. A detailed technical report of the new SELENE design can be found on the Neutron Optics Website. A half scale prototype SELENE bench has been implemented at the PSI (Figure 1). Such a set-up allows measuring the reflectivity of a sample by sending a white beam on the sample. An example of the data collected on the Position sensitive detector is presented on Figure 2. The top figure shows the intensity map as a function of the wavelength (Ox) and the position on the detector (Oy). The bottom figure shows the Monte-Carlo simulations performed using McStas. In order to reproduce the black horizontal lines (not physical), it was simply necessary to introduce a small misalignment of some of the mirrors in the elliptical guide. This shows the degree of refinement reached by the Monte-Carlo simulations.

From these two dimensional patterns it is possible to reconstruct the neutron reflectivity of a sample. A real demonstration experiment was performed on a thin nickel film of size 10x10mm² (Figure 3). The gains in flux obtained with the SELENE setup are on the order of 10 with respect to a conventional setup.

High flux reflectometry using refractive optics

It was proposed that the energy analysis of a white neutron beam could be performed using the refraction in a prism. A large MgF2 crystal (100mm long) was bought at the ILL in order to build such an energy dispersive spectrometer. It has been shown that data of similar quality can be obtained compared to the ToF technique. The implementation is straightforward on any existing time-of-flight reflectometer (Figure 4).
ToF technique. The implementation is straightforward on any existing time-of-flight reflectometer (Figure 4). The deflection achieved by using a single MgF2 prism are however small (<1°) so that in order to resolve the spatial dispersion it is necessary to either use a high resolution detector or to set-up a normal detector at a large distance.

Demonstration experiments were performed at the PSI on the AMOR reflectometer using a prism set 0.742m after the sample, a 3He detector (6m from the sample) / resolution 2.4mm FWHM and a CCD camera / 5.1m from sample / resolution 0.2 mm / efficiency 10%. The sample used was a Ni/glass layer (50 x 140mm²).

Figure 5 shows the comparison of the different results measured of a thin nickel film using the standard setup (red), the prism setup with He3 detectors, the prism setup with a CCD camera. The quality of the data is equivalent in the three cases. The efficiency is not comparable. For high resolution experiments gains in the range 30-90 can be achieved. This can be useful for kinetic experiments or for measurements on small samples.

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In the setup presented above one of the limitation is given by the limited efficiency of the refractive effect of a single MgF2 prism which only provide very small deflection angles (<1°). HZB has developed a fabrication process of arrays of Silicon prisms using a chemical etching process. This allows the fabrication of perfectly aligned and smooth silicon prisms (see figure 6). The use of several tens of prisms allows to multiply the refraction effects by the number of prisms and thus to increase proportionally the deflection angles.

Such prism wafer have been stack and characterized on the EROS reflectometer at the LLB to check that they behaved as an energy analyzer.

It was proved that it was indeed possible to achieve a measurable energy dispersion over a bandwidth ranging from 2 to 8A° (figure 7)

Unfortunately, it is presently not possible to exploit longer wavelengths due to spurious refractive effects. A possible solution has been devised (coating of the bottom side of the wafers with Gd). The new stacks shall be tested during the spring 2013 on the reflectometer EROS at the LLB.

Task 17.3 Advanced Focusing Techniques

Multichannel focusing guide

Phil Bentley developed genetic algorithms applied to the optimisation of neutron optics. The programs are available @http://philbentley.com/

Genetic algorithms have shown that is was possible to design focussing guide which were 30% more efficiency than human designed guides.

Adaptive Optics for extreme Environments

Some new McStas components were successfully used to model adaptive optics. A 1D parabolic focussing system has been extensively modelled using this component.

Full scale adjustable focussing devices were built and tested. The results agree with the numerical simulations. Two prototypes were built : one with one adjustable point and a second one with 5 motors to tune the mirror shape.

A proper control software has been written to avoid breaking the mirror when changing its shape.

Detailed reports of the performances of the device can be found in:
Detailed reports of the performances of the device can be found in:
• http://optics.neutron-eu.net/Optics/W17_Meetings/May2010

A more advanced 2D focussing device was built for the instrument TOF-TOF at FRM2. Its characteristics are the following: Total length = 495 mm, Entrance cross section = 23x52.18mm² Exit cross section = 12.4 x28.13 mm², coating m-factor= 3.5 4 piezomotors with holders to tune the mirrors curvature. On the TOF-TOF instrument, this device allows changing the curvature of the supermirrors as a function of the wavelength, in order to keep the focal point at the sample position.

Gain in flux of a factor 2 could be achieved at the sample position.

High resolution imaging using reflective optics

Use of elliptic neutron guides

It was demonstrated by means of Monte-Carlo calculations that elliptic neutron guides lead only to minor distortions of the phase space and can thus be efficiently implemented for neutron radiography and tomography. Monte-Carlo simulations have been performed for various imaging geometries using a straight guide, a convergent guide and an elliptic guide (see Figure (a) below). A small section of elliptic guide (0.5m long) has been used to demonstrate the principle of image magnification so as to be able to achieve gains in spatial resolution. A significant improvement in image resolution has been obtained as shown on Figure (c).

The results have been published in

Neutron tomography using an elliptic focusing guide

Use of capillary optics

A new type of high resolution neutron imaging detectors was designed and constructed at HZB (N. Kardjilov et al, Nucl. Instr. and Meth. A, 651, Issue 1, 2011, Pages 95-99). The small pixel size of the detector requires a high flux density for performing imaging experiments. A focusing device based on Kumakhov-type lenses was realized for high-resolution imaging applications. The neutron optic group at HZB (group leader Thomas Krist) has designed and optimised Kumakhov-type lenses in order to focus the neutron beam with a cross-section of 2 cm in a diameter on a small Field-Of-View of 2x2 mm. Two lenses were tested by Roland Bartmann at the neutron imaging instrument at HZB, Figure 5.

The beam focusing by a Kumakhov lens has provided a flux gain of 20x at a field-of-view of 1 mm² which was essential for the application of a high resolution detector with a pixel size of 2 µm. In this way realistic exposure times of several minutes were achieved. The image quality has been degraded due to the non parallel beam resulting in some spatial resolution reduction. In order to study this effect further investigation will be performed. The results of this investigation will be published soon.

Upgrade of the CONRAD imaging station

In the design of the new imaging facility CONRAD-2 at HZB a neutron guide system was used to transport the beam to the sample position. The neutron guide configuration is shown in Figure 5.

The neutron transport is done with the help of curved neutron guide section with a length of 15 m and radius of 750 m. The super-mirror coating of the outer wall of the guide is m=3 and the inner wall as well as top and bottom walls are with m=2 coating. The curved section is followed by straight section with a super mirror coating of m=2 used for better beam homogenization. The original idea was to use an elliptic focussing guide instead the straight section as it was described in the deliverable 17.41. Unfortunately due to financial restrictions this could not be realised. In the full scale set up a straight guide was installed. At
Financial restrictions this could not be realised. In the full scale set up a straight guide was installed. At the end of the guide arrangement a pinhole was placed. The sample position is allocated at a distance of 10 m behind the pinhole. The beam intensity distribution at the sample position for a pinholes D= 3 cm is shown in Figure 6a. The guide structure provides stripes in the image. In order to reduce the beam heterogeneity a graphite diffuser of 5 mm thickness was used. The results are shown in Figure 6b. The measured neutron flux at the sample position with pinhole of 3 cm shows 2.7x10^7 n/cm²s. The beam size was estimated to be larger than 20 cm x 20 cm. The first imaging experiments were performed with the presented setup as shown in Figure 7.

The designed and constructed imaging facility by using reflective optics (neutron guide system) provides a beam quality which can be used for imaging purposes. For future investigations the last guide section of the facility can be replaced by focusing guide and the parameters of the facility can be studied again. The obtained results are prepared for a publication in a peer-reviewed journal.

Focussing SANS using reflective optics

A new concept of neutron focalisation on SANS spectrometers using a combination of curved super mirrors (SM) was proposed. The aim is to design a focusing system which is achromatic and has no absorption. The proposed design combines advanced neutron optical element such as parabolic and elliptic SM. Figure 1 presents the device design. A parabolic SM focuses the beam from the exit of the guide to make it a point source at its focal point Fp. An elliptic SM with its primary focal point (Fe1) lying at the same position as Fp images Fe1 to its secondary focal point Fe2 according to the properties of ellipses. Now, if a sample is placed after the elliptic SM and a detector is located at Fe2, then we build a focusing system with working on reflection (around 85% for m=3 SM) and achromatic. Therefore, SANS instruments could benefit of this technique in terms of flux at the sample.

A test device bench has been fabricated at the LLB and tested at PSI in September 2011 on the optical test beamline BOA.

For a given resolution (direct beam size on the detector), the elliptical device provides 10 times more flux than the pin-hole set-up (see Figure 10). This is however a 1D design. The present device provide an improved performance only in 1 direction. The overall setup could be more performing if focusing could be achieved in 2 directions as shown below. This type of set-up is technically not feasible today.

The optical components of such a set-up have been tested at BNC. Two 500mm elliptical mirrors were nested to build "half" of the above structure. The device was tested on the optical beamline at BNC. While the device provides roughly the expected performances, Optical imperfections are too large for SANS experiments.

Thus for the new Focussing SANS instrument at BNC, a KirkPatrick -Baez arrangement combining two 1m long elliptical mirrors will be used.

The results of this work have been published in S. Desert et al, to appear in J. Appl. Cryst. SANS using parabolic-elliptic focusing optics.

Focussing SANS using refractive optics

It has since long been proposed to use refractive lenses to implement focussing SANS so as to enable to measure scattering pattern down to much smaller Q values.

JNCS has been working in improving the idea of this concept. A first issue was to have aspherical lenses built so as to avoid aberrations for large diameter lenses. The following figure shows a sketch of the lenses with have been ordered for JCNS from Zeiss. The lenses are made of MgF2 because of its high optical index and low absorption. The polishing of the lenses was crucial to minimize diffuse scattering from the lenses. The right figure shows one stack of such MgF2
Crucial to minimize diffuse scattering from the lenses. The right figure shows one stack of such MgF₂ lenses for the implementation on KWS1 at FRM2.

The second issue which had to be solved was that at room temperature phonon scattering significantly reduce the transmission of these lenses. Thus a dedicated cryostat was built so as to accommodate three lenses stacks (as shown above).

The third issue to be solved was to implement proper data processing tools. Monte-Carlo simulations were performed to quantify the aberrations introduced by the lenses system (see Figure 3. The conclusion is that it optical artefacts from the lenses are negligible compared to gravity effects.

In parallel the data processing programs for the 3 SANS instrument has been upgraded to calculate the resolution effects for SANS measurements. The package qtiKWS developed by V. Pipich (http://iffwww.iff.kfa-juelich.de/~pipich/dokuwiki/doku.php/qtikws) treats all SANS data; the internal SANS data of JCNS instruments KWS-1, KWS-2, KWS-3 is preferred. The detailed modeling of the instrumental resolution function with the lenses has however not yet been implemented.

Task 17.4 Monte-Carlo simulations of complex optics
Modelling of interacting optical elements

There was a wish among users to avoid writing new components to describe new geometries / devices since there are already many existing, useful components to build from. The obstacle is McStas using intrinsically a linear flow. A solution has been devised to handle assembly of basic optical elements to build a new McStas component.

The technique has been demonstrated on a “meta-component” including a guide with an embedded, wedged, polarizing mirror system of the HZB type. A publication describing the implementation has been written.


Optical simulation work bench

A McStas/VITESS schools was organized in May 2010 in Ven, by Peter Willendrup, Linda Udby, Klaus Lieutenant, and Emmanuel Farhi (see www.essworkshop.org)

Another workshop, for more specialized use of McStas was organized in 2011.

The partners of the projects contributed several components to the McSTAS library.

Deuteration (WP18)
Task 18.2 Optimisation of deuterated biomass production

A large number biological neutron studies rely on the biosynthesis of deuterated biological macromolecules using deuterated carbon sources. The cost of these often limits experiments severely. In this task protocols were developed for the optimisation of algal biomass production. Since algae grow photosynthetically, relying only on D₂O medium, CO₂, and light, they are ideal candidates for cheaper production of deuterated components. Major downstream applications in neutron scattering are obvious for these in vivo products. Figure 1 shows examples of deuterated biomass production from phototrophic (green algae) and heterotrophic (E. coli and P. pastoris) micro-organisms.

Task 18.3 Labelling of proteins using Pichia pastoris

Most proteins used in neutron scattering studies are produced in bacteria such as E. coli. This type of protein production has had a huge impact on studies of biological systems using a wide variety of techniques. In many cases the use of E. coli is limited by folding/post translational modification problems. Some proteins have to be produced in lower eukaryotic expression systems. However there are difficulties in adapting such cells to growth in deuterated media. Here we have developed methods whereby labelled
In adapting such cells to growth in deuterated media, here we have developed methods whereby labelled proteins can be produced (intracellularly or exported) in yeast (see Figure 2). The successful development of such systems is now opening up completely new areas for neutron-based biomolecular studies.

Task 18.4 Segmental labelling of proteins

There is a huge requirement for proteins where extended regions/domains/subunits are selectively deuterated. Protein splicing approaches do exist for this type of segmental labelling, but methods for 2H labelling have not been developed. Development the method for deuteration now allows contrast matching studies to be carried on a far wider range of sample systems. Over the course of the project we have established two model systems (U2AF65 and TIA-1) for implementing and optimizing protein ligation techniques and subsequently demonstrated the expression of fragments and the ligation using protein trans splicing techniques. The production of segmentally isotope-labeled proteins was first established using segmentally 15N-labeled proteins. The optimized protocol was then used for segmental deuteration of TIA-1 RRM2-RRM3. The purified protein was used for SANS measurements with contrast variations at Institut Laue-Langevin (ILL) Grenoble to document the utility of segmental deuteration. Based on the results obtained in this project a protocol for the production of segmentally deuterated proteins has been developed, which serves as a guideline and recommendation for the neutron community. The experimental protocols and optimizations of the production of segmentally deuterated proteins have been exchanged with the Life Sciences group at the ILL and will thus be available for the general scientific community of neutron researchers. The implementation of the protocol is being prepared for publication.

We have also started to explore the use of sortase-mediated protein ligation, which has been reported to yield better ligation efficiencies compared to intein-based methods. For the TIA-1 model systems, this work is still in progress. However, for another multi-domain protein we have successfully implemented sortase-mediated protein ligation with very high yields. Figure 3 summarises one of the segmental labelling protocols that has been developed, and Figure 4 shows an electrophoresis analysis of the expression, ligation and purification of a segmentally labelled protein.

Task 18.5 Low cost production of deuterated glycerol

The high cost of deuterated carbon sources for the expression of D-proteins in E.coli is still a stumbling block for the application of neutrons in biology. In this task, methods have been developed for the production of deuterated glycerol by algae under salinic stress. A novel protocol based on “milking” algae of the glycerol produced, dramatically reduces costs since the same biomass and D2O can be used repeatedly. Approaches have been developed using Dunaliella salina and Chlamydomonas reinhardtii (a freshwater algae that could be competitive with Dunaliella). Dunaliella accumulates up to 6M glycerol in the cell and this task has focused on efficient release of glycerol into the media. Methods tested included high temperature treatment, cell immobilization and mild sonication.

Task 18.6 Deuterated membrane proteins

Membrane proteins perform a wide range of essential cellular functions and play key role in (for example) transportation, energy management, signal transduction, photosynthesis. They are also implicated in a number of genetic diseases and have considerable therapeutic importance (70% of drug targets). This sub-task has focused on the development of methods to optimise deuteration of membrane proteins. Model membrane proteins have been identified and bacterial expression systems in high cell density cultures used for deuteration. The deuterated membrane proteins will be used to reconstitute membrane systems with hydrogenated lipids for neutron studies and to test new classes of surfactants for their capacity to stabilize functional assemblies. Figure 5 shows an example of results obtained during screening of experimental conditions used for deuterated membrane protein synthesis.

Task 18.7 Deuterated lipids
One of the major limitations for the application of neutrons to the study of biological systems is the availability of deuterated lipids. Membrane biology is a particularly important area and a new range of powerful experiments could be carried out with the availability of selectively labelled lipids. The provision of unsaturated perdeuterated lipids with a range of head groups required the development of an optimised route for the production of oleic acid and conversion to the target lipids.

The methodology developed for the production of full (C8D17CD=CDC7D14COOH) and part deuterated (C8D17CD=CHC7H14COOH) oleic acid is described here. Briefly, azelaic acid (d-nonanedioic acid, HOOCC7H14COOH) undergoes deuteration on a platinum catalyst surface in the presence of D2O and sodium peroxide. Over three further steps one of the carboxylic acid groups of deuterated azelaic acid is converted to a methyl ester while the other is converted to a deuterated aldehyde group to produce deuterated methyl-9-oxononanoate (DCOC7D14COCH3). A Wittig reaction between the deuterated methyl-9-oxononanoate and deuterated 1-bromononane (C9D19Br) converted to its triphenyl phosphonium salt (C9D19P+PhBr-) produces methyl-(9Z)-octadecenoate (C8D17CD=CDC7D14COOCH3), which is then converted to oleic acid ((9Z)-octadecanoic acid) (Figure 6).

Coupling of the acids to phosphocholine head group is straightforward chemistry that is accessible to a wide range of academic and commercial groups. We plan to pass the material to a range of partners to both spread the load and develop a wider range of sources for the produced material. The phosphoglycerols (and phosphoserines) are synthetically accessible from the phosphocholines so the PCs will be the main focus.

Polarized Neutrons (WP19)

Task 19.2 Wide-angle neutron polarimetry

The realization of large solid angle neutron polarimetry will allow for the use of large solid angle detectors, which enable the simultaneous data acquisition over a wide range of the transferred momentum. This results in an enormous gain in the efficiency of neutron polarimetric experiments and opens new horizons for detailed understanding of the mechanisms involved in multiferroic compounds, photo induced and molecular magnets, magnetic nanostructures, spin electronic and new superconductors, which are at the forefront of condensed matter research.

A detailed analysis of different possibilities for the wide-angle analyser at the diffractometer has been performed Super 6T2 at LLB. It is found that existing solutions that employ the radial array of polarizing super mirror (SM) analysers are competitive with similar devices based on the 3He spin filters only for long wavelengths, \( \lambda > 2.5 \text{Å} \), that limits considerably the application of SM analysers in single crystal diffraction and clearly favours the polarized 3He technique for to the single crystal diffraction applications. This technique is based upon the strong spin dependent neutron absorption of the highly polarized 3He gas that makes it an effective neutron spin filter: it is transparent for neutrons with one spin direction and is opaque for neutrons with the opposite spin direction.

FZJ developed a very compact 70cm diameter magnetic system capable of producing uniform field in three orthogonal directions over a very large solid angle. A pioneer method for manufacturing of doughnut like containers for 3He gas from the dedicated GE180 glass has been also developed at FZJ.

Task 19.3 and 19.4 Further developments of Larmor labelling methods for inelastic neutron spectroscopy, SANS and reflectometry

Neutrons may be used to study dynamics on a molecular scale by measuring the neutron’s energy gain or
Neutrons may be used to study dynamics on a molecular scale by measuring the neutron’s energy gain or loss during the scattering process from the sample under investigation. Examples of these studies are determining Li diffusion through a battery system or hydrogen transport through a fuel cell. In order to determine the energy change of the neutron, the energy before and after scattering must be known. Present state-of-the-instruments select one particular energy of the incoming neutrons, throwing away more than 95 % of the available neutrons, and determine the scattered-neutron’s energy by the time-of-flight (TOF) technique.

In the proposed new TOFLAR technique (TU Delft) the complete neutron spectrum will be used and the neutron’s energy is determined by a modulation technique: a polarised neutron beam pass through a magnetic field so that the Larmor precession of the polarisation vector, thus labelling the neutron’s energy. Combining the Larmor labelling and the TOF technique will result in a quasi-elastic neutron-scattering instrument with high neutron intensity and large accessible range of length and time scales on the molecular level (Fig.3). During the NMI3 project, the theoretical background is described, a proof-of-principle experiment is performed on a prototype instrument at the Reactor Institute Delft, and computer simulation have been performed.

Neutron spin-echo spectroscopy is a method to analyze slow motions and relaxations on the length scale of atoms, molecules and molecular aggregates. In particular in soft-matter (polymers, proteins, complex fluids like microemulsions, etc.) the combination of neutron diffraction (SANS) and spectroscopy with the contrast generation by selective replacement of H-atoms by deuterium enables deep insights in the structure and mobility of these systems. The neutron spin-echo spectrometer has a unique resolution to detect very small velocity changes of the scattered neutrons. This resolution is about 3 orders of magnitude higher than that of any other neutron spectroscopic method. Currently the limiting factor to extend the resolution even further is the difference of the factors determining this timing between various possible paths the neutron may take from sample to detector. The variety of paths is necessary to have sufficient intensity, the difference in time-keeping result from differences in the precession magnetic field along the paths. This field drives the rotation of the neutron spins and the differences can be reduced by correction elements in the beam path. The nature and quality of these elements determine the residual errors. To further improve the resolution and the transmission of neutron-spin echo spectrometers new correction elements that have a good transparency for neutrons and at the same time can hold the large currents that are necessary to perform the correction have been developed in FZJ. The challenge is to combine good neutron transmission with high current density and high accuracy of the electric current distribution that is responsible for the corrective action. Both arms (before and after the sample) of the spectrometer contain 3 of these elements, i.e. a complete set consists of 6 elements with different active area. The only practically suited material is aluminium, which combines good neutron transmission with high electrical conductivity. The best theoretical performance is expected from radial current distributions. These were tried first with painstaking effort, however, their practical performance stayed behind the expectations. Thus an idea already employed at the ILL for elements with smaller area was adopted and extended to larger diameter and current density. These so called “Pythagoras coils” consist of crossed current wedges (Fig. 4). Their combined action resembles that of a radial distribution. Despite the fact that their theoretical performance is somewhat non-ideal their realization meets the theoretical expectation and they are the best performing correction elements that currently could be obtained. Following this new design complete sets of coils for the spin-echo spectrometer J-NSE in Garching and the SNS-NSE at the JCNS outstation in Oak Ridge have been produced and are now used there.

Monte Carlo simulations are playing a very important role in the context of the design and optimization of neutron scattering instrumentation. An accurate, carefully benchmarked computational model of a neutron...
An accurate, carefully benchmarked computational model of a neutron instrument allows to underpin the design of new instruments as well as to enhance the efficiency of the existing ones. This makes the development of powerful Monte Carlo instrument simulation codes very important for the progress of neutron scattering research. A significant contribution to these developments has been made in the frame of this project: FZJ in collaboration with Joint Institute for Nuclear Research in Dubna, Russia has extended the possibilities of the simulation software package VITESS allowing for the simulation of spin dynamics in time-dependent magnetic fields. This paved the way to simulations of practically all existing spin-handling devices and Larmor labelling based neutron scattering instruments. An important step was to simulate the performance of real rather than ideal spin handling devices, i.e. those with magnetic field distributions deviating from the assumed ideal ones. Illustration to this is given in Fig. 5, which demonstrates remarkable possibilities of this new software on the example of thin neutron spin turners that are employed for the rotating magnetic fields NSE technique.

**Task 19.5 Development of Large Solid Angle Resonance Spin-Echo**

This technique yielding to design and construct Large Solid Angle (LSA) resonance coils for the implementation of a multi detector system on a NSE spectrometer and gain two orders in solid angle detection.

The aim of the project was to design, develop and construct Large Solid Angle (LSA) coils for neutron resonance spin echo spectrometer. In the first option, one can use two flat LSA coils for the primary spectrometer, each of them include two radiofrequency coils inserted in static coils (Fig. 6). The main problems to overcome were to obtain an appropriate homogeneity of the field distribution inside the coils, to reduce as far as possible the stray fields outside the coils, to develop an appropriate cooling system (water and air) to avoid mechanical deformation (2kW per coil) and to get an appropriate inductance of the RF coils manage high powers in the frequency range of measurements. For the secondary spectrometer, in order to achieve a measurement over a very wide angle, a curved coil has been developed with the aim to cover simultaneously 15° of scattering angle (Fig. 7). The characteristics of the coils should be similar to the one of the flat coils for the first arm with an additional difficulty related to the fact that we loose a plan of symmetry, and the surface to be covered is wider. In another approach developed in TUM the curved coils are not winded to a body, but cut from one Al piece by means of electrical discharge machining (see Fig.8).

The coil design and the construction were performed at the LLB and TUM and the test has been carried on the spin echo spectrometer G1bis located close to Orphée reactor of the LLB Saclay (Fig. 9).

**Task 19.6 Polarized neutron technique for measurements of triplet correlation functions**

In the present day neutron experiment one determines the mutual position of two scattering objects in the sample: the distance between these objects is the length scale at which we probe the sample (so-called pair correlation function. However, using the NRSE technique one can split the initial neutron wave into four waves, so that in the precession path of the first NSE arm these four neutron waves will produce phase shifts corresponding to three different distances: these neutron waves probe the sample simultaneously on three length scales. The detected intensity will now depend on distances between three scattering objects in the sample (so-called triplet correlation function). The prototype setups for the Four-Wave Neutron Resonance Spin Echo (FW-NRSE) experiments and Spin-Echo Small Angle Neutron Scattering (SESANS) has been built at the reactor of PNPI, in Gatchina, Russia.
Subtask 19.6.1 Ultra-Small-Angle Polarized Neutron Scattering (USANS POL)
The characterization of magnetic structure of matter and the study of its evolution in varying external conditions is a particular strength of neutron research. A new option for investigating the magnetic microstructure is the USANS POL technique, which relies on the high resolution of scattering angles provided by perfect crystal neutron reflection. A corresponding instrumental configuration was set up at the S18 instrument at the ILL, Grenoble (Fig. 10-11). This instrument was equipped with magnetic prisms for neutron polarization and a dedicated sample environment, which provides 3D control of an external magnetic field configuration ranging from a zero-field environment via continuous intermediate settings up to the magnetic saturation of the samples. In addition, this sample environment enables us to apply external mechanical forces for the study of magnetostriction in novel technologically relevant materials that are used in modern sensors and actuators. Exemplifying test experiments were performed which demonstrated the potential of the new technique (Fig. 12). Measurement results allow for an assessment of the native sample state which follows from a specific manufacturing process and the evolution of its microstructure in external magnetic fields and under mechanical stress according to its particular magnetic properties. Thereby, USANS POL experiments offer a picture of the structure which may be related to material functionality and eventually lead to technological improvement.

Subtask 19.6.2 Development of an ultra-flexible neutron magnetic resonator
Spectral and temporal tailoring of neutron beams is an important issue for advanced neutron sources like the European Spallation Source project. Spatial magnetic neutron spin resonance as basis for the famous Drabkin-resonator demonstrated its potential for defining the spectrum of a polarized neutron beam already in the 1960s. With the novel idea of controlling each element of the neutron resonator separately, a concept was invented that allows for polarized neutron beam tailoring of unprecedented flexibility regarding key parameters like incident and final neutron energy, spectral width of the incoming beam, or its energy resolution. We have built two prototype resonators according to that concept and tested them experimentally at a polarized neutron beam line at the Atominstitut TRIGA reactor of the Vienna University of Technology (Fig. 13-14). The experiments demonstrated the flexible spectral definition of the neutron beam with variable resolution in continuously operated mode which may be applied in diffraction and fundamental physics experiments. They also included the first realization of a travelling wave mode of operation where short neutron pulses in the microsecond range are produced by synchronized magnetic field pulses. This operation mode offers new possibilities for neutron spectroscopy as it decouples the energy resolution from the time-of-flight resolution of the neutron beam. In addition, a Ramsey-type resonator setup was conceived and also tested which offers promising potential for advanced neutron spectroscopy techniques.

Muons (WP20)
Spin polarised muons are an important probe of materials at the atomic level. Applications of the muon technique (μSR) are remarkably diverse, encompassing studies of magnetism, superconductivity, and spin and charge transport, while providing a highly sensitive hydrogen analogue to probe semiconductors and proton conductors. The technique has an important role beyond condensed matter physics, offering chemists a valuable method for investigating the fundamentals of reaction kinetics while enabling the study of organic radical structure and dynamics in solids, liquids and gases. Researchers frequently use μSR in tandem with techniques such as neutron scattering and magnetic resonance; the techniques provide complementary information and only through a combination of measurements can a detailed understanding of a system be obtained.
The Muon Joint Research Activity (JRA) involved the two European muon facilities, ISIS at STFC – Rutherford Appleton Laboratory in the UK and the Swiss Muon Source at the Paul Scherrer Institut in Switzerland, together with academic partners from Parma and Babes-Bolyai Universities. Its aim has been to extend the capabilities of the muon technique for the benefit of the user community through the development of new source instrumentation, novel measurement techniques and advanced computational methods. A significant aim of the JRA has been the development of the technologies required for μSR spectroscopy in high magnetic fields. The importance and success of this work is evidenced by recent grant awards to both facilities to develop high field instruments that, working together, are making a significant impact on the European muon user programme.

Specifically, the JRA has encompassed the following tasks:

- Technologies for high field instruments: particularly new detector technologies for fast timing in high fields and array designs, supporting the development of high field spectrometers.
- Technologies for μSR at high pressures: solving problems unique to μSR to develop cells for high pressure gas phase and condensed matter measurements.
- Novel resonance techniques and simulation codes for complex experiments: exploring the application of NMR-style pulsed RF techniques in μSR and the use of novel simulation codes.
- Muon beamline control and monitoring: developing new beam diagnostic techniques and codes for instrument simulation, extending metadata included in the NeXus instrument definition.

Task 20.2 Technologies for high field instruments

The development of new instruments for high field spectroscopy is vital for providing the user community with the tools necessary for future research. However, μSR in high fields is uniquely challenging. Both the implanted muons and detected decay positrons are charged and their trajectories are modified by the applied field, while the detector systems need to be field insensitive yet capable of providing fast-timing. Work within this task area supported the development of new muon instruments capable of measuring in fields of up to 9.5T and has included:

- Development and commissioning of a prototype fast-timing detector array based on Geiger-mode APDs [P1-P6]. The array was optimised for high transverse field experiments planned at PSI which required a timing resolution better than 140ps. In fact, during testing, a resolution better than 80ps was achieved and, most importantly, the detector (shown in Figure 1) was demonstrated to be insensitive to magnetic fields. Performance was confirmed by measuring the ~1.3GHz precession of diamagnetic muons (μ+) stopped in a silver target, with impressive results also being obtained during a study of muonium (a bound μ+e- system) transitions in a synthetic quartz crystal where frequencies up of ~3.5GHz were measured. A detailed account of the design and performance of this array is available on the JRA website, completing deliverables D20.2.1.1 D20.2.1.2 and D20.2.2.1 with results presented at the MuSR 2011 conference and published in the proceedings [P2]. The complex behaviour of the muon and positron trajectories in high magnetic fields made the design of both the spectrometer and detector array challenging, and the simulation codes developed both during FP6 and as part of the present task 20.5.2 proved essential for completing this work.
- Successful testing of a prototype veto detector system designed for integration into the dilution refrigerator. Operation of a dilution refrigerator in high magnetic fields is particularly problematic because the small spiralling radius of the decay positrons (~1cm at 9.5T) requires that veto/validation detectors are positioned close to the sample. To overcome this problem, a highly novel device has been developed using scintillators operating within the dilution refrigerator at cryogenic temperatures with light readout realised using a lens system [P7].
• Publication of a paper describing the performance of the ISIS 5T longitudinal field spectrometer [P8]. The detector array for this instrument was developed using beam and instrument simulations coded during FP6. Scintillation detectors were by necessity positioned close to the sample position; however, extended light guides were successfully used to move the field sensitive photomultiplier tubes to a low field region. Commissioning of this instrument required new technologies for direct imaging of muons stopped at the sample position, to understand how the muon spot evolved in position and shape with applied field. This was achieved through the development of a field-insensitive beam camera (D20.5.1.2 in task 20.4) which enabled a detailed performance evaluation to be completed (D20.2.3.1) with results being published in Review of Scientific Instruments [P8] (D20.2.3.2). The instrument (shown in Figure 2) is now fully integrated into the ISIS User Programme and is being used in a broad range of studies that have led to a number of journal publications [P9-P14].

• A high field workshop brought together facility staff and users at The Cosener’s House in Abingdon, UK (September 2010) for a two day meeting to consider novel applications of high field μSR. Sessions covered superconductivity and magnetism, semiconductors, and applications in chemistry and soft matter. More recently, the development of novel detector technologies and high field techniques were the theme of a joint meeting of PSI and ISIS instrument scientists.

Task 20.3 Technologies for μSR at high pressures

The aim of this task was to develop new pressure capabilities for μSR. Pressure is an important parameter in the study of the phase diagram of condensed matter systems and its study can often reveal new and sometimes exotic physical properties of materials. In the gas phase, compared to other resonance techniques μSR provides a uniquely sensitive tool both for studies that can reveal spectroscopic information and enable a direct measurement of chemical reaction kinetics. Work within this task has focussed on solving problems unique to μSR. These include the need for thin beam entry windows, a requirement to minimise cell mass to avoid significant degradation of the decay positrons and a design that ensures muons are stopped in the sample region with a low measurement background from the cell walls.

Work has included:

• Development of a solid-sample pressure cell designed for pressures beyond 2.5GPa with a low measurement background. This work was led by Babes-Bolyai University with a PDRA being appointed for the project. Because relatively thick windows are required to withstand the pressures the cells were developed for the high energy muon beam available at PSI. Computer simulations of the muon stopping range in the cell were developed, enabling the signal (from the sample) to noise (from the pressure cell walls) ratio to be evaluated for various cell configurations and beam conditions (including the muon momentum and beam profile). From modelling it was concluded that piston cylinder pressure cells, having a comparatively large sample volume, were the best choice for μSR experiments, and work focussed on improving their characteristics for use in existing cryogenic environments. A number of cell designs and pressure transfer fluids were tested to complete deliverable D20.3.1.1 evaluating the merit of openings on one or both ends and for using a single or two-layer construction. The cells are now available to the facility user programme and have already been used in studies of heavy fermion systems and an investigation of the phase diagram of the FeSe1-xsuperconductors [P15-P17]. Results from this work have been collected in a report available on the JRA website to satisfy deliverable D20.3.1.2.

• Development of a 50 bar gas-phase μSR pressure cell, designed with an integral radio frequency (RF) coil for resonance measurements on the ISIS high magnetic field instrument. Initially, cells capable of measuring high pressures on a high energy muon beam were planned; however, this part of the project was refocused after discussions with facility users. They suggested that, scientifically, there would be
was refocused after discussions with facility users. They suggested that, scientifically, there would be considerable interest in developing gas pressure cells for high field spectroscopy. Initial design work focussed on the need for thin windows to admit a ‘surface’ energy muon beam to the cell, with a laminate of seven 25μm foils proving optimal. A metallic cell was required both to withstand the pressure and to ensure a clean environment for the gas sample. However, this design required the radio frequency cavity (formed from a three turn saddle coil) be mounted inside the cell and connected using a high pressure RF feed through. A sliding mount was used to position the cell within the high field magnet. The gas cell (shown in Figure 3) was commissioned on-beam (D20.3.2.1) with initial experiments demonstrating that useful spectroscopic information could be obtained by measuring avoided level crossing resonances for ethene and isobutene. These successful measurements demonstrate that information about muoniated radical structure and dynamics can readily be obtained in the gas phase. Work continued to commission the RF cavity. In this case the gas pressure had to be carefully controlled to ensure the muon stopping profile was centred in the coil. However, with this achieved, strong paramagnetic and diamagnetic RF resonances were measured for muons stopped in nitrogen gas, demonstrating a novel technique that is essential for making final state spectroscopic studies and investigating chemical reaction kinetics. The outcome of the commissioning work and demonstrating experiments is available in a report on the JRA website (D20.3.2.2).

Task 20.4 Novel resonance techniques and simulation codes for complex experiments

The aim of this task was to develop novel experimental and software techniques to assist with the study of complex systems using μSR. NMR-style pulsed resonance techniques, and particularly simultaneous stimulation of the muon and nuclear spins, has been explored as a means of obtaining new information from the μSR experiment. An in-situ NMR capability has also been developed, both to support the multi-nuclear experiments and to provide a unique experimental system. Software development has centred on exploring how simulation codes can be used to support the analysis of complex μSR experiments, and particularly how DFT codes can be used to enable the muon site to be identified within the sample. Work within this task included:

- A demonstration of RF μSR experiments using NMR style pulsed techniques. Advantage has been taken of the ISIS beam pulse structure in order to investigate the application of high power RF pulse sequences for novel μSR methods in a collaborative project with University of East Anglia. ISIS is uniquely suited to these measurements since the RF excitation can be timed to the intense muon pulse, avoiding problems associated with RF heating while simplifying the timing of complex pulse sequences. Two sequences have been demonstrated during this project to satisfy deliverables D20.4.1.1 and D20.4.2.2. Firstly, a double resonance technique has been demonstrated where both muon and nuclear spins are simultaneously irradiated to decouple the nuclear dipolar interaction, thus providing unique information about the muon site and dynamics. Secondly, a composite spin inversion sequence has been explored [P18] as a means of improving the efficiency of RF spin rotation in the RF μSR experiments. Intriguingly, because the muon spin polarisation is detected by positron emission, μSR provides a unique way of monitoring the spin evolution during RF excitation, providing a unique insight into the effect of the RF field on the spin polarisation.

- Development of in-situ NMR spectrometer (D20.4.2.1) was essential to support the development of RF pulse sequences. Good results have been obtained using both dedicated NMR coils and RF cavities typically used for RF μSR experiments and a detailed report (D20.4.2.2) is available on the JRA website. From the work developing RF pulse sequences the need for good engineering of RF probes is apparent to ensure the reliable application of suitably intense pulses. To this end, the NMR system has been used for off line tests to develop cavities without impacting on facility beamtime, and a dedicated high power RF...
Off-line tests to develop cavities without impacting on facility beamtime, and a dedicated high power RF insert has been developed for the ISIS high field spectrometer.

- A study was carried out to assess the suitability of simulation codes for supporting analysis of complex μSR experiments in an area of work led by the University of Parma through the appointment of a PDRA. Calculation of electrostatic potentials and magnetic dipolar fields within magnetic materials was considered particularly valuable since the estimated value of the local field and its orientation in the crystal lattice could then be compared to experiments to help assign muon sites (shown in Figure 4). Density Functional Theory (DFT) simulations provide a framework to estimate the muon’s zero-point motion, the local structural and magnetic perturbations, and the muon interstitial sites in a growing set of compounds. The ab initio strategy may provide a particularly powerful method for making muon site assignments provided the computational complexity can be solved, and were used to advantage in a recent journal publication [P19]. An overview of the planned work was presented as a poster at the MuSR 2011 conference and is available on the JRA website (D20.4.3.1). Feedback from the community was very positive and the ideas were taken forward in software development. The strategy for determining a-priori muon sites(s) in a given compound by simple DFT calculations was clarified and checks performed choosing iron pnictides as a test case. The same strategy was replicated with different free and open software DFT suites, including all electron (Quantum Expresso, SIESTA, ELK) (deliverable D20.4.3.2). To engage the community, a discussion meeting was held April 2012 (hosted by ISIS) bringing together a number of groups from Europe, Indonesia and Japan interested in using simulation methods to determine the muon site in materials. A further meeting was held in Penang, Malaysia, and it is hoped to continue this series of meetings to help focus development of methods in this important area.

Task 20.5 Muon beamline control and monitoring

Muon beamlines are complex and require many hours of set-up to enable correct transportation of the primary muon beam to the sample. Beam parameters can greatly affect measurements both through the profile of the muon spot and beam transport in the instrument. A greater understanding of beam and instrument properties, gained both through better diagnostic tools and simulation codes, is therefore highly desirable both to reduce commissioning time and bring new insight to the experimental results. This task has involved:

- Development of techniques for beamline diagnostics. This work started by making a comprehensive assessment of methods for providing better beam diagnostic information, and a discussion document is available on the JRA website (D20.5.1.1). The work was particularly timely as a number of the techniques researched are being included in the design of a refurbished ISIS muon beamline planned for 2014. The development of the CCD beam camera to image the muon spot in high magnetic fields was completed early in the project (D20.5.1.2) as it was essential to making a detailed performance evaluation of the ISIS 5T instrument required to complete deliverable D20.2.3.1. The camera used a cooled commercial CCD sensor and lens to image light produced as the muon beam impacts a scintillating element mounted at the sample position. Excellent results were achieved with a detailed understanding of the evolution of the spot profile with magnetic field, instrument and beam parameters being obtained. A report discussing the performance of the camera is available on the JRA website and results are included in the Review of Scientific Instruments publication [P18].
- Development of the simulation code ‘musrSim’ to become a general tool for simulating almost any μSR apparatus including sample environment equipment (D20.5.2.1). Development of this code continued the work started during FP6 and was led by PSI following the appointment of a PDRA. The software has successfully been used at the facility for the development/optimisation of four instruments – the High Field Instrument (Figure 5), LEM, ALC and GPD. At ISIS, Dr Bakule of the RIKEN RAL facility used the
Instrument (Figure 5), LEM, ALC and GPD. At ISIS, Dr Bakule of the RIKEN-RAL facility used the program extensively both in the development of the low energy beamline and as a means of understanding the operation of the ARGUS collimator. The code also played a crucial role in the interpretation of a combined laser stimulation/μSR measurement made by Prof. Fleming (of the University of British Columbia). While ‘musrSim’ is relatively simple to run, the analysis of the simulated results to a graphical output (histograms, μSR spectra, etc) required an analysis program to be coded specifically for a given instrument. Therefore, in an extension to the work associated with sub task 20.5.2 a general tool for analysing simulation output has been developed. The program, ‘musrSimAna’, enables the simulated data to be analysed and tested for varying acquisition parameters, and this software suite proved essential for the development of the new High Field instrument at PSI (sub task 20.2.2). The work was presented at MuSR 2011 and is published in the conference proceedings [P20].

- Work to finalise a NeXus Instrument Definition suitable for both ISIS and PSI. Agreement between ISIS and PSI was reached on a common Instrument Definition that contains a comprehensive dictionary of metadata for properly describing muon experiments (D20.5.3.1). An account of the definition was presented at the NOBUGS 2010 meeting. Within this definition, a subset of essential entries was agreed to enable the worldwide muon community to use the definition as a Common Exchange Format. The utility of this exchange format has been demonstrated with PSI data being viewed with ISIS analysis codes and vice versa. The standard definition was formulated as an NXDL file and the NeXus validation tool (‘NXvalidate’) used to demonstrate validation of muon NeXus data files, an effective way of ensuring they conform to and can be read as a Muon Common Exchange file. A paper discussing the NeXus format was presented at MuSR 2011 and is published in the conference proceedings [P21].

Sample environment (WP21)
Task 21.2 High Pressure
Partners: ISIS, Laboratoire Léon Brillouin (LLB), Institut Laue-Langevin (ILL), and Helmholtz-Zentrum Berlin (HZB)

The aim of this task was to provide a range of containers (cells) for high pressure gas samples and suitable pressure-generating equipment.

The technical challenge faced by the LLB and ISIS groups in completing this task was the need to make the high pressure gas cells strong, and thus safe, whilst making them sufficiently ‘transparent’ for neutrons. An added complication was the corrosion produced by hydrogen, limiting the choice of suitable cell construction materials still further. An extensive investigation into potential materials was carried out, supported by material testing carried out by students at Imperial College London. To complement the test data the collaboration used experimental results from the Engin-X diffractometer at ISIS and extensive finite element analysis (FEA) to aid design.

Sourcing a high-strength, neutron-compatible, hydrogen-resistant material proved to be a challenging endeavour, but the data obtained was used by the teams to choose the best available materials to construct the new cells. All the cells specified were made and tested successfully. Most were made from beryllium copper (Figure 1), but for high temperature 4 kbar hydrogen Inconel was used (Figure 2) as the data showed beryllium copper is not suitable at elevated temperatures. For 8 kbar hydrogen a composite cell with a hydrogen-resistant beryllium copper liner and a neutron-transparent outer of titanium zirconium was used in order to increase the neutron transmission through the cell (Figure 3).
To enable the full exploitation of this suite of high pressure cells, a support network of safety features, testing facilities and gas handling systems was also produced. This equipment included gas ‘intensifiers’ which compress the gas to pressures over 10 kbar - 10,000 times atmospheric pressure. The ISIS test area was updated and strengthened, and has already been used by the LLB for testing their high pressure cells. The LLB produced a cryogenic system in order to fully test their cells at low temperature (Figure 4). The LLB and ISIS procured 10 kbar inert gas intensifiers (Figure 5) and ISIS extended the range of their hydraulic intensifier to over 13 kbar. Both the HZB and ISIS constructed 10 kbar hydrogen intensifiers (Figure 6).

These new pressure cells and equipment have doubled the pressures available to LLB users. The hydrogen pressure available to ISIS users has increased from under 4 kbar to 8 kbar. Several of the cells have already been successfully used for experiments at ISIS and HZB.

Task 21.3 High Temperature

Partners: Institut Laue-Langevin (ILL), Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM-II)

Levitation furnaces are used for the study of small samples of molten materials, too hot to be held in a container. For this workpackage, two furnaces were developed for different sample types: an aerodynamic version at the ILL and an electrostatic version at FRM-II. An aerodynamic furnace uses high speed gas jets to suspend the sample; an electrostatic furnace levitates charged samples using electric fields.

Aerodynamic furnace

Existing aerodynamic furnaces were not suitable for experiments on neutron beamlines because of sample instability and sample access: only two-thirds of the molten sample volume was generally visible to the neutron beam. The neutrons scattered by the nozzle also created unwanted background scatter, leading to data analysis problems. These were significant problems to overcome but after many trials of different gas nozzle types, geometries and flow rates, a solution was found. The novel four-nozzle technique developed allows the stable levitation of a sample up to 6 mm in size, unobscured by the nozzle. It is also now possible to change the atmosphere in which the sample is heated, for example by the introduction of a small proportion of oxygen or carbon dioxide. Figure 7 shows the furnace and Figure 8 shows a levitated sample during heating. Experiments may now be carried out at temperatures up to 3000 K, a temperature never before obtained on a neutron beamline. 3000 K is over 2700°C – more than 1000°C hotter than lava leaving a volcano, to put it in context.

Due to the complex technical challenges faced during the development of this prototype furnace the decision was made not to continue with the final stage (the electrode-less technique deliverable) until further resources are available.

Electrostatic furnace

The main task facing the FRM-II team working on the electrostatic furnace was to adapt an existing system to fit the spatial constraints of a neutron scattering instrument. The system also needed an upgrade to levitate the larger samples required for the neutron beam, as well as improvements to portability.
to levitate the larger samples required for the neutron beam, as well as improvements to portability, reliability and user handling.

Working in partnership with the German Aerospace Centre, DLR, an improved and compact furnace has been made. It has been tested and used for neutron scattering experiments on beamlines at both the FRM-II and ILL. The system has fulfilled all its specifications and the addition of a laser pre-heating stage now removes unwanted organic material from the surface of the sample as well as dissolved gases and other contamination of the bulk material. This results in a more reliable and faster melting process and aids the processing of new sample systems. Figures 9 and 10 show the electrostatic furnace.

Task 21.4 Gas Adsorption
Partners: Helmholtz-Zentrum Berlin (HZB), ISIS, Laboratoire Léon Brillouin (LLB) and Institut Laue-Langevin (ILL)

An ambitious set of gas adsorption systems for both volumetric and gravimetric analysis was promised, and delivered. Gas adsorption is the process by which components of a gas adhere to the surface of a sample. Volumetric analysis determines the extent of adsorption by measuring the change in sample volume; gravimetric analysis by measuring the change in sample weight.

The greatest challenge to the HZB team was overcoming the complexity of automating the supply of an accurate measure of gas to the sample for the adsorption process. The difficulties of providing a range of multipurpose apparatus, suitable for neutron beamline use, which was safe, user-friendly and flexible were also significant. New construction materials had to be investigated and were rigorously tested under extreme conditions before approval. Important safety measures had to be taken to provide protection against possible material failures. For example, high pressure hydrogen vessels were surrounded by containment tubes filled with a non-flammable gas atmosphere.

It was not always possible to design a single device to cover the whole pressure or temperature range required. Thus, to avoid compromising accuracy or performance, specialised equipment was developed for specific sample conditions.

Volumetric Systems
This range was initially increased with the development of systems for the in-situ measurement of gas adsorption at a specific temperature, at low pressure and in the temperature range 1.5 to 600 K (-271.5 to 327°C). New equipment includes a cryo-furnace insert and a mini mechanical cooler version for use on neutron beamlines with restricted access (Figure 11). In addition, accessories to facilitate the supply of gas to the sample have been developed including a glove-box insert and a self-locking sealed sample can (Figure 12).

A gas handling system with automated control was then built, operating at up to 200°C and 300 bar (Figure 13). This comprehensive system incorporates an oven to heat the gas supply tubes to the sample, ensuring that the vapour condenses in the correct place for analysis. A residual gas analyser has also been adapted for the system to provide chemical composition information for experiments related to reactions and catalytical processes. This gas handling system has been in successful operation for experiments since July 2012.

Gravimetric Systems
Gravimetric Systems

For gravimetric analysis an existing magnetic suspension balance has been adapted for neutron scattering experiments. A magnetic suspension balance weighs samples without contact, separating the weighing instrument from the sample which may be in a corrosive atmosphere or under extreme temperature and/or pressure conditions.

Firstly, to guarantee a reproducible sample position with respect to the neutron beam, a mechanical depositing rack has been added (Figure 14). This has given repositioning reliability better than 0.1%. Secondly, a high pressure hydrogen vessel for the balance has been designed and made, incorporating a hydrogen-resistant liner and a neutron-transparent outer casing. Thirdly, a control system allowing the application of either variable gas mixtures or humidities has been developed. This system can remotely regulate the gas flows, the temperature (to 500°C) and the pressure (0.5-35 bar) of the sample container on the balance. To this was added a high pressure (up to 300 bar) gas handling system, built together with an industrial partner, which allows very precise sample pressure control (Figure 15). Finally, the working range for gravimetric analysis on the neutron beamline has been extended still further down to cryogenic temperatures, -250°C and below. A customised helium flow cryostat had to be designed as no existing system was suitable. The sample holder is cooled by contact with the cryostat heat exchanger and magnetically coupled to the suspension balance by a thin fibre to minimise heat transfer, and then lifted for sample weighing. A series of thermal radiation shields helps to maintain a constant temperature around the sample whilst allowing almost 360° neutron beam access to the sample.

The advanced performance and automated control of these adsorption systems has successfully increased the rate of experiments at the HZB.

Standardised gas handling centresticks

In addition, to complement the equipment described above, the ILL (in cooperation with HZB and ANSTO, Australia) has developed an improved version of a gas adsorption stick. This stick combines volumetric, continuous flow and gas mixing applications together with a standard sample cell design (Figure 16). This stick is easy to use and maintain, and provides users at different neutron facilities with a standardised piece of equipment. It has already been successfully used in several experiments.

Detectors (WP22)

Task 22.2 Gaseous Scintillation Proportional Counters

When a neutron is detected in a GSPC filled with a gas mixture of 3He-CF4, it gives rise to two light pulses emitted in the wave length region between 150 nm and 750 nm. A ‘primary’ light pulse following the absorption of the neutron in the nuclear reaction with 3He and a much brighter ‘secondary’ pulse when the charge released in the gas reaches the charge amplifying region of a micro pattern device, e.g. a MicroStrip Gas Counters (MSGC), are generated. In a GSPC configuration as depicted in Fig. 1, this secondary light pulse is recorded through a transparent window by an arrangement of photon detecting devices, e.g. by an ANGER Camera type array of individual Photomultiplier tubes (PMT). If a proper processing algorithm is applied to the PMT signals the neutron impact position can be determined with sub-millimetre precision.

The performance of a GSPC strongly depends of the photon yield, the spectral response and the light pulse duration. A main objective was to measure the absolute primary and secondary photon yields of CF4.
A main objective was to measure the absolute primary and secondary photon yields of CF4 between 200 and 800 nm and the decay time properties in the typical conditions of operation of a GSPC detector. A series of precise studies performed at LIP Coimbra and ILL have confirmed the release of ultraviolet and visible light in the emission band of CF4. Emission spectra of CF4 fully corrected for spectrometer and PMT sensitivity were obtained for various gas pressures and the result is shown in Fig. 2. With increasing CF4 partial pressure the intensity of the secondary light emission is increasing drastically in the UV and the visible part of the spectrum. A ratio of ~0.19 emitted photons to electrons produced in the charge avalanche of the MSGC is achieved at 5 bar shown in Fig.3 for the UV and visible part separately. This allows a light yield of 105 -106 photons / neutron capture in a realistic GSPC configuration which is a hundred times brighter than the light yield of Li-glass. Very short decay times of only a few nanoseconds for the UV-part and ~15 ns for the visible part could be confirmed for both the primary and secondary scintillation light of CF4. These values guaranty a dead time shorter than 100 ns per event in a real operational system.

To reach the envisaged performance of sub-millimetre position resolution and MHz-count rate capability a potential GSPC has to be operated with a gas mixture of at least 4 bar 3He pressure and 6 bar CF4 pressure. While under these conditions it is difficult to achieve sufficiently high charge gains with other micro pattern devices like single GEM or Micromegas it could be demonstrated that MSGCs can be safely operated in such a GSPC at a charge gain of several hundred. Two specific types of MSGCs optimized for use in a GSPC have been designed at ISIS. They exhibit 8µm Cr-Anode stripes with 500µm pitch fabricated on 1 mm thick Schott S8900 conductive glass with 32 x32 mm2 and 90 x 73 mm2 active area respectively.

Apart from the CF4 scintillation properties; the performance of a potential GSPC mainly depends on the light readout scheme as well as optical and geometrical parameters, such as photon detection efficiency, readout pixel geometry and position reconstruction. All these parameters have been taken into account in the comprehensive simulation package “ANTS”: A simulation package for gas scintillation Anger camera in thermal neutron imaging developed at LIP Coimbra. The simulation module of ANTs enables to evaluate different GSPC detector designs, to predict their performance and to study the influence of individual physical or detector parameters. The analysis module of ANTS allows to process either simulated or experimental data using sophisticated algorithms like Centre-of-Gravity or Maximum Likelihood for calibration and position recognition. It is an excellent toolkit to design a GSPC with optimized performance and enables to directly compare experimental results with simulation.

Light detecting devices for a GSPC

The principle of ANGER camera readout for a Gas Scintillation Proportional Counter using single cathode Photomultipliers (PMT) has already been demonstrated in the MILAND detector JRA in NMI3 FP6. A proper choice of PMT parameters (photo cathode, window, size, etc) is crucial for optimizing the GSPC performance. In this context the simulation package ANTS allows single cathode PMT parameters including photocathode type, shape, area and spatial geometry to be selected and provides information on detector performance criteria as a function of this selection. To compare the simulated data with experimental data, different single cathode PMT types have been tested and compared. Two types of 25 mm PMTs with S20-photocathodes and 10 stage dynode have been studied at ILL regarding sensitivity and linearity. The ET9113WB PMT from ET Enterprises has a UV window and is sensitive to the CF4 emission peak at 300 nm, while the Hamamatsu R5070A has a glass window with a cut off at 300 nm, so only half the 300 nm CF4 peak can be detected efficiently. Though the ET9113WB provides higher light yield at low gas gain the R5070A reveals better linearity at high gas gains and higher sensitivity in the visible region. Therefore, this PMT type was chosen to be used in the large size demonstrator detector.
visible region. Therefore, this PMT type was chosen to be used in the large size demonstrator detector equipped with a glass window built at ILL.

At LIP and at FZ Jülich, experimental setups have been built to measure spatial uniformity, wavelength and angular dependence of the sensitivity of PMT photo cathodes. Mounted on high precision x-y linear stages, highly collimated LEDs emitting short light pulses have been used to determine gain variations, spatial uniformity, wavelength and angular dependence of the sensitivity of the R5070 PMT photocathode. Significant variations of up to 20% could be observed in both spatial uniformity and angular dependence. The same setup equipped with a specifically designed isotropic light source is used to precisely determine the Light-Response Function (LRF) of the individual PMTs in the real GSPC ANGER Camera setup, which is required for a proper processing of the position determination algorithm.

To study different light readout schemes and to compare simulated with experimental data, three small size GSPCs shown in Fig. 4 have been built at FRM II and distributed to FZ Jülich and ISIS. This “standard” device approved for 10 bar fill pressure can be equipped with an ANGER Camera readout of four or seven PMTs with 38 mm or 25 mm diameter respectively.

Two types of 38 mm PMTs labelled “red” (ET 9972WSB) with UV-window and S20 photo cathode and “blue” (ET9102SB) with glass window and Bialkali cathode mounted in this device have been studied at the ROTAX beam line at ISIS. Compared to the “blue” PMTs, the “red” PMTs show an improvement in position resolution of 15 – 25%, corresponding to an increase in light collection efficiency of 30 - 50% in good agreement with simulation calculations performed with ANTs. Consequently the GSPC was equipped with the newly developed MSGC and a UV transparent sapphire window to study the influence of gas gain and CF4 partial pressure on the achievable position resolution up to 6 bar partial pressure. The detector was readout with an array of four or seven PMTs respectively and the PMT signals were recorded with an 8-bit Aqiris fast digitizer system and analyzed with ANTs v.06. At a CF4 pressure above 5 bar, sub-millimetre spatial resolution close to 0.6 mm (FWHM) has been obtained as demonstrated in Fig. 5.

Task 22.3 Front end pulse processing and readout electronics

Two different readout electronics architectures including signal processing schemes have been evaluated for an ANGER camera array of single channel PMTs to be used in the GSPC demonstrator detector. At ISIS a system has been developed which is able to collect and process the data of a 7-PMT setup in real time. A commercial signal processing system has been selected based on a Terasic Altera TR4 FPGA Development system and Terasic 150 MHz sampling ADCs. Position reconstruction with this system is based on an algorithm using neural networks, which can be incorporated into the detector signal processing electronics and carried out in real time without the need to send the data to a PC. The neural network algorithm has been carefully constructed so that it can be processed in the FPGA. The position resolution of the GSPC has been measured with both the Terasic system and the digitizer system using a Centre-of-Gravity (CoG) position reconstruction algorithm in each case. The results show the Terasic system is working well achieving a spatial resolution close to the digitizer based system.

A second attempt to read out the Anger Camera array of the GSPC pursues an architecture based on a charge sensitive preamplifier, pulse shaping stage and a sampling ADC for each PMT channel with data storage to a PC. While the 8-channel preamplifier modules have been built at FRM II a dedicated 32-channel readout electronics for an Anger Camera based GSPC has been built at FZ Jülich. It consists of two LVD pulse processing and one controller board mounted in a crate. The self-triggering system provides for each channel CR-RCn shaping of the preamp input pulse, pulse height detection via a 80MHz ADC (12bit) and FPGA based pulse processing. The system allows raw data storage on disk via a GBit...
ADC (12bit) and FPGA based pulse processing. The system allows raw data storage on disk via a GBit optical interface for the development of reconstruction algorithms. Online event reconstruction could be implemented in the FPGA or on a Graphics Processing Unit connected to the readout system. The study of the potential use of a NVIDIA GeForce GTX570 GPU for implementing an online maximum likelihood based reconstruction algorithm has been started at FRM II showing promising results.

GSPC 19 demonstrator detector
Based on the results achieved during the programme a large area prototype with Anger Camera readout has been designed and built at ILL which acts as demonstrator for the GSPC technology. The 40 cm x 40 cm pressure vessel with a 5 mm thick Al-entrance window of 10 cm diameter is equipped with a Borofloat glass rear window of 3.3 mm thickness only and has been successfully pressure tested up to 25 bar fill pressure. For first measurements the detector shown in Fig. 6 has been filled with a gas mixture of 1 bar Helium-3 and 6 bar CF4. It is equipped with the 9 cm x 7.3 cm active area MSGC (substrate S8900 Schott glass) developed at ISIS and is read out by an array of 19 Hamamatsu R5070A PMTs.

In October and November 2012, the 32-channel readout electronics and the digitizer readout system presented above were integrated to the demonstrator and a first test with neutron beam performed at the CT2 beam line at ILL.

Fig. 7 shows the resulting 2D-position spectrum recorded with the 32-channel readout system when the detector is homogeneously illuminated with 2.5A neutrons with a multi-hole / slit Boron-nitride mask mounted in front. The hole diameter is 0.5 mm on a 10 mm pitch, while the slit width is 0.2 mm. A position resolution of $\Delta x \sim 0.6$ mm (FWHM) close to the physical limit is achieved by analysing the data with ANTv.06 using a maximum likelihood reconstruction.

Potential Impact:
The NMI3 project under FP7 is conceived as an efficient tool for further building the European Research Area. Neutron scattering and muon spectroscopy rely inherently on large-scale facilities. These are distributed all over the world, with the major concentration being in Europe. Improvements in the return on investment can be expected from coordination of the use and development of the facilities, while at the same time keeping competition as an important regulator. NMI3, as a comprehensive consortium of European neutron and muon providers, will act as the facilitator of this necessary integration process. It will work to ensure that national spending in the neutron and muon area produces optimized scientific output. This integration requires by definition a fully European approach. The considerable number of facilities, and their geographical distribution, make it impractical to achieve such European coordination on a local or bilateral basis.

The NMI3 web page is the information and communication hub for neutron scattering and muon spectroscopy in Europe. Via the supported schools NMI3 is able to monitor and pilot the training of young researchers in Europe. Foresight studies on energy and food had highlighted the expectations from these sectors for neutrons and muons. The foresight study on a long pulse source prepared planning of next generation pan-European facilities like ESS.

Joint development of technology and methods allows taking the right choices for investment in future instrument upgrades. Through concerted action in the area of instrument construction, the financial burden of such necessary development is shared by the partners, thus enhancing European competitiveness in this sector.

Transnational access funded by NMI3 was only provided within the first 24 months, but continues to enhance the user base through better service provided. Attracting new users by encouraging mobility.
enhance the user base through better service provided. Attracting new users by encouraging mobility makes new demands for better performance at the facilities. This can be achieved by specialisation, i.e. by building on each facility’s strength but also by providing better service. Access thus has a real structuring power on the landscape of facilities and user base. Compared to national funds allocated to development of neutron scattering and muon spectroscopy, and especially in the context of the future multinational facility ESS, NMI3 is a small player in terms of funding, but a strong catalyser. In the area of collaborative R&D, NMI3 covers certain aspects of methodological and technical development like neutron optics, deuteration, sample environments, polarized neutrons, muons and detectors. The scientific and technical developments find their application in updates of existing instruments or influence the design of future generations of instruments’ to be built at ESS and elsewhere. The high demands from the user community can only be satisfied in the long run by continuous development on the instruments side as well as on the sample environment side. Technical developments challenge our business partners in the same way the facilities are continuously challenged by the changing expectations of their user community.

The commercial market for neutron scattering instrumentation and components is very limited. Effort therefore has to be made to find companies willing to develop products, and to provide them with a stable market; excessive IPR protection can actually lead to some developments never reaching the real application stage. The main principle within NMI3 is therefore rapid publication of results in the open literature to ensure that they can be of as widespread benefit to as many facilities as possible. The same principle will apply to collaborations between NMI3 and non-European countries, and is a condition of those countries participating in technical JRA meetings. The significant investments in neutron scattering and related developments currently being made in the USA and Japan mean that NMI3 partners have more to gain by collaborating than competing with these countries. Only in those rare cases where a development may find a broader commercial application beyond neutron scattering, will the management of IPR need to be more protective.

All software development is open source.

Neutron optics:

The work conducted within the WP17 Neutron Optics JRA will have immediate and long term impacts. Immediate impacts which have already been made available as routine options for regular users are the following:

• upgrade of the TOF-TOF instrument at FRM2: gain of a factor 2-3 at the sample position by using an adaptive-optics, 2D, focusing device.
• upgrade of the CONRAD imaging station at HZB providing a much more intense and homogeneous flux
• Lens option on KWS1 at JCNS allowing measurements down to 10^-4 A°^-1 on a regular SANS machine. This is a 10-fold improvement over existing machines and bridges the gap with existing USANS machines
• Multichannel elliptical focusing optics is now proposed on a commercial basis (by Swiss Neutronics for example)

The McSTAS Monte-Carlo simulation code has been upgraded to better match user needs. This will have long term benefits for the modeling of instruments which are becoming more and more complex. McSTAS 2.0 was released a few months ago.

The work has also triggered large scale projects which are funded and are presently being built.

• New focusing, small angle instrument at BNC which will benefit from advanced reflective 2D focusing optics
• Triple-axis instrument using an multiple crystal energy analysis principle at PSI
• The BOA beamline has been built and made available for friendly users to test advanced optical concepts.

Some concepts which have been demonstrated within the JRA have led to proposals for new innovative instruments:
• Energy analysis using prisms in reflectometry is being considered within the next ILL upgrade program as an option for a new instrument
• A time-of-flight instrument using multiple crystal analyzer has been designed and modeled using Monte-Carlo simulations. It is proposed for the new ESS neutron source (CAMEA project)
• The SELENE concept has triggered 2 workpackages for new types of reflectometers at the ESS
• The investigation of various new concepts for neutron imaging have triggered a project for very high resolution imaging (within FP7). New imaging facilities are likely to be built using these principles.

As a conclusion, the project has triggered research and ideas which have already been made available to users. Some technical solutions have already been transferred to private companies which will make these advances available to most neutron facilities.

The network has also made it possible to propose ambitious new projects by allowing the demonstration of several innovative concepts.

Deuteration:
The tasks carried out as part of this JRA have provided new capabilities in the area of biological neutron scattering and this is having a significant impact in widening capabilities throughout this part of the user community. This can be seen (i) from the fact that a number of them have already found their way into the user programmes of user facilities throughout Europe. For example, the use of yeast-based systems (Pichia pastoris) and biomass systems has, during the period of this JRA, become widely used at the Deuteration Laboratory within ILL’s Life Science group, and has resulted in the supply of deuterated proteins to several users of ISIS, ILL, FRM-II (ii) the publications that have exploited the new methods (iii) the dissemination at workshops and international conferences throughout the world.

Polarized Neutrons:
Polarized neutrons that can be considered as elementary magnets that change their direction when interacting with a magnetic field in the sample, allow the magnetic field distributions on atomic and nanoscale to be determined. This information is vitally important for the understanding of complex electronic properties of nanomaterials that are the basis of the next generation of electronic and computing devices, including spintronics, providing a still higher density of recorded information. On the other hand, polarized neutrons are used for the development of high time and angular resolution neutron scattering techniques, facilitating new studies of dynamics of polymers and proteins that constitute the basis of living organisms and augmenting the knowledge base for a new generation of medicines and methods of their delivery to damaged biological cells.

Muons
Impact at the facilities: For the two European muon sources, the work of this JRA has made a significant impact on the instrument suite available to their communities. Recently, both facilities received grants to develop high field instruments, and work during both FP6 and the present JRA has underpinned these...
Develop high field instruments, and work during both FP6 and the present JRA has underpinned these projects through the development of the technologies essential for high field µSR. Of particular importance is the development of G-APD fast timing detectors that are insensitive to magnetic fields – excellent performance has been obtained and nothing similar is currently available worldwide. The instrument simulation codes are unique and proved essential for modelling the high field instruments prior to construction. Their use has enabled the facilities to reduce the instrument build and commissioning time, and to improve the performance of the complete spectrometer. The development of the NeXus data format provides a basis for storing muon data with comprehensive metadata to properly describe the experiment, a facility that will become increasingly important with the move to open access journals and data repositories. JRA funds enabled the muon community to play a full part in the NeXus International Advisory Committee, steering the development of this data format in collaboration with the neutron and X-ray communities. The agreement on a common muon exchange format should be beneficial to users as they move between facilities, and make it easier for the facilities and user groups to share software development effort. The JRA has given a focus to these activities, providing resources to work collaboratively to develop high quality long term solutions.

Impact on the scientific community: Work within this JRA has led to the development of novel sample environment equipment, new experimental techniques and software capable of bringing a new insight to data analysis. University user groups have been involved in each of these developments, and have exploited the technical innovation to benefit their own research, evidenced by publications in peer reviewed journals. Thus, the JRA has provided new equipment and methods, and then advertised the potential offered by these new techniques to the wider scientific community. The software codes developed during the JRA have made a significant impact worldwide. This is particularly true for the techniques developed for determining the muon site. Well received at the MuSR 2011 conference, this work has stimulated the application of DFT methods both for muon site determination and the calculation of radical state hyperfine parameters, and has stimulated the worldwide muon community to collaborate to develop this area of research through a series of discussion meetings. The impact of the JRA also extends beyond the muon community. For example, resonance measurements in the gas phase and the study of spin evolution during RF excitation are both applications that are difficult or impossible to realise using established magnetic resonance techniques, and the muon results obtained have been received with interest by that community.

Sample Environment Science
The greatest impact this sample environment JRA will have is on science – moving boundaries and extending experimental ranges. High pressure research is one of the fastest growing areas of natural science, and one that attracts such diverse communities as those of physics, bio-physics, chemistry, materials science and earth sciences. For example, the advances in high pressure equipment will enable further exploration in the areas of condensed matter physics, planetary and geo-science - studies of high pressure gases which mimic conditions on other planets or inside our own - and high pressure hydrogen research, which may yet provide the answer to global energy problems. The development of two types of levitation furnace will allow studies of high temperature melts across a broad range of both conducting and non-conducting materials not possible before. Studies of the molten state are not only of interest for fundamental research, but are also very important for technology. It is an essential stage in various industrial processes such as glass-making, semiconductor technology and iron and steel production.
The suite of new gas adsorption equipment will contribute significantly to many areas of science including the development, characterisation and improvement of proton conducting materials, gas sensors, nanostructured porous materials and catalytic converters. This will aid research into improved drug delivery, hydrogen storage solutions and catalysts used to speed up industrial and chemical processes.

**Education**

The JRA funding has allowed a number of students at under- and post-graduate level to participate in practical research work. It has aided the re-distribution of skills and knowledge amongst the participating technical teams. Overall, it has contributed to the significant role that the neutron facilities already play in higher education by providing improved tools for researchers.

**Industry**

The availability of high pressure, hydrogen-certified parts is now much improved thanks to the broader market opened up by the JRA. Through the continued requests of the JRA partners, European suppliers of high pressure equipment (including Harwood, Nova Swiss and Sitec) recognised the need for the development of products like valves, fittings and transducers guaranteed for work at high hydrogen pressures.

In addition, companies such as Oxford Instruments, Hiden Isochema and Pfeiffer Vacuum are now more aware of the common needs of the sample environment community, leading to mutually beneficial developments and a consensus on standards.

**Collaboration**

The JRA project has led to radical changes to the relationship between the sample environment teams. Before the project communication was sporadic, with few joint activities. Now, a well-defined international sample environment community exists.

The European partners have led the way with the formation of a global society, the SE@NSF. There is now a forum for sample environment discussion shared by almost 40 collaborators worldwide, including those at facilities in Japan, USA and Australia. Information-gathering visits with specific aims have already taken place between facilities.

Leaders of the neutron institutes recognise that collaboration by technical teams, such as sample environment, should be supported as it makes for a highly effective use of resources and promotes elevated standards across the neutron facilities.

**Detectors:**

Within the framework of this Work package, the potential of a rather new technology for neutron detection has been intensively explored, stimulated by the results achieved during the MILAND programme in FP6. A lively and very effective collaboration has been formed and now shares a lot of expertise on Gaseous Scintillation Proportional Counters (GSPCs) between the partners, bringing together different technologies available in the individual groups. This collaboration is reflected in the various joint training schools and experiments that have been performed together with participants from all partners.

With the MC-simulation package ANTs, which is made freely available to interested groups, a very powerful training toolkit has been developed which already found interest and application in other fields than neutron detection, e.g. dark matter search or medical application. Apart from ANTs, all important knowledge on the performance of GSPCs that has been gathered during the project was made available...
Knowledge on the performance of GSPCs that has been gathered during the project was made available to the scientific community in six publications.

List of Websites:
nmi3.eu

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