ESS Instrument Construction Proposal
High Resolution Neutron Spin Echo
ESSENSE

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This work is the result of work unit SD002DE.

ENCLOSURES

• Configuration and operation mode for very short Fourier-times
• Compatibility with extra π/2 flippers
• Prolongation effect on currents
• XYZ polarization analysis
• Magnetic shielding: Compatibility and effects
• Comparison between superconducting and water-cooled copper main solenoids
• Other instruments
• Costing (supplement)
• Pulse shaping chopper

LETTERS OF INTEREST

REPORT FROM THE NSE-WORKSHOP
EXECUTIVE SUMMARY

ESSENSE is an ultrahigh-resolution, high intensity neutron spin-echo spectrometer (UNSE) with a gain factor of 30 compared to the best present instrument. NSE is unique in enabling the observation of slow dynamical processes from pico-seconds to micro-seconds extending the spectroscopic range 3 orders of magnitude beyond the backscattering limits. ESSENSE will be essential to round off the spectrometer suite of ESS to be ready for the contribution of neutron-scattering to the grand challenges for science and society, ranging from safe energy supply in the future, novel information “green” and quantum technologies, new functional materials, molecular understanding of life, transfer of functional principles of nature to rational design of materials and pharmaceutics. Solving these grand challenges needs to address the complexity of the required novel materials as well as that of living matter. For many of these topics neutron techniques are unique in determining the dynamic processes. However, since in general the involved entities are large, such motions are very slow, at the very limit, of what can be resolved by the most advanced neutron methods, namely ultrahigh resolution neutron spin echo spectroscopy. UNSE is an essential tool to detect and quantify molecular, atomic mobility and spin dynamics. For example mechanical flexibility as, described in terms of hinge bending, sliding or torsion in protein molecules is not seen in mere structure descriptions, but is important for interplay with cofactors, substrates or drugs. Response to stimuli depends on molecular motion in functional “intelligent” materials, as does the mechano/rheological response of polymeric materials, composites and complex fluids. It becomes increasingly clear that mobility, selective compliance and fluctuations are essential for function. Combining UNSE with molecular dynamics (MD) will form a powerful implement to obtain detailed and verified insights into the micromechanics and molecule docking environments in proteins, mechanism in functional materials or slow diffusion processes. With its gain factor of 30 and employing new developments to drastically enhance the evanescent neutron field that probes a macroscopic surface layer, ESSENSE also has the potential to provide dynamical views on flow boundary layers, lubrication and tribology. ESSENSE will play a prominent role in the understanding of biomolecule flexibility and its role in drug design and intelligent material response and flow and lubrication. Beyond that it has the potential to yield important contribution to a plethora of other problems ranging from dynamic processes in ionic liquids, novel polymers and composites to diffusion in fuel cell and battery electrolytes. Further, slow paramagnetic fluctuations, as present in systems ranging from nanoparticles for medical diagnosis and treatment to quantum phenomena in frustrated spin systems and molecular magnets, can be observed with full resolution. The intensity limitation restricting resolution and extent of observations of magnetic scattering will be releaved, such that new realms become accessible.

ESSENSE is based on a highly optimized configuration of the well-established generic high-
resolution spin-echo configuration and uses proven and effective technical realisation concepts for each of it’s components. The key innovation element of the secondary spectrometer is the new design of the precession coils. The coil configuration has been optimized to have the lowest feasible field-integral inhomogeneity; this measure yields factor 2.5 improvement in resolution. ESSENSE uses the full source pulse over a wavelength frame of 8 Å width and a frame start that can be set to any wavelength between 3 Å and 20 Å using the flexible frame overlap chopper system. The neutron guide system contains a polarizing kink and a curved guide section to avoid the direct line of sight twice. In the vertical direction slight elliptical focussing enables the realisation of a 1.5 fold intensity increase from the cold "pancake" moderator compared to the TDR reference moderator. Variable slits will allow to cope with different sample shapes and reflectometry type operation modes and other divergence adjustments, whenever needed. The intensity gain factor of the instrument will be 30 compared to today’s most intense instrument IN15. The improvement of 2.5 in resolution will allow to extend the useful Fourier-time range from 1ps to 1000ns. Pushing the resolution enhances the performance of ESSENSE over the larger part of Fourier-times since thereby any given time can be measured with a lower wavelength than before, i.e. with much higher intensity –a gain on top of the aforementioned factor 30–. This feature e.g. is particular important for the biodynamical application. There highest intensity and accuracy at intermediate times is vital. Further ESSENSE will open new unprecedented realms of sample conditions; e.g. it will be possible to cope with the intensity loss imposed by high-pressure cells with small area windows or with other sample volume restrictions by specialized sample environments. Resonator-enhanced evanescent wave scattering by surface layers will benefit from the intensity gain such that novel and unprecedented comprehensive views on local, molecular interface dynamics can be obtained; the macroscopically accessible interfaces may be subjected to external fields. The orders of magnitude leap in intensity and the comprehensive coverage of the time domain enable new systematic studies of effects of structure- and parameter-variation that will result in a game-changing boost of emerging information and synergy with MD computations. The significantly reduced data collection times enable the completion of experiments on more delicate (bio)-molecules before degradation sets in. Even kinetic experiments on the minutes to hour time-scale of the stimulus triggered response of complex living matter, new functional materials or chemical reactions in polymers will become possible. The amount and quality of information obtained by any spin-echo experiment always depends heavily on intensity, restricting the amount of always needed parameter variation and entangling it with the size of statistical errors in $S(Q, t)$. Accuracy is a key for the discrimination and identification of specific dynamical processes in $S(Q, t)$. The practical limit for the maximum Fourier time depends on instrument resolution and intensity. Pushing both: intensity and resolution to their ultimate limits is the signature of ESSENSE to achieve a new game-changing rate of information output.
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1 INSTRUMENT PROPOSAL

1.1 Scientific Case

The High Resolution Challenge.

Within a worldwide consensus the following themes are considered as grand challenges:

- The energy supply in the future in connection with the resulting hazards for the environment.
- The development of information technology from green IT towards novel quantum technologies.
- The development of functional materials and novel technologies.
- The search for a molecular understanding of disease towards the physics of life.
- The transfer of functional principles of nature to the world of materials and pharmaceuticals.

Solving these grand challenges needs to address the complexity of the required novel materials as well as that of living matter. Novel materials are often nano-structured with functions distributed over hierarchical levels. In the realm of "nano-structured materials", fluctuations are decisive for the evolving materials properties. Furthermore, transport properties are of great importance for devising novel energy materials such as advanced fuel cells or batteries.

Concerning biological molecules the dynamic dimension of function is becoming evident with consequences also for pharmaceutical approaches. In biomedicine research on the molecular causes for disease will need to consider the dynamic dimension.

For many of these challenges neutron techniques are unique in determining the dynamic processes. However, since in general the involved entities are large, such motions are very slow, at the very limit of what can be resolved by the most advanced neutron methods, namely ultrahigh resolution neutron spin-echo spectroscopy (UNSE).

Such experimental investigations are paralleled by the advancement in atomistic molecular dynamics simulations that approach similar space-time regimes [1, 2]. The frontier of materials exploration –as well as of bio-dynamics both with simulations and with neutrons is in the ultrahigh resolution regime where the fluctuations of complex matter take place [3, 4].
Life Science, dynamics pf proteins and drug design

Neutron scattering, in particular SANS and high resolution NSE providing the information on molecular motions and flexibility will contribute to our knowledge about the delivery and function of drugs and anesthetics, understanding the molecular aspects of diseases such as neurodegenerative Huntington’s and Alzheimer’s, viral and bacterial infection, and toxin decontamination. The transport of products and enzymes of the molecular factories inside the crowded cytosol of a cell depends on the mutual interactions and interdiffusion of many components. In biotechnology and biomaterials, neutron scattering in general and high resolution NSE in particular, providing substantial input to model the molecular mechanics of proteins, enzymes and aggregates, will contribute to the rational design of new drugs, industrial enzymes and new bio-inspired materials and sensors.

Understanding molecular micromechanics and dynamics in proteins is essential to enable rational computer aided drug design [5, 6, 7, 8]. Whereas, until recently, most of molecular biology was discussed in terms of structure, and particularly structures were derived using X-ray crystallography, there is now near universal recognition that the next major advances in molecular biology will arise from understanding disorder and correlated dynamics. The characterization of intrinsically disordered proteins and the relative motions of domains with flexible linkers have been identified as of critical importance in several biological and biomedical fields. The time- scales and length-scales relevant to biological function are those probed by ESSENSE. Whereas in the 1990s drugs, such as Tamiflu and HIV protease inhibitors, were designed using static crystallographic structures and the lock-and-key principle, within the last 10 years the state-of-the-art has come to involve ‘ensemble docking’, meaning that metastable protein states identified in molecular dynamics (MD) simulation are individually targeted. This dynamic view led to Merck’s last blockbuster, raltegravir, and has now become a standard approach in the USA. Drugs designed to be allosteric inhibitors for G protein-coupled receptors (GPCRs) function in a similar way. Critical to the furtherance of ensemble docking will be a detailed characterization of the motions between the metastable states targeted. No experimental technique other than NSE can directly measure these correlated motions; X-rays cannot, NMR cannot, and single-molecule spectroscopies cannot. In opening this window ESSENSE will be THE tool for calibration, tuning and verification of state-of-the art MD-methods in general and in particular for computer aided drug design.

The high neutron flux of the new ultra-high resolution NSE spectrometer will allow experiments requiring significantly less total counting time and less amount of proteins. Thus the instrument will enable systematic investigations, which add an entirely new quality to the approach to the functional dynamics of enzymes. E.g. the effect of point mutations and drugs on the functional domain motions of enzymes.
may be investigated systematically [9, 10]. During functional domain motions in enzymes, specific amino acids are brought into close contact [11]. In that way the chemical reaction is enabled, which determines the biological function of the enzyme. The importance of specific amino acids for the chemical reaction mechanism can be evaluated by measuring different point mutations. Finally the effect of pharmaceuticals and drugs on the function related motions of medically relevant proteins can be tested even if only a small amount of mutated protein or drug is available for the experiments.

**Interface and surface dynamics, tribology and lubrication**

Mesoscopically structured system, in particular of the hard/soft type, depend on the influence of the interface. Modifications of conformation and dynamics of the polymeric or fluid components at close contact are decisive. They are present in embedded nano-particle systems like filled rubbers or encapsulated metal hydride, polymers in nano-pores as e.g. templates for polymeric nano-“wires” or on all kinds of polymeric coatings from displays to photovoltaic cells. Complex fluids in close contact to solid surfaces also determine flow properties in porous systems, e.g. oil recovery or lubrication.

Wear and friction are ubiquitous in machines and vehicles, where they cause huge economical losses. Friction and drag are responsible for about 1/3 of the total energy needed to run machines. Proper lubrication is essential and must work over large ranges of temperatures, pressures or chemical environments. In biological systems like joints with glycoproteins controlling the friction between cartilages, loss of effectiveness can be painful. Understanding the role of solid-surface fluid boundaries on molecular scale is essential to optimize or develop new lubrication systems. Information on the mobility and response of the lubricant molecules close to the surface is vital for understanding the force transmission into the liquid or in the regime of boundary lubrication. Dynamics of such boundary layers are accessible by neutron spectroscopy, not only in nanoporous systems, but also at smooth extended flat surfaces due the newly developed grazing incidence NSE technique, which will further gain by a resonator sublayer. Recently it could be demonstrated that in grazing incidence geometry with total reflection of the incident beam a NSE signal could be measured that carries the fluctuation of a surface layer [12, 13]. Scattering origins from the evanescent neutron wave function extending a few 100 nm into the liquid phase side. With resonator enhancement by more than an order of magnitude and general ESSENSE related gain factors (30 ) the latter method will allow systematic and routine surface dynamics investigations. Flat surfaces will also allow to apply external fields (flow, pressure, electrical...) to the boundary layer. Tribology is one example of a huge field which relies strongly on the understanding of surface dynamics, and which could be transformed by joint application ESSENSE and thereby boosted molecular dynamics simulations.
Functional and responsive matter: Self healing, control of transport

Novel materials tailored for specific functions require the combination of different properties from various building blocks. Supramolecular structuring is an essential element for advanced function. Self-healing materials are an emerging class of functional materials with strong potential in technological applications. The healing functionality of such materials enables the recovery of fracture and of barrier properties or improves corrosion resistance under harsh conditions, e.g., in surface materials or in coatings. Robust functional materials with high resilience and the ability to cope with local damage by reversible physical association, chemical crosslinking or a combination of both are of increasing interest. Self-healing elastomers are the ideal candidates for robust and long lasting dynamic sealings or vibration damping with huge possible economic impact due to mainly longevity, costs-saving seals for vehicles, heavy-duty seals for wind turbines, vibration abatement systems for roads and bridges, noise abatement systems or even asphalt mixtures. The candidate materials with the desired properties essentially consist of dense polymeric networks with flexible linkages that rely on various association mechanisms like reversible H-bonds, reversible polymerization or chain (re)-entanglement. The recovery process is highly dependent on the mobility and diffusion of the polymer chains inside the material. Timescales in these melt, gel or rubber like polymeric systems extend from ns to s. High resolution NSE will enable to explore the essential linker mobility and association. ESS-SENSE is an ideal tool to investigate the relevant molecular mobilities and diffusion properties that are prerequisites for the healing mechanisms.

Further functionality can be achieved by controlling material properties by external parameters (temperature, pH, light, ...). [14, 15]. As building blocks, tethers, filling and functional parts of the emerging –synthetic as well as natural– complex materials, macromolecules play an overwhelming role. Association with other nano-particles, structured templates or aggregates formed with equal or different molecules may be routes to function. This comprises self-healing, adaption to external stimuli or tuning properties by combining functions from different building blocks to form a new smart and specific system property [16, 17, 18, 14]. Most of these materials may be categorized as soft matter, where the overall challenge is to understand the competing effects of physical interactions and the role of entropic contributions that determine the behavior of large assemblies, based on the known properties of the individual building blocks as well in the bulk material as under low-dimensional confinement or in self-organized phases of complex fluids and in composites. [19, 20, 21].

Further hot topics

Energy storage: Polymeric electrolytes, fuel cells and hydrogen storage

Understanding the interplay of ion conduction and polymer mobility and the effects of mesostruc-
tures is vital for the development of new generations of battery and fuel cells. E.g. introducing nanostructures into the electrodes or separating electrolyte membranes can improve the performance of batteries. New synthetic systems with nano- or mesoscaled structures enable new high-performance materials, e.g. particle loaded polymer electrolytes and electrode membranes for batteries [22, 23, 24, 25]. Novel ionic liquids are new candidates for composite electrolytes [26]. Transport and interaction with polymeric or gel type membranes containing higher viscosity fluids urgently will need the ultimate dynamical resolution in neutron scattering experiments.

Complex fluids: emulsions, microemulsions and more

Complex fluids that contain a number of molecular and macromolecular mesoscopic components with specific and peculiar macroscopic properties are abundant in living matter as well as in technical fluids. Emulsions and microemulsions are numerous in food, medical formulations, cosmetics, paints, cleaning fluids and formulations for chemical synthesis. The physical state, entropy, mobility of the emerging aggregates and incorporated polymeric or nano-mesoparticles can be inferred from fluctuations in the ns-μs window [27, 28]. Production of functional coatings with protecting, biocompatible or specific selectivity depends on the interaction of complex fluids with interfaces as accessible with the GINSE-resonator on ESSENSE. Understanding the key physical factors in these systems will help to optimize the efficiency of bio/med-technological as well as technical fluids.

Dynamics of membrane proteins

Up to one third of all proteins with important functions as receptors, transporters or enzymes are embedded in biological membranes. Membrane proteins can be solubilized for neutron scattering experiments by detergent molecules or by the use of recently developed "nano-discs", which mimic cell membranes [29, 30, 31]. Applying high intensity, high resolution NSE on membrane proteins in "nano-discs" will allow to explore their molecular mechanics and functional dynamics.

Motions in protein complexes and large macromolecular machines

Protein complexes with each other and different binding partners such as DNA and RNA form a cornerstone in many biological processes and operate as large molecular machines [32]. Cells are using very large macromolecular assemblies for different biological functions such as the ribosome for protein synthesis or the bacterial flagellum for cell propulsion. Due to their large size the function of large macromolecular assemblies is determined by very slow dynamics. Thus dynamics in macromolecular complexes calls for the ultimate NSE resolution.
Biosynthetic hybrids

Recently solvent free protein liquids were described that consist of aggregates of polymeric surfactants and surface modified globular proteins [33]. They form water free liquids at ambient temperature with enzymatic activity. Understanding interplay of protein and polymeric mobility in these systems will lead to new insights into the prerequisites of enzymatic function.
Magnetic fluctuations

Up to now about 2% of the spin-echo works pertain magnetic fluctuations. One main reason is the typically low intensity of magnetic scattering [34]. ESSENSE in paramagnetic mode will provide new opportunities in terms of possible systems and resolution due to its large intensity gain factor of 30. The natural energy scale in spin systems is the exchange coupling with typical values in the meV regime. However, cooperativity slows this down by several orders of magnitude [35]. Materials with frustrated spin interactions may have highly degenerate ground states, which provide room for fluctuations and that lead to a variety of phenomena [36, 37] as the formation of "spin ice" with magnetic monopole type excitations or e.g. "spin-liquids". Some of these systems stay highly dynamic down to mK temperatures [38]. On the other hand frustration leads to spin-glass type relaxation characteristics [39, 40], which upon approach of the glass transition become arbitrarily slow (the characteristics of any glass). New types of spin-glasses [41] are investigated with possible relevance for future spintronics applications in mind. Also in "spin-ice"-type structures sub-ns to ns dynamics at temperatures in the 100 K region slow down to relaxation times beyond 10’s of ns at temperatures of a few K or below, where new interactions, possibly with nuclear spins, enter the stage, see e.g. [42, 43]. The observation limit of only a few ns of current investigations is dominated by the need to use short wavelength to overcome the severe intensity limits. ESSENSE will extend this regime considerably due to its combination of resolution parameters and in particular its huge intensity gain. Very novel 2D magnetic materials with promises for new magnetoelectronic/spintronic devices emerge from associating magnetic ions with graphene [44], with yet unexplored microscopic spin dynamics. Organic ligands allow the preparation of low dimensional spin systems like 1D chains as e.g. the Haldane antiferromagnet NDMAP: Ni(C₅N₂H₁₄)₂N₃(PF₆) or even isolated (0D) molecular magnets like e.g. the Single Molecule Magnets (SMM) with giant spins (S=83/2), [45, 46]. SMMs exhibit a rich dynamical behaviour with relaxations from picoseconds up to milliseconds [47], only NSE covers a large part of this time domain. Among future applications of such high nuclearity clusters are magnetic cooling and quantum information processing. Molecular spin-crossover materials, in which the transition of a low-spin state to a high-spin state of a magnetic ion is connected to vibrational/mechanical degrees of freedom of the molecules, offer new perspectives [48]. Further the properties of surface absorbed molecular magnets gain interest; here ESSENSE in combination with the resonator enhanced grazing incidence technique will enable an unprecedented view on the dynamics.

The dynamics of systems of magnetic nanoparticles exhibit slow paramagnetic fluctuations as was impressively demonstrated in a NSE investigation by Casalta et al. [49]. Superparamagnetic particles in combination possibly with organic surface modification and in fluids find rising interest for technical and biomedical applications [50, 51]. In ferrofluids [52] and suspensions for medical use magnetic nanoparticles serve as drug carriers or energy absorbers for local

11 (88)
hyperthermic treatments. A part of the dynamics pertains to magnetic domain fluctuation and a part to orientation relaxation in the embedding medium, e.g. the cytosol of a cell. The effect of the medium on the particle relaxation will provide important input on the role of anisotropy and surface properties on the dissipation and transport mechanisms of such particles.

In general NSE has the advantage –compared to backscattering or TOF spectroscopy– that the associated paramagnetic scattering signal is unique, because in the proper NSE operation mode without \( \pi \)-flipper only paramagnetic scattering will give rise to an echo signal. This gives a clear distinction from nuclear scattering intensity contributions. ESSENSE will enable to analyze paramagnetic scattering from any of the above and other systems without restrictions. By combining ESSENSE’s advances in resolution and intensity gain a significant extension in coverage in \((Q,t,T)\) and range of possible samples will be achieved.
Relevant time and length scales

The length scale of natural, emergent or engineered structures in functional complex materials extend from single molecule size 0.5-1 nm over typical macromolecular or protein dimension (5-20 nm) to the larger extensions of association complexes, engineered templates, higher hierarchy levels in bio-materials and living matter. In the realm of neutron scattering the accessible structure range is that of SANS (small angle neutron scattering). The time scale, where displacements due to molecular motions become visible, depends on the spatial resolution (i.e. the neutron momentum transfer, $\hbar Q$) and the size dependent diffusivity of the observed structures. Further, the time-scale scales with the local viscosity. Thus even at a length scale of only a few nm typical relaxation times of many 100 ns and more are observed. Ideally relaxations should be followed towards the end in order to e.g. distinguish them from possible static correlations (i.e. 3-4 times the relaxation time would be required). This would also allow to precisely decomposing the contributions to more complex relaxation processes. Even with many 100 ns time range, for most soft matter systems, this ultimate goal is difficult to reach if the length scales ($\pi/Q$) exceed about 3 nm. Systems with activated diffusion (e.g. slid electrolytes) or systems approaching a glass transition –ranging from glass forming polymers to frustrated spin systems– are prone to become arbitrarily slow upon cooling. Thus it is of paramount importance to extend the Fourier-time (resolution) of neutron spectroscopy to the ultimate technical limit. This is essential to address the important length scales of nano- and mesoscopic structures and close the gap to dynamic light scattering as much as possible. The only known and proven neutron spectroscopy technique, which has the potential that allows efficient measurements beyond a few 10 ns is the generic IN11 type high-resolution spin-echo configuration. ESSENSE is a fully optimized instrument of this class pushing the possible resolution to its limit beyond the 1000 ns margin.
Required Instrument Parameters

The most prominent parameter used to describe a high resolution NSE spectrometer is the maximum Fourier-time, $\tau_{\text{max}}$, it may reach. In that sense we might characterize ESSENSE as a $\tau_{\text{max}}>1\,\mu s$ instrument. However, such a characterisation is imprecise and not well suited to assess the virtues of an NSE instrument for a specific scientific problem. The relevant parameters are rather:

- $J_{\text{max}}$, the maximum field integral.
- $H$, the resolution determining homogeneity parameter. ESSENSE pushes this value to the ultimate technological limit.
- $\Delta\Omega_{\text{in}}$, the illumination solid angle (divergence).
- $\Delta\Omega_{\text{det}}$, the detection solid angle.

The maximum useful Fourier time depends on the neutron wavelength and is

$$\tau_{\text{max}} = \min(0.18J\lambda^3, H\lambda^2)$$

provided the flux at the minimum required wavelength is large enough to yield a sufficient detector count rate. For a 3% statistical error of one $S(Q,t)$ value as derived from any selected detector area and wavelength band a total number of about 25000 counts is needed. As for any neutron instrument maximizing the flux up to the limits imposed by resolution in $Q$, and $\omega$ or $\tau$ is a priority issue.

The requirements for the large scale dynamics of proteins are inferred from the following consideration. The internal dynamics is observed as excess relaxation on top of the translation and rotation diffusion of the whole molecule. The major contribution is the translation diffusion (typical values $D_{\text{com}} = 1\cdots 10\,\text{Å}^2/\text{ns}$). Large fluctuation of protein domains contribute around 10% to the fluctuation signal intensity with relaxation times of similar order as those of the diffusion processes. At a typical observation wavevector $Q \simeq 0.1\,\text{Å}^{-1}$ the centre-of-mass diffusion related effective relaxation time is between 10 and 100 ns. The relevant internal dynamics signal is seen as slight modification of this relaxation. Therefore these investigations are to be dealt without aiming to the very high Fourier-times, however, they require that $H$ is pushed to the limit and $J$ can reach large enough value to cover the 1 to 100 ns regime with the shortest possible wavelength. This is essential because of the steep flux increase with decreasing wavelength, $\Phi(\lambda) \propto \lambda^{-5}$ in the large $\lambda$ limit. E.g. with the ESSENSE value of $H=2.5\,\text{ns/Å}^2$ a Fouriertime of 100 ns can be reached with $\lambda = 6.5\,\text{Å}$ and $J=2\,\text{Tm}$. The extra effective intensity gain due to the high resolution type extension of $H$ and $J$ to the limits is
nearly one order of magnitude. In combination with the general 30 fold intensity of ESSENSE this will enable such type of experiments

- with much shorter counting times, extending the possible number of system towards those that are more sensitive to degradation
- with less concentration, allowing to include systems that tend to aggregate
- with less amount of sample, extending the possible number of systems towards those that are scarce
- using a large number of variants or mutations in order to perform systematic studies

Interaction of (polymer)molecules with surfaces in nanoporous or nanoparticle systems show modified dynamics of the polymers, which contain the information. Thus the basic time scale of observation is similar to that known from bulk polymers. In addition immobilisation and retardation due to the surface and topological interactions will occur. Depending on momentum transfer in the typical SANS domain \( (Q=0.01\cdots0.3 \, \text{Å}^{-1}) \) characteristic times ranging from many thousands of ns at low Q to several ns at the large Q side are anticipated. In particular in the more complex composite systems elastic scattering from the scaffold or other static components will occur. A safe decomposition is only possible if the fast component can be followed towards complete relaxation. The same holds in the case of self-healing, responsive respectively "functional" systems, the often nanosized/macromolecular structures that effect the functions have sizes of a few nm and contribute to \( S(Q) \) mainly at the low Q side, where again the above mentioned timescale of up to many thousand ns holds. Even with the high resolution capability of ESSENSE, which is limited by current technology, this will only partly be possible.

At intermediate \( Q \) the relaxation time goes down and so does the coherent (SANS) intensity. Here the intensity advantage due to the extra ability (due to maximized homogeneity, \( H \), and field integral \( J \) values) to use a smaller wavelength, i.e. higher neutron flux, enhances the efficiency of the instrument to the point where a new quality in terms of systematic studies on parameter variations becomes a realistic experiment mode.

Analysis of slow diffusion, e.g. by proton jumps in solid electrolytes or similar, requires observation at large \( Q \) (of the order of 1/jump length), which again issues the need for high resolution at a low wavelength. i.e. \( Q = 2 \, \text{Å}^{-1} \) needs less than about 5Å, where the ESSENSE parameters would allow to reach times up to 45 ns. A WANSE (WASP type) would there be limited to \( 2\cdots3 \, \text{ns} \).

\[1\]With a diffusion constant of \( 1 \, \text{Å}^2/\text{ns} \) the relaxation time of \( S(Q,t) \) at \( Q =0.01 \, \text{Å}^{-1} \) is 10000 ns.
The dynamics of complex fluids and adsorbed soft layers close to a macroscopic interface as available in the Grazing Incidence NSE is mainly intensity limited. It will need – as the protein dynamics – the combination of high Fourier integral with the high intensity available at shorter wavelength. Variable slits will allow to establish the necessary reflectometer type illumination of the GINSE sample cell. A neutron prism is used to keep the surface perpendicular component $Q_z$ virtually constant over the wavelength frame.

Systems with paramagnetic scattering at NSE generally benefit from the fact that in paramagnetic mode ($\pi$-flipper off) the NSE echo signal is purely due to paramagnetic scattering, a clear distinction to nuclear density fluctuations is automatically obtained. The unprecedented high intensity of ESSENSE is the ultimate prerequisite to extend observations of the intrinsically weak magnetic fluctuation scattering to times beyond the currently achieved few ns. Freezing of spin-glass phases or frustrated spin systems (kagome, spin-ice, ...) at lowest temperatures may become arbitrarily slow, however, the basic time scale of frustrated spin systems is given by the exchange coupling $J_{i,j}$ which typically is in the meV range, a 1000 fold slowing yields a ns-timescale. Again, intensity and Q-range require use of short wavelength. Super-paramagnetic fluctuation in nanocomposites with magnetic particles or ferrofluids mingle with soft matter dynamics that controls the rotation diffusion with the fluctuations of magnetic domains. Without compromising any of the resolution properties ESSENSE will immediately allow paramagnetic mode operation over the full range. Normal (nuclear) spin-echo can be collected in the same run.
Synergy: Ultra high-resolution NSE and MD simulations

The ESSENSE development also matches with the advances in the ability to perform molecular dynamic calculations on larger more complex objects (e.g. polymers with architecture beyond linear chains, molecular aggregates, interaction with confining nanostructures, bio-molecular aggregates, protein complexes, ...) over increasingly longer times. For most of those systems simulations are challenging because very large unit cells, containing many ten thousands or more atoms, are required in order to tackle the essence of the problem under question. But the ongoing development of computing capabilities promises that we will soon be able to use the required atomistic models in simulations that extend over many hundreds, approaching thousands, of ns in a more routine way. Currently atomistic computations start to match with the times reached by high-resolution NSE and detailed comparisons will be possible. So a synergetic neutron-MD methodology can be applied to the wide range of intriguing systems considered in the whole soft matter field [1]. The interplay between neutron experiments and realistic simulation may be used to adjust model parameters and simulation procedures [3]. Thereby high resolution NSE will become the decisive tool to verify and calibrate state-of-the art complex matter MD simulations. Once the calibration yields results that match those from NSE-experiments, otherwise inaccessible insights into the system can be constructed from the validated MD-trajectories, thus supplying a detailed microscopic view. A strategy that proved already successful –at shorter time scale– for polymers and biopolymers and other biological systems based on smaller molecules like e.g. phospholipid membranes. At the ESS, the associated data center in Copenhagen will be an ideal partner hosting computing facilities and providing simulation support in combination with the NSE data evaluation and interpretation. Thus synergies will emerge that enhance the impact of both, the neutron instrument ESSENCE as well as that of the simulation and computing facilities.

1.1.1 User base

Currently, in Europe there are 3 comparable high resolution instruments in operation (IN11, IN15, J-NSE ) In addition European (German) users have access to the JCNS operated NSE at the SNS in Oak Ridge. Worldwide there are further NSE spectrometers at NIST (a clone of J-NSE) and the iNSE in Tokai. The requests during the last 5 years for the high resolution instruments have average overload factors of 2.2, 3.9, 1.8 for IN11, IN15 and J-NSE & SNS-NSE. The use and output of the instruments is basically limited by the available beam times, an effect that is also reflected by the development of the NSE publication counts over the years that reflect with the usual time delay of 2-3 years the availability of instruments.
Figure 1: Number of neutron spin-echo related publications as function of publication year. The raise around 2000 is due to the fact that several new instruments (J-NSE, IN15, NSE at NIST) became operational in the period 1996-2000. The publication rate is limited by the available beam time rather than by the request.

In the period from 2010 to beginning of 2013 there were about 350 authors that published at least one NSE-experiment related paper and 190 of them had at least two and 135 three related publications. These are considered to be the core of the present user community. Naturally the present numbers are rather limited by the worldwide available beam time. On average a paper needs about 3 weeks of spin-echo beam time. This may be significantly reduced at the ESS spectrometer utilizing the gain factor of 30 for shorter counting times even if it is also partly used to enable the measurement of novel, presently still too difficult samples or exploration of a larger Fourier-time range. The experiment turn-around time will go from weeks to days enabling the buildup of an order of magnitude larger user experiments and a corresponding grows of the community.
1.2 Description of Instrument Concept and Performance

1.2.1 NSE Choice of Technique

The spin-echo technique as such covers a dynamic range that is both very difficult to access with other experimental methods and of utmost importance both for soft and biological matter and also extends the ability to tackle a number of hard matter problems. Thus, the technique has high potential for providing an indispensable capability to the ESS. Among the known neutron spectroscopic methods NSE surpasses all other options by 3 orders of magnitude in effective energy resolution. The next closest approach to high resolution is achieved by backscattering with practical energy resolutions of around 1 \( \mu \text{eV} \), whereas that of an ultra-high resolution NSE instrument corresponds to neV. In the time domain this is the step from 1 ns to 1 \( \mu \text{s} \). Beyond any question ultra-high resolution spin-echo spectrometers are the only neutron instruments that are able to explore the otherwise inaccessible dynamical range from a few to beyond 1000 ns with nano-meter spatial resolution.

Among the known NSE instrument types, high-resolution instruments of the generic IN11 type (i.e. spin-coding in a magnetic precession coil) are unique in the potential to approach and surpass the micro-second margin with real-world scientific samples\(^2\). ESSENSE is the latest fully optimized member of this family. The design that minimizes the resolution limiting inhomogeneities and utilizing the high flux of ESS will enable experiments at Fourier times exceeding the 1000 ns margin. This is the ultra-high resolution that is required for most of the challenges of the science case.

Wide angle NSE, in the form first demonstrated by the SPAN (HZB), adopted and expanded for the WASP (ILL) spectrometer, also uses spin-precession coding in a magnetic field, however, with different symmetry. The anticipated resolution performance of the most advanced design, WASP, is expressed by a maximum time of \( \tau_{\text{max}}=40 \text{ ns} \) (at \( \lambda = 12 \text{ Å} \), i.e. \( Q < 1 \text{ Å}^{-1} \)) decreasing if larger \( Q \)-values shall be reached to \( \tau_{\text{max}}=1 \text{ ns} \) (at \( \lambda = 3 \text{ Å} \), i.e. \( Q < 4 \text{ Å}^{-1} \)). The advantage of WASP is the approximately 20 times larger detection solid angle that extends over a large range of scattering angles. In the scale of the \((Q, t)\) diagram (figure 2) we indicate the range extension available by installing a Wide Angle NSE as green zone, which has to be compared to the much larger yellow field pertaining to the substantial genuine range extension supplied by high resolution NSE.

\(^2\)The ultimate limit of resolution can only be reached by a combination of measures, which all must come together. They are: 1. highest intensity at long wavelength, 2. lowest possible intrinsic effective field integral inhomogeneity, 3. best available correction for the unavoidable inhomogeneity, 4. stability over sufficiently long counting times. At the spectrometer side intensity can only be increased by using sufficient divergence for the illumination of an as-large-as-possible sample area, low intrinsic inhomogeneity can only be achieved by an optimized effective field shape.
Figure 2: Ranges covered by different neutron instruments, adopted from the ESS Technical Design Report (fig. 2.1). The possible range of wide-angle NSE is indicated by the green frame whereas the yellow zone shows the coverage of an ultra-high resolution NSE-spectrometer.

It is the yellow zone (high resolution NSE) that significantly extends the coarse broad diagonal path in the diagram that pertains to the general trend that larger structures respond on larger time scales. Most of the realm of wide angle NSE can –if needed– also be covered by the high resolution instrument, however, with less counting efficiency. 3

Currently established Neutron Resonance Spin-Echo techniques (NRSE) are limited by the difficulties to correct for path-length variation that severely restrict resolution or solid angle or –in the case of elliptic focussing– beam area, i.e. intensity. For MIEZE the sample extension and the path length variations to the detection points are further, even more important limitations to the maximum Fourier times. In practice presently operating state-of-the art NRSE instruments are restricted to times below 10 ns. Even the assumption of a 10 fold increase of

3For more details on the discussion about the priority of a high resolution NSE over a wide angle NSE at ESS we refer to the attached report of the workshop (see enclosure) hold in Copenhagen in August 2014.
the currently possible parameters as may be anticipated for the most advanced RNSE design at J-Parc (VIN-ROSE) would boost the time just slightly beyond the WASP range, but with much less solid angle coverage.

The high resolution neutron spin-echo spectrometer (NSE) is the only proven means to extend the scientifically usable resolution range of neutron spectroscopy significantly beyond the limit of several tenths of a $\mu\text{eV}$ - as obtained by advanced backscattering techniques - down to the neV range. In contrast to backscattering or normal time-of-flight spectroscopy the spin-echo yields the intermediate scattering function $I(t, Q)$ rather than $S(\omega, Q)$, which are related via a Fourier transform. The main resolution parameter for spin-echo therefore may be expressed in terms of the maximum Fourier-time ($t = \tau_{\text{max}}$) that can be obtained or even better in terms of the mostly limiting homogeneity parameter $H$. The Fourier-time is proportional to the third power of the wavelength, $\lambda^3$ times $J$, the magnetic field integral over the neutron path or -for larger wavelengths- proportional to $\lambda^2$ times $H$, the achievable field integral homogeneity. The lower value of both alternatives applies.

The performance of the proposed instrument (ESSENSE) profits both from the high neutron flux of ESS and the resulting high intensity and the innovation of the magnetic design towards a higher usable field, where the challenge of the latter pertains to the minimization of the field-integral inhomogeneity.

\footnote{The planned specifications of the VIN-ROSE spectrometers ($\tau_{\text{max}} = 2$ ns for the MIEZE part and 100 ns for the NRSE part) are quoted in the QENS/WINS2014 contribution of H. Endo et al. (see \url{http://www.ill.eu/html/press-and-news/events/qens-2014-wins-2014/booklet/}).}

\footnote{This relation holds if the resolution is limited by the field integral inhomogeneity; if the limitation is rather the maximum field integral $J_{\text{max}}$ that can be generated then $t_{\text{max}} \propto \lambda^3$ holds.}
Figure 3: Overview of the whole spectrometer with the dimensions and its main components. These are discussed in detail in the following sections. To avoid the direct line of sight two times, the guide after the kink will be a curved guide with radius of curvature of 500 m (max. 1000 m). The direction of inclination of the spectrometer in the figure is only indicative.
1.2.2 Instrument Layout: Primary Spectrometer

High Resolution NSE relies on the use of long wavelength neutrons. The neutron guide of ESSENSE will view the cold “pancake” moderator \(^6\). The moderator-detector distance will be slightly flexible, to be able to cope with bulky sample environments: A minimum distance of 35 m, extendable to a maximum distance of 36 m, yields a wavelength frame-width of \(\Delta \lambda = 7 \cdots 8 \text{Å} \). This frame width is sufficient to effectively harvest the pulse gain factor, which is limited by the steep dependence of the neutron intensity with the wavelength. Due to the finite width of the pulse the wavelength-spread at any instant is 0.3 Å.

The choice of the distance is motivated by balancing different conditions. Here indeed there is no simple single parameter that yields an extremum at \(L=35-36\) m but –as for many aspects of NSE instruments– it is a kind of good compromise. The main ingredients to find a best distance are

1. gain due to large frame bandwidth.
2. wavelength uncertainty due to bandwidth by the pulse length.
3. influence on neighboring beam lines (space, distance..), NSE needs some width !
4. to lesser extent: cost.

Concerning 1: with the nominal frame width of around 8 Å we span a broad beam intensity range, such that optimum counting time will often become quite imbalanced between \(\lambda_{\text{min}}\) and \(\lambda_{\text{max}}\), more frame width would not help too much to increase information output per hour of measuring time. Some more length (5..10 m) would not hurt too much here.

Concerning 2: we have about 10\% \(\delta\lambda/\lambda\) for 35 m at 3 Å, less for longer wavelength. 10\% is a soft limit as 3 Å is a wavelength rather on the short side. Thus one might choose a length slightly shorter or longer. However, there is not much space between the last chopper and the secondary instrument.

Concerning 3: this requires a consideration of placing the instrument together with shielding and neighbouring instruments needs. As said above, some meters extra length to cope with possible collisions would be possible, which, however, would (slightly) increase the cost as stated as point 4.

\(^6\)In autumn 2014 ESS decided to move from the TDR reference 12x12 cm\(^2\) cold moderator to a 3 cm high, flat “pancake” moderator. This required a modification of the beam transport in order to re-optimize the flux at the sample. Therefore at some points in the following we quote the design based on the TDR and the gain factor (\(\sim 1.5\)) obtained by the brilliance increase, mitigated by the necessarily incomplete guide illumination.
The reference features of the primary spectrometer were first worked out for the 12 cm×12 cm ESS-TDR reference moderator with a guide system starting at 2 m distance from the moderator and ending at 27 m. Based on that the modifications for the recently decided 20 cm×3 cm cold “pancake” moderator are assessed and adopted to the proposed instrument design. The sample is positioned at 31 m and has a typical dimension of 3 cm × 3 cm. The dimension of the transport system, the positions of the chopper system and of the polarization device are shown in Figure (3).

![Figure 4](image-url)

**Figure 4:** To illustrate the chopper transmission characteristics the virtual flux from the moderator through a straight guide system containing the choppers in direct straight view at detector position resp. distance is shown.

The chopper system  Frame selection (Figure 4) is realized by a system of 4 disc choppers in the distance range between 14 m and 23 m (e.g. C1 at 14 m, C2 at 16.7 m, C3 at 20.12 m, C4 at 23 m). With a rotation frequency of 14 Hz and apertures of 110.9°, 138.7°, 173.8° and 203.5° respectively, the choppers make use of the whole pulse. Such a system is able to select any frame within (and beyond) the useful operation wavelength range between \( \lambda = 3 \cdots 4 \text{Å} \) and \( \lambda \approx 25 \text{Å} \) without any contamination of neutrons with wavelengths shorter than 80 Å. The frame boundaries can be chosen freely using the proper chopper phasing, e.g. one may center a frame also around 10 Å or any other desired wavelength without impairing the suppression of contaminating neutrons from other pulses. This will enable also a background suppression strategy by selecting the wavelength frame such that the arrival times of neutrons

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7Sample size between 4 cm × 4 cm down to only a few mm will be possible. The illuminated area is controlled by a variable slit system in front of the sample. Small samples will receive the full illumination divergence.
from the frame boundaries coincide with the times T0 of the prompt pulse. A distance of 14 m for the first chopper is the largest distance that yields a viable frame selection with no more than 4 choppers.

As option we propose a pulse shaping chopper (see also the enclosure). It would be located at a distance of 6 to 7 m and consists of two closely spaced synchronously co-rotating disks each with two symmetrically placed 90° sectors. By phasing of the two disk any effective sector width between 0° and 90° can be set. The chopper opens twice per revolution, its frequency range is between $n \times 7 \text{ Hz} \to 7 - 168 \text{ Hz}$ with $n = 1, 2, \ldots, 24$. With that one can reduce the wavelength spread to virtually any value between 0.03 to 0.3 Å. This e.g. would allow to avoid Bragg reflex contamination in large unit cell (para)magnetic compounds (molecular magnets, spin-ice, ..) as well as in compounds as zeolithes or other cage compounds with diffusing molecules. Further details are given in the enclosures.

The additional costs (not included) for the PS chopper would be 450 k€.

**Beam extraction: the guide system**  
The neutron guide has been initially optimized for the TDR reference moderator ($12 \times 12 \text{ cm}^2$). The sample has typical/maximal dimensions of 3 cm \times 3 cm and is placed at 4 m from the end of the guide. A full transmission of the TDR reference moderator intensity to the sample position can be achieved for $\lambda > 5 \text{ Å}$ with a 8 cm \times 8 cm guide with coating $m = 2$, as shown in Figure 5. A guide cross-section of 8 cm \times 8 cm still guarantees efficient brilliance transfer for $\lambda$ larger than a limit wavelength of about 4 Å within maximum illumination divergence at the sample of ±0.8°. The saturation at 5 Å suffers a small drop of efficiency towards 4 Å but – given the moderator spectrum and its wavelength dependence in a frame from e.g. 4-12 Å – it is totally reasonable for the anticipated operational wavelength-range of the instrument from 4 Å to 25 Å.

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8Alternative solutions with the first chopper at 6-8 m and keeping the last one at 23 m require only 3 choppers, the second chopper is located at about 10 m.

9The brilliance transfer of the straight guide is calculated w.r.t. a moderator surface of the dimension of the guide cross-section placed 4 m away from the sample.
Recently the moderator concept was changed to a flat cold ("pancake") moderator with only 3 cm height but increased brightness. Therefore the beam transport, which was first devised for the TDR standard moderator, needed reconsideration and adaption. The simulations show that ESSENSE will be able to harvest a gain of intensity at the sample from the “pancake” moderator. The gain with respect to the TDR moderator obtained with optimized modifications of the neutron guide ranges up to 50% depending on the degree of guide adaption, see figure 5. We considered three different solutions: The first one consists of a combination of a tapered guide (3-5 m long) and a straight guide, the former with a starting height of 6 cm opening to 8 cm at the end and the latter, as before, with a cross section of $8 \text{ cm} \times 8 \text{ cm}$. In the second solution the vertical profile of the guide system is replaced by an elliptical shape with one focus on the moderator and the other on the sample positions; the height at the exit of the guide on the sample side is fixed to 8 cm. Both solutions are based on the idea that the vertical transport is decoupled from the horizontal one and that only an adjustment of the vertical shape of the guide is necessary. Mads Bertelsen has proposed a third solution obtained with an optimization algorithm for McStas called Guide_bot. This solution presents a combination of an elliptical and a tapered guide, however both for the vertical and the horizontal profile and—differently from the previous two solutions—assumes an exit aperture of the guide.
larger than 8 cm × 8 cm. In conclusion, with elliptical vertical focusing ESSENSE will enhance its effective intensity by a factor $1.4 \div 1.5$ with a moderate increase in guide complexity.

**Beam extraction: neutron transport and polarization** For an efficient performance of the instrument a good polarization of the beam at the sample position is essential, together with a high neutron flux and avoidance of the direct line-of-sight. The polarizing device consists of an inclined polarizing mirror (kink). With a total length of 2.7 m, it is a sufficiently compact insert that can be placed between the 8 m after the moderator and shutter and before the first chopper at 14 m. As supermirror a coating with Fe/Si ($m=4 \cdots 5$) multilayers is envisaged \(^{10}\). The kink consists of a neutron guide with an inclination $\theta = 1.7 \degree$ of the lateral mirrors, as shown in Figure (6). The aperture of the device is not constant: It shrinks from 8 cm to 4 cm in the center and then it opens to 8 cm at the end again. The aperture reduction contributes to some extent to the reduction of the background from the source due to very fast neutrons and $\gamma$-radiation. For the slow neutron flux at the sample this geometry provides an intensity gain of $\sim 10\%$ with respect to an inclined guide with constant cross section.

![Figure 6: Geometry of the simulated kink with $\theta = 1.7 \degree$. The red line represents the polarizing mirror.](image)

With the inclination of $\theta = 1.7 \degree$ and a length of the polarizing mirror of 2.7 m the kink provides virtually perfect polarization up to a wavelength $\lambda \simeq 15 \AA$ dropping to 80% at 20 Å. The effective transmission of the neutrons with “proper” polarisation reaches 50% at 4.4 Å (3.5 Å for $m=5$) and rises to a plateau value of 80% above 6 Å (5 Å), Figure (7). This transmission ($T_\uparrow$) is a measure of the brilliance transfer from the moderator onto the

\(^{10}\)FeCoV layers for the polarizing mirror is to be avoided due to the otherwise occurring radiation hazard by strong neutron activation of the cobalt in the intense primary beam.
sample through a system of neutron guides 25 m long, including the 2.7 m long kink, and with dimension $8 \text{ cm} \times 8 \text{ cm}$ with respect to the virtually perfect transport of a straight $8 \text{ cm} \times 8 \text{ cm}$ reference guide of the same length.

For an unpolarized beam the transmission, $T$ of an ideal instrument is $1/2$. Then the figure of merit (FOM) for the performance of the beam transport may be written as

$$Q = P \sqrt{T}$$

the optimum value is $Q = 1/\sqrt{2} \approx 0.707$. With the kink only, the polarization at long wavelength beyond 15 Å becomes insufficient. To improve the FOM $Q$, i.e. the performance in the important long wavelength range, a further measure to improve polarization is needed. For this purpose a transmission polarizer (FeSi multilayer on Si-wafers) acting on long wavelengths will be inserted in the neutron guide between choppers.

![Figure 7](image)

**Figure 7:** Left: Transmission, polarization and figure of merit at the sample position for the kink solution, $\theta = 1.7^\circ$ and 2.7 m. The polarizing mirror has coating FeSi, $m_u = 4$ and $m_d = 0.6$, the other mirrors have coating $m = 2$. The curves obtained with a second polarizer are simulated for a mirror with an inclination of 4.6° and with $m_u = 4$ and $m_d = 0.6$. The dashed line indicates the theoretical limit, the performance of an ideal neutron guide. Right: Transmission, polarization and figure of merit for a flat moderator ($12 \times 3 \text{ cm}^2$) with the elliptoc solution of figure 5. The reference configuration for the transmission is a straight guide.

The transmission polarizer has to be preceded by a broadband adiabatic RF flipper to comply with the reflected polarization direction of the kink. The mirror of the transmission polarizer

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11 A similar solution is installed in IN15 at ILL with good performance.
will have a relative high angle of inclination, i.e. \( 4.6^\circ \). This inclination will selectively improve \( P \) only at wavelengths larger than 11 Å but without absorbing too many neutrons, because the neutron path through the silicon layer (0.3 mm thick) will be short (12 mm). This combination allows for a polarization of more than 95\% at 25 Å and improves the FOM even if the transmission is slightly reduced (Figure 7).

Figure (8) shows the neutron distributions and their divergence at the sample position for different wavelengths. The black rectangle indicates the dimension of a sample 3 cm \( \times \) 3 cm, while -as shown on the right- the divergence is already limited to the maximum divergence accepted at the sample. Only for the case \( \lambda = 4 \) Å significant distortions due to divergence limitations from surpassing the \( m=4 \) reflection limit in the kink mirror are visible. Using the highest available \( m \)-values (currently \( m=5 \)) will shift the occurrence of this effect toward still lower wavelength. The adaption of the guide system to the “pancake” moderator and the restriction that the earliest guide start is at 2 m moderator distance leads to some modulation in the vertical divergence distribution. For the quality of the measured \( S(Q,t) \) data this plays a minor role.

![Figure 8](image_url)

**Figure 8:** Distribution of the positions (left) and of the divergence (right) of the neutrons at the sample position for different wavelengths for the kink solution without second polarizer. The position monitor is 9 cm \( \times \) 9 cm, the black rectangle indicates the shape of a 3 cm \( \times \) 3 cm sample (but also smaller samples can be used), the divergence monitor accepts divergences between \( \pm 0.8^\circ \) both in \( X \) and \( Y \) direction. The rightmost column displays the “natural” divergence.

The alternate option of a polarizing channeled bender with a coating of FeSi with \( m_u = 4 \) and \( m_d = 0.6 \) instead of the polarizing kink would yield a worse polarization at the sample...
position. For this reason, and because of its more simple and stable geometry, we finally opted for the kink.

The possibility to go out of line of sight two times can be realized through a curved guide with a radius of curvature of 500 m, maximum 1 km. The curved guide shall start after the kink and end at 27 m, before the secondary spectrometer. Simulations have shown that the flux at the sample for $\lambda > 5 \text{Å}$ will remain virtually unaltered.

Analyzer The analyzer in front of the detector will have the dimension of the detector (30 cm diameter) and it shall accept the divergence given by the typical sample size. We propose a 40 cm long analyzer with 4 mm wide and 30 cm high channels with (FeCoV multilayer coating with $m_u = 3$ or higher and $m_d = 0.35$) on both vertical walls of each channel. The implementation of FeSi with higher $m$ (e.g. $m_u = 4$) would require stronger working magnetic fields that are less compatible with the magnetic requirements of the spectrometer. To compute the FOM (Eq. 2) the effective transmission is evaluated as ratio of neutron intensity from the sample entering the analyzer channel and the (total) intensity leaving the analyzer channel. For a good polarization a proper angle of inclination (i.e. the channels are oriented towards a source position at some centimeters off the real one) has to be chosen. Thus the performance of the McStas models of a tapered guide and of the curved guide with aspect ratios of 4:300 have been compared (in the enclosure the analysis case for FeSi is shown, a mirror with coating FeCoV shows qualitatively the same performance). The theoretical performances of the curved and tapered channeled analyzer are quite similar so we opted for the mechanical simpler tapered guide solution. If the angle of inclination is properly chosen both solutions reach a figure-of-merit close to the optimum for long wavelengths (25 Å). The instrument design will allow for automatic control of the analyzer inclination angle. With possibility of selecting the best angle of inclination for a selected wavelength frame, the solution with the tapered guides as channels can cover the whole range of $\lambda$ up to 25 Å. The analyzer will have to be set according to the requirements of the experiment, Figure (9), for example $1.1^\circ$ ($0.86^\circ$) for $\lambda < 14$ Å and $1.9^\circ$ ($1.29^\circ$) for $14$ Å $\leq \lambda \leq 25$ Å.
Figure 9: Figure of merit for an analyzer with tapered focusing channels for a FeSi supermirror with $m_{up} = 4$ (left) and for a FeCoV supermirror with $m_{up} = 3$ (right). The angle of inclination is explained in the text.

Detector  The detector will have a dimension of 30 cm × 30 cm and with a moderate (2D) position resolution (better than 3 cm or 1 inch), high efficiency and high maximum count rate (better than 5 KHz/cm²). A robust possible solution would consist of an array of 100-200 front end counting tubes ($^3$He) with square cross-section. A pixel size of several cm matches the effective spot size due to sample illumination divergence. Alternatively a staggered array of 50 linear position sensitive counting tubes (1 cm diameter, $p(^3$He) = 4 bar) may be used, which –with current technology– would allow for 1···2 KHz/cm² at 10% deadtime.

1.2.3 Instrument Layout: Secondary spectrometer

The technical limit for the Fourier-time ($\tau$) is given by the residual field-integral inhomogeneity, which remains after the action of correction elements in the beam paths (“Fresnel” correction coils). At the current state-of-the-art the correction elements seem to be resistant to further improvement, therefore the most promising means towards the ultimate limits of resolution is a reduction of the intrinsic inhomogeneity of the main solenoids, a measure that has been first selected at the ILL to enhance the IN15 properties within a currently conducted refurbishment. The potential of the application of this strategy is about a factor between 2 and 3 inhomogeneity reduction compared to existing instruments. Reduction of intrinsic inhomogeneity is achieved by a somewhat enhanced field in the center of the solenoids (resembling C. Zeyen’s optimal field-shape solution for a narrow beam [53]) and enlargement of the solenoid diameter. The latter, however, is limited by the requirement to avoid extensive fringe fields and to keep the total length of the instrument within feasible limits. Optimization consists in finding the best compromise among these contradicting requirements. By using superconducting partial solenoids, that are fringe field compensated in a similar way as the solenoids of the SNS-NSE spectrometer, these requirements can be fulfilled with a distance of
4 m from the sample to the $\pi/2$-flipper. When using water-cooled copper solenoids instead only a partial compensation—to ensure a working spin-echo configuration—is possible (see appendix). For a (in)homogeneity (measured by a parameter $H$) limited NSE-spectrometer the resolution determining parameter $H$ yields $\tau_{\text{max}} \simeq H \lambda^2$, i.e. for a given construction the resolution depends on the square of the wavelength. An improvement of $H$ either allows usage of shorter wavelength for a given Fourier-time or usage of larger Fourier-time at a given wavelength. The anticipated homogeneity improvement would pave the way for a Fourier-time $\tau = 1000 \text{ ns} (\simeq 0.7 \text{ neV})$ at $\lambda = 20 \text{ Å}$.

Figure 10: The picture shows a horizontal section of the magnetic coils on a plane containing the coil axis. In the right arm the system of concentric, fully compensated, superconducting coils is put in evidence: the coils with $+NI$ are colored in red while the compensating ones with $-NI/2$ are colored in blue. The green solid lines indicate a normal conducting coil, the dashed green line delimits the space needed by one of the short-time option. The largest dimensions for one arm are reported. The robustness of field homogeneity for this configuration has been tested for a position of the $\pi$ flipper up to 20 cm from the sample.

The coil assembly. We present here a solution for superconducting solenoids [54]. For a comprehensive comparison of the properties, the advantages or disadvantages of superconducting versus water-cooled copper coils we refer to the enclosure. A decision in favor of one of the two solutions will be taken on the basis of the information obtained from the refurbishments of IN15 and J-NSE. The family of solutions is represented by the typical configuration sketched in Figure (10). The coil assembly is about 2.4 m long with a maximum coil radius of 0.68 m and consists of five fully compensated, superconducting parts. The solutions are robust against adjustment of coil length and winding numbers needed in order to facilitate manufacturing using constant winding pitch according to wire diameter and such that an even number of full layers results (here: assuming the 0.9 mm diameter wire, as was used in the SNS-NSE). The optimizations were performed with a $\pi$ flipper positioned between 10 cm to 20 cm from the sample. If required by bulky sample environments or special setups more sample space can be supplied by the possibility to include extra distance pieces between spectrometer arms and
sample stage.

![Magnetic field profile diagram](image)

**Figure 11:** Profile of the magnetic field along the axis for both arms of the coil assembly of Figure (10). The dashed line is a 40-times magnification of the field. The point-dashed green line is also a 40-times magnification of the field along the axis but for a configuration with an extra free sample space of 30 cm radius.

The coils of Figure (10) are characterized by an intrinsic inhomogeneity $\Delta J = 3.4 \times 10^{-4}$ for a neutron beam with 10 cm radius at the $\pi/2$ flipper or by $\Delta J = 5 \times 10^{-4}$ for a radius of 12 cm, corresponding to a divergence of the beam comparable with that at MLZ or at SNS. Figure (11) shows the magnetic field along the axis for both arms, the typical asymmetric triangle shape that is common to all optimized solutions is visible. It has also been checked that the field remains sufficiently homogeneous across the $\pi/2$-flippers, in particular this is important for the efficiency of the large flipper at the end of the second arm.

**Residual inhomogeneity and improved resolution** Without further correction a factor 2.5 times lower intrinsic inhomogeneity is obtained for a beam of 20 cm diameter at the $\pi/2$-flipper, Figure (12). The still necessary corrections will be performed by two correctors at optimized positions in each of the main solenoid sets. The layout of the main solenoids is such that assuming linear increasing radial current densities at the corrector positions an inhomogeneity of about 1ppm can be achieved. The magnetic landscape was optimized for a field-integral setting of 1 Tm but ensures proper working of all components in the range from $\approx 0.001$ to 1.5-2 Tm. It yields a depolarization-free and working NSE-compatible field map over the whole beam path. This is feasible without larger external compensation by the auxiliary current rings, which stay at low power/current. Further, it allows easy access to large
scattering angles\textsuperscript{12}, e.g. for 45 degrees the computed corrected inhomogeneity (by the above mentioned 2 quadratic ideal current distribution type correctors) is increased by magnetic cross-talk between both spectrometer arms merely from 1ppm to 4ppm. By shifting the correctors by less than 0.5 mm this can be reduced to 2ppm again. Further, the fringe fields are compatible with a magnetic shielding enclosure\textsuperscript{55}. Thus the proposed instrument will have some similarity with the SNS-NSE spectrometer, however, with a larger, more sophisticated main coil that has significantly improved homogeneity properties and considerably more neutron flux and more than twice the frame bandwidth.

\textbf{Figure 12:} The relative intrinsic inhomogeneity of the optimized coil configurations for ESS (black) is plotted together with that for SNS (red) and MLZ (blue) as a function of $r$, the distance from the axis of the neutron trajectories at the last $\pi/2$-flipper. The spread around the mean parabola due to the different starting point of the trajectories at the sample is also reduced.

In the design optimization and assessment of the main coils it was assumed that ideal radial coils with quadratic correction effects are in place. That allows for a correction of the uniformity of the precession field to less than 1 ppm, i.e. then deviation of the main field from quadratic errors are sufficiently low and the necessary quadratic correction strength is reduced —corresponding to the reduced intrinsic inhomogeneity properties of the new coil design. In reality, the possible realization methods of such coils are limited and suffer from insufficient

\textsuperscript{12}If there is sufficient space to allow large scattering angles for the secondary arm, this will allow to reach $Q \approx 2 \text{Å}^{-1}$ with $\tau_{\text{max}} = 20$ ns.
accuracy of the necessary representation of the current density. The theoretically approximating but non-ideal Pythagoras coils can handle the required current density. They rely on the combination of two linear elements with quadratic corrector effects that provide an overall quadratic radial correction. Operation experience at existing spectrometers [55] showed that the Pythagoras coils can be made close to their theoretical performance whereas the realization of the theoretically more ideal radial coils stays significantly behind the expected performance. Magnetic simulations show that the reduction of the intrinsic field integral inhomogeneity is about 2 ppm for a divergence of the beam of 0.02 rad. For the same divergence, a simulation of the coil configuration of J-NSE with three Pythagoras correction coils (of the same dimensions) yields a corrected inhomogeneity of 4 ppm; a gain factor (for the shorter J-NSE compatible configuration) of two is confirmed.

**Short times option.** Two options (“shorty”) to reach very short Fourier times down to pico-seconds are foreseen, see also enclosures. Two methods will be implemented:

1. Within the magnetic layout it has been verified that two $\pi/2$ flippers can be positioned in the sample space without compromising the efficiency of the spectrometer, the space needed for this solution is shown in Figure 10. The main solenoids, operated at low current, then serve to generate a guide field, the proper NSE precession will be performed in short coils inside the sample space. This mode is used at the J-NSE (and NIST-NSE and at IN15 at ILL) spectrometer, where it supplies a tenfold reduction of the minimal useful field integral.

2. Inserting extra $\pi$-flippers between the main coil ends and the “normal” $\pi/2$-flippers and adding short extra coils in the space between these flippers will enable an operation where, the effective field integral, i.e. the Fourier-time can be set to arbitrary small values. This is achieved by inverting the precession angle in the second $\pi$-flipper thus subtracting the field integral inside the main coil (at very low current) from that generated by the short extra coil. This mode has already been proven at the SNS-NSE spectrometer. The shortest time here is not given by the arbitrarily small effective field integral but rather by the condition that the field integral $\delta J_\pi$ variation, necessary to probe at least 1/2 echo oscillation is less than 10% to 20% of $J_{\text{eff}}$, which yields $\tau_{\text{min}} = (J_{\text{eff}}/\delta J_\pi)(m_n/2h)\lambda^2$, about 1 ··· 2 ps at $\lambda = 4$ Å.

Depending on the technical details, we will evaluate for both “shorty” options whether it is feasible to move the $\pi/2$-flippers out of the beam when they are not in use.

**Magnetic scattering** The instrument has been optimized for “standard” spin-echo measurements on non-magnetic samples. Paramagnetic scattering can be observed in this “normal
mode" with full resolution. A set of xyz-magnetic field coils shall be installed that can be used to control field direction at the sample position to enable proper normalization of paramagnetic echo-scans (see enclosure).

Ferromagnetic scattering (without intensity modulation) may be performed at lower resolution with the insertion of two extra $\pi/2$ flippers in the sample environment space.

The option to enlarge the sample environment and to extend the length of the spectrometer to 36 m, will supply enough room for such a setup.

**Sample stage** Adjustable spacers connecting the sample stage to the spectrometer arms will allow to go from 10 cm radius available sample space up to 50 cm. This will enable the use of spacious special sample environments. The total length of the secondary spectrometer will accordingly increase by 100 cm (see enclosure).

**Magnetic shielding** A magnetic shielding around the spectrometer is foreseen. It consists of a double walled mu-metal enclosure with a space of about 0.3−0.5 m between the layers (thickness $\approx$1.5-2 mm). The space in-between will host the radiation shielding around the spectrometer. The basic parameters of this type of shielding are known from the SNS-NSE installation [56]. In the enclosures a further discussion of the pro’s and con’s of a magnetic shielding and estimates for the effect of the retroaction of the induced magnetization in the shielding walls on the homogeneity are given, they indicate that a distance of 2 m between shielding and magnetic axis is sufficient.

The magnetic shielding has also the function of protecting the neighbouring instruments from the stray field generated by the NSE. Thus, such a shielding is unavoidable if these instruments are sensitive to magnetic fields, even if the rest of the neutron hall is magnetically quiet.

The alternative to a passive $\mu$-metal shielding would be active compensation of static environment fields (modified earth field). However, changes in the order of a few milli-Gauss (fractions of a $\mu$T) may cause changes of the symmetry phase. If that happens during a sequence of an experiment the final results will suffer from additional noise or even become invalid. Unshielded instruments typically lose significant time, e.g. by stopping data acquisition when the crane moves too close or if larger magnets are used at neighbor instruments. The choice of the threshold to stop acquisition always is a compromised between the amount of data distortion versus the amount of lost acquisition time. To our experience it is only possible to use data from an unshielded NSE instrument (i.e. J-NSE) if during evaluation the symmetry phase is readjusted based on the echo signals from the sample. This method, however, needs sufficient amplitude and statistics in the sample signal; it fails for weaker signals and smaller background contributions. In contrast the data from a shielded instrument (i.e. SNS-NSE) can be evaluated with symmetry phases as fixed by a reference scan.
Software  The basic framework of the instrument software may be adopted from our SNS-NSE instrument. Interfaces have to be modernized. Depending on available software developer capacities in Jülich or at the ESS (DMC) this may also include the code structure. Data analysis will be immediately possible with an adaption of the modernized present analysis programs (which is currently performed for the SNS-NSE evaluation program). User interfaces and possible code adaption to ESS standards will require additional work.

Sample environment  As “standard” sample environments the following equipment is foreseen:

- “Bio-oven”: supplying temperature control in the temperature range between -20°C and +120°C, sample room at ambient pressure (suitable for Hellma cells). It will serve all biomolecule dynamics work, complex fluids and microemulsion, gels, polymer solution and a part of polymer melt investigations.

- “Humidity cell”: controlled humidity (solvent partial pressure) cell, possibly add-on for the “Bio-oven”.

- “Cryo-oven”: multipurpose cryostat with extended upper temperature limit, temperature range: 5 K to 700 K. For general work needing low temperatures and/or large temperature variation, e.g. glass dynamics, diffusion in energy materials, paramagnetic scattering.

- “Polymer-oven”: simple oven for sealed niobium or aluminum cells, temperature range: ambient - 250°C. Suitable mainly for polymer melts, partly complex fluids, ionic liquids, solutions if only temperatures above ambient are needed. The advantage is a rapid sample change and rapid temperature equilibration.

- “GINSE-cell”: grazing incidence, resonating layer cells with integrated prism and temperature control in the range between -20°C and +120°C. Enables experiments addressing the dynamics close to extended macroscopic surfaces addressing e.g. lubrication, flow at boundaries etc..

- “High-temperature-oven”: temperature range: ambient - 1000°C. Enables investigation of e.g., diffusion in high temperature energy materials, dynamics of inorganic glasses. This will probably be NSE specific since a heating method that does not create magnetic fields must be used.

- “Pressure cell”: for supercritical liquids, range: p=0-500 bar, T=10°C-90°C. Enables investigation on microemulsions and solution incorporating e.g. supercritical carbon-dioxide as “green” solvent. The pressure range is such that a full sample size can be
illuminated. For higher pressures up to 5000 bar a SANS type cell with effective sample area restriction to less than 1 cm diameter may be used. The corresponding intensity loss would be overcompensated by the ESSENSE intensity gain factors.

all sample environments must be nonmagnetic. More specialized sample environments (supplied by the user) may be hosted, possibly using the prolongation option to increase the available sample space.

For (para)magnetic scattering a cryostat capable to reach some mK will sometimes be required. This sample environment will be used infrequently and is expected to be supplied by the ESS pool.

For a more detailed estimate of the costs of the equipments for the sample environment we refer to the costing supplement in the enclosure.

1.2.4 Performance

Concerning the performance of the instrument there are two main distinct but still entangled aspects: effective flux and resolution.

The resolution (R) issues do not depend on the nature of the neutron source and are independent from its pulse structure. However, a high neutron intensity at long wavelength is essential to reach the highest Fourier-times. The longest useful wavelength largely depends on available intensity and together with field integral homogeneity and/or the maximum available field integral, determines the largest Fourier time. The resolution of a NSE spectrometer is expressed in terms of the maximum Fourier time and is determined by the resolution function

\[ R \propto \exp\left\{-(\tau/(H\lambda^2)^2)\right\}, \]

where \( H \) is a measure of the relative field integral homogeneity. In the regime, where the maximum field integral is the main constraint to the resolution (short \( \lambda \)), the \( \lambda^3 \) scaling is the dominant one (\( \tau_{\max} = 0.18 \text{[ns/(Tm Å³)]} \times J_{\max} \lambda^3 \)). In this case, with a maximum field integral of the (superconducting) coil assembly of about 1.5 – 2.5 Tm \(^{13}\), the maximum Fourier time will be between 17 ns ·· 23 ns for 4 Å. However, in the regime where the drop of \( R \) below a certain factor (i.e. 1/e) limits the range, the dominating scaling is given by \( \tau_{\max} \propto H \lambda^2 \). Pertaining the resolution we expect a parameter \( H = 2 \cdot 2.5 \text{ns/Å}^2 \) leading to a maximum Fourier time of 800 ·· 1000 ns at \( \lambda = 20 \text{ Å} \) (1200 ·· 1600 ns at \( \lambda = 25 \text{ Å} \)) and of \( H\lambda^2 = 40 \text{ ns} \) for \( \lambda = 4 \text{ Å} \). The improvement in \( R \) of 2.5 is independent of the specifications of the beam transport.

The moderator brilliance together with the beam transfer determine the available flux spectrum at the sample. The flux at the sample has huge influence on the data quality that can be obtained. As shown above, in the relevant wavelength range plain neutron optics yields efficiencies in the range of 80%-90% brilliance transfer from the TDR standard moderator to sample with polarization better than 0.9. For the new “pancake” moderator the average

\(^{13}\text{Depending on manufacturing margin.}\)
brilliance transfer to the sample is lower but the reduction is still overcompensated by the increase in moderator brightness. The main realm of the high-resolution NSE will be between λ = 6 and 20(max. 25) Å.

The average flux at the sample for the new ESS cold source model is given in table 1. The simulated fluxes are multiplied by attenuation factors coming from the (assumed) 4 cm Al, 5 m He and 1 m air that the neutrons will inevitably find on their path in the real instrument. A gain between 3 and 4 (TDR reference moderator) and 4 to 6 for the final “pancake” moderator with respect to IN15 is observed.

<table>
<thead>
<tr>
<th>λ/Å</th>
<th>simulated Φ $10^8$ n/s/cm²/Å</th>
<th>attenuation factor</th>
<th>Φ [ESSENSE] $10^8$ n/s/cm²/Å</th>
<th>Φ [IN15] $10^8$ n/s/cm²/Å</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.3</td>
<td>1.3</td>
<td>0.77 x 0.84 x 0.98</td>
<td>0.82</td>
<td>1.1 ÷ 1.2</td>
</tr>
<tr>
<td>7</td>
<td>0.9</td>
<td>0.76 x 0.81 x 0.97</td>
<td>0.54</td>
<td>0.76 ÷ 0.81</td>
</tr>
<tr>
<td>17</td>
<td>0.025</td>
<td>0.56 x 0.73 x 0.94</td>
<td>0.01</td>
<td>0.01 ÷ 0.015</td>
</tr>
</tbody>
</table>

Table 1: Fluxes at the sample position (31m) for polarized neutrons. Polarizing device is the kink. The simulations have been performed for λ in $[\lambda - 0.5\text{Å}, \lambda + 0.5\text{Å}]$. The estimated real flux (fourth column) is obtained after multiplication by the attenuation factors for 4 cm aluminum, 1 m air and 5 m He, respectively. The fluxes simulated for the TDR reference moderator are consistent with the ‘source-ESS-2012’ (Zanini) of Vitess. (*) Courtesy of B. Farago. The estimated (by applying the combined scaling factors, 1.4 ÷ 1.5, due to moderator brilliance and guide transport) fluxes for a flat “pancake” moderator of 3 cm height are also reported.

Finally the larger frame width yields a gain factor, $g$, compared to reactor based instruments which is

$$g = \frac{\ln(\lambda_{\text{max}}/\lambda_{\text{min}})}{w},$$

where the effective relative selector width of the reactor instrument is $w$. Assuming $w = 0.15$ for an instrument with 15% resolution like IN15 and a wavelength window from 7 to 14 Å the gain factor is $g \approx 5$. $g$ will be larger for smaller wavelength and less for larger wavelength band center, i.e. $g(4 - 11\text{Å}) = 10$, $g(13 - 20\text{Å}) = 4.3$. This $g$ is the maximum effective gain factor due to extension of the wavelength band of a frame; depending on the sample scattering and the type of investigation the useful gain factor may be less. The intensity gain factor can be estimated as the product of $g$ with the gain factor in flux at the sample. Thus, the new high-resolution NSE will have an improvement factor ranging from 16 up to 60 (geometric average is 30) with respect to IN15, independent of the performance of the precession coils. This factor translates to less counting time requirements and/or a higher accuracy of the experimental data.
In Figure (13) a complete experimental cycle with the scattering intensity computed for standard polymer samples from h/d mixtures of polyethylene or polyethyleneoxide has been simulated with the data of new ESS spectrometer and for IN15, taking already into account the expected performance of the new coils. Transfer functions (moderator-sample and sample-detector) have been taken from tables generated by McStas simulations and multiplied by transmission of the estimated lengths of Al, air and He. Resolution functions were modeled by the Gaussian approximation given above, assuming $H=2.5 \text{ ns/Å}^2$ for the new ESS spectrometer and $H=1 \text{ ns/Å}^2$ otherwise. The considered detector area was 100 cm$^2$ in all cases. The counting time assumed was the same for ESS and IN15.

The first example of Figure 13 shows incoherent scattering from a fully protonated PE sample with 0.5 mm thickness (size 3 cm $\times$ 3 cm) and it demonstrates the advantage of a large wavelength frame. The 3-4 times larger intensity yields two times smaller error bars in the corresponding ESS curve (red points). In both cases the field-integral range was 0.001-1 Tm (ESSENSE) or 0.001-0.25 Tm (IN15, pertains omission of the last 4 tau-points). The second example shows a h/d-mixture of PEO in the anticipated "bread-and-butter" range of wavelength and scattering angle. Finally a comparison for the h/d PEO melt in the long wavelength regime centered at 20 Å is shown.

In each case the dynamical features were assumed to be simple Rouse type polymer dynamics, in detail real polymers will show somewhat different, yet similar $S(Q,t)$ behavior. The comparisons show that beyond the flux ratio of 3-4 (x up to 1.5 after adaption to the flat high brilliance “pancake” moderator) a big advantage of the ESS spectrometer lies in the fact that between 7 and 3 effective experiments, all yielding useful data, are performed simultaneously. The significant increase in error bars at the large Fourier-time side are due to the approach of the resolution limit (residual inhomogeneity of the main coils). For a comparison with the SNS-NSE spectrometer see the enclosure.
Figure 13: Simulations of an experiment with polyethylene and PEO at the future ESS spectrometer (left) and at IN15 (right) with either the optimized (for ESS) or the new, refurbished (IN15) specifications of the instrument, both cases with 15% wavelength-band resolution using data from 100 cm² detector area. The assumed counting times per field-integral setting for the ESS and the IN15 cases were equal. Form top to bottom: incoherent scattering at $\lambda = 7$ Å (16 hours total counting time, 0.5 mm sample thickness, 11 hours with the new ‘pancake’ moderator) and, below, coherent scattering for $\lambda = 12$ Å and for $\lambda = 20$ Å on the last row (0:47 hours the first, 5 hours the second, total counting time for the experiment, PEO 3 mm sample thickness, or 0:31 hours and 3 hours with the ‘pancake’ moderator, respectively) and Fourier time ($\tau$) up to 1 $\mu$s for the 20 Å. The red symbols mark the set of data among those for ESS with the same $q$ as the data for IN15.
1.3 Technical Maturity

The design of the instrument has been developed on the basis of the existing technology and on the experience accumulated with the construction of other spectrometers (i.e. MLZ, SNS). Thus the risks are minimized.

Below, a list of the system components is added; a risk evaluation and a risk mitigation is discussed for the most relevant components.

1.3.1 Overview of the system components

All components of the secondary spectrometer must be nonmagnetic!

The proposed instrument will contain the following main functional components:

1. Neutron guide in target block and shutter (8cm x 8cm, m=2), elliptical in the vertical direction.
2. (Possible option: pulse shaping chopper)
3. Shutter fulfilling the minimum condition of accessibility of the instrument at the sample area during full operation of the source
4. Polarizing mirror, with 3-3.5 degrees deflection angle
5. Neutron guide section connecting polarizing mirror with the secondary spectrometer (8cm x 8cm, m=2 non-magnetic, guide field vertical)
6. Within neutron guide section3: 4 frame overlap choppers (14 Hz, disk diameter 70 cm-80 cm)
7. Within neutron guide section3: adiabatic RF spin-flipper to enable the use of an additional long wavelength transmission polarizer
8. Within neutron guide section3: transmission polarizer for long wavelength
9. Within neutron guide section3: spin turning section (1m) from vertical to longitudinal direction
10. Neutron guide section on secondary spectrometer carrier
11. Spectrometer arms (carrier) on air pads, sample stage, motions for scattering angle and sample rotation
12. Diaphragms, monitor at beam entrance
13. Flippers (rectangular coils, Al wire)
14. Main solenoid sets
15. Auxiliary coils (current rings) for field at flipper positions etc.
16. He gas flight tubes
17. Correction elements with piezoelectric position control
18. Background suppression collimator

19. Analyzer with magnetic solenoid

20. Detector, 3-He position sensitive area detector or preferentially 100-200 single tubes with quadratic section (2cmx2cm..3cmx3cm).

21. Option for short Fourier times (additional flippers and auxiliary coils either in sample or between main coils and $\pi/2$-flippers). The additional $\pi/2$-flippers can be also used for the ferromagnetic mode.

22. Option for paramagnetic modes

With the following additional equipment

- 40 high precision variable current sources with currents between 10-100A
- Main coil power supply
- Main coil cooling compressors
- Electronics including slow-control, data-acquisition, computers, UPS
- He gas circuit for flight paths
- Magnetic shielding including degaussing system

Further, radiation shielding, a secondary shutter, Tanzboden-floor and all sorts of general infrastructure will be needed; the cost interface has to be specified. The beam shutter must be so designed as to permit access to the secondary spectrometer while the source is operating.

**Beam extraction**

- Besides the plain optical brilliance transfer, the number of windows, functional components and air gaps has a huge impact on the sample flux (much more than any optics variations). Realistic estimates of Al thickness and air and He path-length, which the neutrons have to overcome between moderator and sample, yield loss factors between 3 and 10 for 20 Å neutrons. The construction goal will be to minimize these as far as possible. Exact values will depend on technical and safety boundary conditions.

- Polarization and deflection of the beam rely on the availability of high quality FeSi multilayer coating with $m>4$. The current simulation uses reference data of mirrors commercially available from Swiss Neutronics. Currently Swiss Neutronics has samples of $m=5$ coatings with 80% reflectivity at the edge. Depending on technological development this offers the chance that at the time of construction $m=5$ or even higher can be chosen, with the effect that the wavelength range is extended towards shorter wavelength, $\lambda < 4$ Å.
Precession coils The performance of the coils depends on the accuracy of fabrication: The two arms must be as symmetric as possible. Experience with superconducting coils at the SNS [55] shows that they perform very well; the observed rms phase fluctuations between experiments is about 3 degrees and this value includes all internal and external (in)stability effects. For details we refer to the enclosure on the comparison between water-cooled and superconducting coils. A rescaled version of the coil configuration as the one developed for this proposal will be realized and installed in 2016 at the spectrometer in Garching (MLZ). Not only will this be an implicit test of the ultimate performance of our design, but it will also allow to recognize possible unexpected sources of errors during the manufacturing or operation and thus it will contribute to a reduction of the risks. A refurbished pair of water-cooled copper coils is currently installed and tested on IN15. A comparison between them and the superconducting coils to be installed on the J-NSE will finalize the decision on which typology is most suitable for the project.

Detector The detector for the NSE is comparatively small and will contain not more than 5-10 liters $^3$He, which even at the currently elevated price will cause no significant problem. The concept with separate counting tubes requires that a manufacturer is found, who is able to deliver tubes with square cross-section in the range between $2 \text{ cm} \times 2 \text{ cm}$ and $3 \text{ cm} \times 3 \text{ cm}$. GE Reuter-Stokes will produce test pieces of such tubes that we will assess with neutrons in during 2015. A conservative estimate for this concept is a safe instantaneous count rate beyond 5 KHz/cm$^2$ and a detection efficiency close to 100% over the interesting wavelength range.

Another concept with linear position sensitive tubes as is presently in operation and construction at several SANS instruments is a possible fall-back alternative.

Magnetic shielding The compatibility and efficiency of a magnetic shielding around the spectrometer has been shown at the SNS-NSE spectrometer. The main risks here may occur from price fluctuations of Ni, respectively mu-metal. For details we refer to the enclosure on the compatibility and the effects of magnetic shielding.
1.4 Costing

At the moment it is only possible to make a rough estimation of the costing. It is based on the experience collected in the SNS-NSE construction. The costing is influenced by the definition of the “interface” between the instruments at ESS (shielding, inserts into the target block, interface points for cooling water, electrical supply etc., personal safety systems). Further the required radiation and activation limits can have a significant impact on the cost of shielding and in-beam components. Here we assumed total beamline cost starting from moderator, however, excluding target block itself. The values known from the SNS-NSE installation allow educated guesses for many components, these were applied in the costing. A detailed list of the parts with estimated investment costs as well as the influence on the costs due to technological choices (e.g. superconductor vs. water-cooled copper coils, magnetic shielding) is given as enclosure.

The table below summarizes the costs for the different options.

<table>
<thead>
<tr>
<th>Option</th>
<th>SC-coils</th>
<th>water-cooled Cu-coils</th>
<th>magnetic shielding</th>
<th>no magnetic shielding</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC-coils</td>
<td>+</td>
<td>NO</td>
<td>18.44 M€</td>
<td>15.99 M€</td>
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<td>water-cooled Cu-coils</td>
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<td>+</td>
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<td>14.2 M€</td>
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<tr>
<td>magnetic shielding</td>
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<td>+</td>
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<td>15.99 M€</td>
<td>14.2 M€</td>
<td>NO</td>
<td>+</td>
</tr>
</tbody>
</table>

Table 2: ESSENSE costing options

The following two tables give the costing for the instrument with superconducting coils either with or without magnetic shielding. The additional costs for the pulse shaping chopper are 450 k€ and they are NOT included in the tables.
<table>
<thead>
<tr>
<th>Item</th>
<th>Project 1</th>
<th>Project 2</th>
<th>Project 3</th>
<th>Project 4</th>
<th>Project 5</th>
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<td>600</td>
<td>900</td>
<td>1200</td>
<td>1500</td>
<td>1800</td>
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</table>

**Subtotal**: 3500
### 1.5 List of Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>BSS</td>
<td>Backscattering spectrometer</td>
</tr>
<tr>
<td>ESS</td>
<td>European spallation source</td>
</tr>
<tr>
<td>FOM</td>
<td>Figure of merit</td>
</tr>
<tr>
<td>FRM-II (MLZ)</td>
<td>Forschungs-Neutronenquelle Heinz Maier-Leibnitz (Garching, Germany)</td>
</tr>
<tr>
<td>HRNSE</td>
<td>High resolution neutron spin-echo</td>
</tr>
<tr>
<td>IMNSE</td>
<td>Intensity modulated neutron spin-echo</td>
</tr>
<tr>
<td>IN15</td>
<td>Neutron spin echo at ILL</td>
</tr>
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<td>IT</td>
<td>Information Technology</td>
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<tr>
<td>J-NSE</td>
<td>Jülich neutron spin-echo at MLZ</td>
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<td>MD</td>
<td>Molecular Dynamics</td>
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<tr>
<td>MLZ</td>
<td>Maier-Leibnitz Zentrum (Garching)</td>
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<tr>
<td>NSE</td>
<td>neutron spin-echo (spectrometer)</td>
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<td>PE</td>
<td>Polyethylene</td>
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<td>PEO</td>
<td>Polyethyleneoxide</td>
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<td>RF</td>
<td>Radio Frequency</td>
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<td>Spallation Neutron Source (Oak Ridge, TN, USA)</td>
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<td>SNS-NSE</td>
<td>Jülich neutron spin-echo at SNS</td>
</tr>
<tr>
<td>TDR</td>
<td>Technical Design Report (ESS)</td>
</tr>
<tr>
<td>WASP</td>
<td>Wide Angel Spin Echo, instrument under construction at ILL</td>
</tr>
<tr>
<td>WANSE</td>
<td>Wide Angel Neutron Spin Echo, generic wide angle NSE</td>
</tr>
<tr>
<td>UNSE</td>
<td>Ultra high resolution NSE</td>
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</table>
PROPOSAL HISTORY

New proposal: (yes)
Resubmission: (no)

References


Enclosures
Remark: Configuration and operation mode for very short Fourier-times

The short-time-mode-2 ("shorty-2") setup shall allow to continue NSE operation down to a few ps. This is achieved by employing an effective field integral that results from the difference between two path segments on each arm. The path segments are separated by an extra \( \pi \)-flipper. One segment collects mainly contributions from the main solenoid and the sample-field coils, whereas the second segments is controlled by the additional "shorty-2" coils between the end of the main solenoid and the \( \pi/2 \)-flipper. This configuration enables various operation modes, i.e. varying only the main solenoid current or only the shorty-coil current or both during a scan. Examples are illustrated in figure 14, the field patterns and geometry of the setup is shown in figure 15.

![Figure 14: Axial field along one spectrometer arm for Fourier-time settings in the ps-regime. Example (left) shows operation with fixed main solenoids (50 mA), the effective difference field integral is controlled by combined action of the sample field coils and the shorty coils. Example (right) shows the situation for fixed sample position field, main solenoids fixed to values between 50 mA and 90 mA depending of Fourier-time. The dashed magenta curve illustrates the need to increase the main solenoid current in order not to create zeroes in the field. The black 1 ps curve leads to \( 3 \mu \text{Tm} \) inhomogeneity whereas the red one for 80 ps yields less than \( 1 \mu \text{Tm} \).](image)

The strategy shall be chosen such that the field stays at reasonable levels over the whole path such that the neutrons do not depolarize, in particular the field shall have no zeroes in the beam zone. On the other hand the field values -especially that of the shorty-2-coils- shall be limited such that the induced field integral inhomogeneity stays low. Achievable values of the integral inhomogeneity are between \( 1 \cdots 3 \mu \text{Tm} \).
Figure 15: Geometry and field pattern of shorty-2 for a 20 ps (at 8 Å) setting. The red line illustrates the axial field curve shape, the dashed horizontal line indicates the 1 Gauss level. The dotted lines show the z-field component due to flippers. Not shown are auxiliary coils that may be used to optimize the π-flipper operation by adding around 0.1 Gauss z-component to the field around the flipper.

There are several advantage of this type of range extension to lower Fourier-times:

- no space required in the sample zone
- no extra length is needed
• since the effective field integral results form a difference, it may even be set to zero without depolarization of the beam.

The price for this is the need for two additional $\pi$-flippers. In the construction phase it shall be considered how these may be remotely controlled moved out of the beam when not in use.

The additional elements in one spectrometer arm for “shorty-2” are the compensated solenoid that is responsible for the peak in the field curve shown in figure 15 and the extra $\pi$-flipper located inside the main coil warm bore.
Remark: Compatibility with extra $\pi/2$ flippers

We have tested that it is possible to insert two extra $\pi/2$ flippers between the main precession coils and the sample without compromising the functionality of the spectrometer and without adding any extra space. These extra flippers can be used either for the shorty-1 option or for the (optional) ferromagnetic scattering operation-mode. The figure below shows, e.g., a possible field configuration compatible with a shorty-1 mode. The extra $\pi/2$ flipper are position at circa $\pm0.7$ m while extra precession coils are inserted to generate the field of 46 Gauss.

**Figure 16:** Longitudinal component of the magnetic field along the axis in the sample region, for a Fourier time of 0.1 ns. The two minima at circa $\pm0.7$ m coincide with the position of the extra $\pi/2$ flippers.
Remark: Magnetic field changes and tuning upon prolongation

As was asked for by several users concerning the installation of special sample equipment or modes for magnetic scattering, the option to prolong the distance between the spectrometer arms and the sample stage shall be foreseen. The extra space will allow to install more bulky sample environments, which may contain specialized setups from the user. Further space may be gained for magnetic modes (ferromagnetic, intensity modulated) even if at this moment only the principle possibility shall be kept open. The mechanical issues of the prolongation shall be solved in a way that no further mechanical adjustments become necessary. Both arms and the sample stage will be on airpads such that only a few Newtons force is needed to move them. The additional space may be realized by inserting pieces from a collections of fixed distance connectors with exact mechanical fittings. This operation should require less that 1h of hands on mechanical work. Besides the provision of the distance pieces the cabling must provide the needed extra length.

Concerning magnetic fields and tuning, only the sample space and the π-flipper is involved. For the prolongation to be effective, the π-flipper is to be mechanical attached to one of the arms that are retracted (say the primary arm). The prolongation affects the current settings of the instrument therefore only for the sample field coils both for the in plane field (since the coils are also retracted) and for the z-component field since this is used for optimal π-flipper operation. The additional measure for larger prolongation acceptance consists of a slight increase in diameter of the z-coils (creating a fraction of a Gauss field at the sample resp. π-flipper location.

In figure 17 the field pattern for situation in standard and prolonged mode are displayed (for 1 Tm and 0.01 Tm field integral).
Figure 17: Axial field in standard configuration (solid line) and in a configuration at $J = 1\text{Tm}$ (black) and $J = 0.01\text{Tm}$ (red, multiplied by 50) with a retraction of 0.3 m at each side (dashed line) –gain: extra 0.6 m sample space.

Figure 18 the values of the currents that have to be adjusted according to the prolongation distance are displayed.
**Figure 18:** Values of the currents in the sample field solenoid pairs (2x200 turns, 2x30 turns) for x- and z-directions (triangles, solid circles).

The phase-zero current value moves by 100 A × turns by the 0.3 m prolongation.
Remark: XYZ polarization analysis

In order to perform (para)magnetic scattering a set of xyz-magnetic field coils can be installed. We have tested that this is compatible with the layout of the secondary spectrometer.

For the generation of a field in the $z$ direction, the existing sample-field coils can be exploited. In the $x$ and $y$ direction extra coils must be installed. We tested a configuration made of a pair of quadratic coils possibly made from a framework of single Al-rods, e.g. two positioned at $y = \pm 0.34$ m before and after the sample and two positioned at $x = \pm 0.34$ m.

This arrangement allows to set the sample field either perpendicularly or parallel to the the vector $\vec{Q}$, as required in the magnetic-operating mode. Our simulations show that this is possible even at large scattering angle (e.g. up to circa 80°, corresponding to a $Q = 1.0$ Å$^{-1}$ at $\lambda = 8$ Å) without collisions either with the precession coils or with the other solsample coils.

Case 1: $\vec{B}_{\text{sample}} \parallel \vec{Q}$

Figure 19 and figure 20 show the realization of a magnetic field at the sample position perpendicular to the the scattering vector for $Q = 0$ and $Q = 1.0$ Å$^{-1}$ and for a magnetic setting corresponding to Fourier time of 40 ns.

![Diagram](image)

**Figure 19:** In the configuration shown here, the scattering angle is zero. The direction of the magnetic field changes adiabatically in the sample environment without vanishing (right panel, black = $x$-component, red = $y$-component, green = $z$-component), thus the polarization is conserved. The left panel shows the orientation of the magnetic field in the sample region; the rectangular coils, in this view from above, are the $xy$-coils. The field is oriented along $y$ like the scattering vector $\vec{Q}$. The dashed horizontal line indicates the longitudinal spin projection along the path, it shows no depolarization effects.
Figure 20: Same as in figure 19 but for a scattering angle of circa $\theta = 80^\circ$. The panel above shows the adiabaticity of the field and the orientation of the latter in the direction of $\vec{Q}$: The green coordinate system is rotated of $\theta/2$. The other two panels show the field components on a path along the axis of the spectrometer before the sample (below left) and after the sample (below right).
Case 2: $\vec{B}_{\text{sample}} \perp \vec{Q}$

The realization of a magnetic field perpendicular to the $\vec{Q}$ is easier because in the standard setup of the spectrometer the field at the sample is already oriented along the $x$ direction. Similarly to the previous case, figure 21 and figure 22 are for $Q = 1.0 \text{ Å}^{-1}$ and $Q = 0 \text{ Å}^{-1}$ and for a Fourier time setting of 10 ns.
Figure 21: The scattering angle is of circa $\theta = 80^\circ$. Differently from figure 20, the magnetic field is in the $x$ direction of the $\theta/2$-rotated coordinate system and thus perpendicular to $\vec{Q}$. The two panels below show the field components on a path along the axis of the spectrometer before the sample (below left) and after the sample (below right).
Figure 22: Configuration for a zero scattering angle. The left panel shows the orientation of the magnetic field in the sample area while in the right panel the components of the field are plotted.
Comparison between superconducting and water-cooled copper main solenoids

The choice of superconducting solenoids for ESSENSE and other NSE spectrometers is primarily motivated by the field design possibilities that are not available for normal conducting solenoids mainly because of the required volume or power densities of the windings. The current densities averaged over the winding zone are >200 A/mm² for a superconducting system compared to 2 A/mm² in a water cooled copper winding (the value correspond to the maximum rating of the J-NSE solenoids). This immediately translates into the ratio of winding volumes, respectively winding thickness. The 100 fold reduced winding thicknesses allow for coil designs with efficient fringe field compensation. Since the superconductor has no resistive losses during operation, the power consumption and dissipation is not affected by these compensations. In contrast, a normal conducting system with a main solenoid creating a certain field needs a factor 2 more current after full dipole moment cancelling fringe field compensation and an additional compensation coil with about half the number of turns and double cross-section that carries the same current. Under the assumption of keeping the conductor type this would require about 7 times the power consumption of the simple coil. In addition, for larger currents, i.e. larger fields, the required winding thicknesses are such that a compensation would collide with or even interpenetrate the main solenoid, making this kind of fringe field cancellation measure impossible. Even if still possible, the freedom of design would be very much restricted and the huge increase in power consumption and copper weight would make it rather impractical and costly. Further the 1 mm diameter wire of a superconducting system can be wound with high precision and the tolerances of the resulting windings are in the sub-mm range. In contrast copper conductors for feasible coil designs with Tm field integrals have diameters in the range of a 1.5-2.5 cm leading to corresponding errors in geometry.

Fringe field compensation is essential for the mutual decoupling of two spectrometer arms in order to reduce deterioration of field-integral homogeneity at larger scattering angles. Fringe field reduction in any direction around the instrument is a prerequisite for a surrounding magnetic shielding.

14 If this is directed only towards the sample side of the coils a partial compensation is also possible at normal conducting systems as the J-NSE or the new IN15 coils.
Figure 23: Fringe field maps of a generic partially compensated normal conducting system (right) and of the proposed fully compensated superconducting system, both shown for a field integral setting of $J=1 \text{Tm}$. The black isolines start at 1 Gauss with a separation of 1 Gauss, the dotted magenta lines cover the range from 0.1 to 1 Gauss ($0.01 \cdots 0.1 \text{mT}$). In a normal conducting system the mutual magnetic influence of the arms leads to the need of significant corrections in order to keep the homogeneity at finite scattering angle.

Low field at flipper positions is required for NSE operation, with good compensation the field at these positions stay low, irrespective of the main coil setting. The latter property contributes a lot to the stability of signals because the main solenoid is one item (rigidly connected and without geometrical temperature drifts in the case of a superconducting system). In that case any movement of the whole solenoid set has very little influence on field integral and field values between and at the flippers. The higher winding accuracy allows for narrower tolerances for the residual fields at the critical positions even at very high field-integrals.

How much the better winding accuracy influences the residual non-correctable field integral inhomogeneities is not exactly known but in any case they will be markedly lower in the superconducting case.

The Fourier-time limit at the very long time end of the scale, using the longest wavelength, is determined by the ability to correct for field integral inhomogeneities—if current technologies are considered. However, at the side of shorter wavelength that have more intensity and are required if the desired Q-values become larger the technical maximum of the field integral is the limit. Extending this requires quadratically increasing power for a normal conducting system or much more copper weight and volume. On the other hand the superconducting systems have an inherent reserve which allows for 1.5-2 $\text{Tm}$ without change of geometry or power consumption.\footnote{15 Maximum current of the powersupply and quench protection may have to be adjusted.}

15 Maximum current of the powersupply and quench protection may have to be adjusted.
Residual fields due to flux trapping or hysteresis in type II superconducting wires are a concern, which has to be considered. The design of the SC-coil system benefits from the following mitigation effects:

- The volume fraction containing superconductor is small (all windings are less than 1 cm thick).
- The wire type is selected to have a low hysteresis (see figure 24).
- Symmetry related windings are wound with wire from the same batch.
- Hysteresis properties are uniform also among different batches as checked by measurement (see figure 25).
- Since hysteresis fields in the windings correspond to currents that have sum of 0 net circulation around the beam axis. Therefore the effect on field integrals is minimal.
- Modelling of the hysteresis fields (figure 25) reveals a total integral effect corresponding to several 10s of degrees of phase and NO detectable effect of the field integral homogeneity (see figure 26).
- The net phase deviation due to hysteresis is compensated by the symmetry of the two (primary and secondary arm) coil sets, which due to electrical operation in series are always subjected to the same current history. Experiment data from the SNS-NSE [57] instrument show an overall phase-variation of less than 3 degrees rms, if sample and reference data are compared after some days of experiment operations. The variations are an absolute upper limit for hysteresis effects since they contain all effects ranging from counting statistics over residual field fluctuations, powersupply stabilities and potential hysteresis field asymmetry or creep.
**Figure 24:** Magnetisation curves of several samples from wires that will be used to wind the SC-coil sets for the renewal of the J-NSE main solenoids.

**Figure 25:** Residual field along the coil axis of the superconducting main coils of the SNS-NSE due to hysteresis (symbols) compared to prediction by a simplified model (line). The field was measured after a current ramp to 250 A and back to 0 A. The simplified model had no gap in the middle of the coils.
Figure 26: Phasescans obtained at different positions on the 32×32 cm² detector at the SNS-NSE with a reference sample at a low field integral setting (J=0.0008 Tm) using a wavelength band from 6 to 9 Å. The low and high data-points at the right side of each echo curve are obtained with $\pi/2$-flippers and all flippers off, respectively, and denote the limits given by polarisation. The setting is one within a series of field cyclings up to high field that comprise the sequence of scans during an experiment. Potential hysteresis fields are expected to be maximal at low field. As the large and uniform echo amplitudes and phase zero positions (green lines) of the depicted phase scans from individual 4×4 cm² detector patches show: there is NO detectable effect of residual fields on the resolution respectively field integral homogeneity.

A further difference between superconducting and normal-conducting coils is the **time needed for a change of field integral**. The superconducting system typically needs longer to charge and discharge. The 1 Tm field integral considered as reference here corresponds to about 0.5 MJ magnetic energy in both cases. With a power of 1 MW in case of the normal-conducting system this energy
is dissipated within 0.5 sec, however, ramp limitations in the large powersupply may extend the full sweep time to several 10s. In contrast, in the superconducting system the maximum current ramp is either limited by the supply voltage (10...20 V) compared to the system inductance (50 H) or by eddy current heating. The latter is the more restrictive limitation. For the SNS-NSE system a safe ramp speed amounts to 0.2 Tm/min, where in principle smaller steps or steps at lower total magnetic field may have up to 1 Tm/min. E.g. during a full scan from low to high Fourier-times in a number of steps a total field change of e.g. 1 Tm has to be performed, the summed time for this –assuming the conservative 0.2 Tm/min– requires 5 min “dead-time”. For a conventional sequence starting the next scan again at lowest fields one has to add another 5 min to ramp down. A realistic assumption on the average duration of a scan at ESSENSE would be about 2h (keep in mind that at ESSENSE each scan yields about 5 times as many data as can be obtained at a continuous source NSE instrument). The additional ramp time thus amounts to less than 10%. We may compare this with the efficiency effect of a 10% improvement of the overall homogeneity parameter, which depends on the coil design, the coil accuracy and the correction elements. With $\tau_{\text{max}} = H \lambda^2$, a 10% change in $H$ would allow for a 5% change in $\lambda$ and since at long wavelength the flux $\Phi(\lambda) \propto \lambda^5$ one could gain 25% intensity respectively counting time for the same sequence of Fourier-times.

The power consumption of a normal conducting solenoid with 1 Tm field integral and only local compensations for low sample and flipper positions is of the order of 1 MW electric input and 1 MW thermal output, which has to be removed by a water flow of approximately 1 m$^3$/min.

The total copper weight of the two coil systems would be 10 tons or more. Cost savings of the mere coil system (about 1.2 M€) must be balanced with the installation cost for 1 MW electrical power installation and a 1 MW cooling water circuit. During operation (assuming realistic operation parameters and times and an overall energy+cooling cost of 0.2 €/KWh) the annual difference in operation cost between the normal conducting and the SC-coils would be 230 K€.

The maximum field integral of normal conducting solenoids is limited to values below $J=1$ Tm by the steeply increase of dissipated power and copper volume and weight for larger J. Superconducting coils on the other hand can be configured for twice this value with very moderate extra effort concerning powersupply and quench diodes. E.g. the SNS-NSE coils are rated up to 1.8 Tm. With currently available correction elements the 1µs will only be reached with 20 Å neutrons and then requires a field integral of only 0.7 Tm. However, measurements at shorter times using shorter wavelength with much higher neutron intensity can considerably benefit from the ability to use larger field integrals. Figure 27 illustrates the resulting gain one may obtain in the intermediate resolution ranges by using this (virtually for-free option of a superconducting coil system).

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16Within obvious limits one always may trade copper weight with power consumption.
Figure 27: The comparison illustrates how an additional $\tau$-range at smaller wavelength becomes accessible by an extended field integral range. The highest $\tau$-points of the longer wavelength band would need better correction and therefore exhibit large errors at the end of the range. However, the field-integral extension is virtually “for free” for a superconducting system, whereas prohibitive for a normal conducting coil system.
Remark: Magnetic Shielding: Compatibility and effects

Compatibility

To estimate the influence of a magnetic shielding on the properties of the spectrometer the effect of mirror images from magnetic planes on the homogeneity were considered, see figure 28.

Figure 28: Top view of the salient coil configuration with first order mirrored coils to estimate the effect of a magnetic shielding with walls in 2 m distance from the magnetic axis. Further images are on top and below (bottom and roof of shielding).

The figure in fact represents a more benign case than the situation of just one mirror plane (due to the additional asymmetry). The starting point is the solenoid system equipped with two ideal correction coils, such that the computed variance of the field integrals is 0.7 ppm (including numerical noise). Keeping positions and settings of the correction elements the effect of a shielding plane parallel to the axis has been computed as a function of distance wall-axis. Table 3 show the results.

Table 3: Influence of magnetic shielding walls on the field integral homogeneity.

<table>
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<th>planes</th>
<th>distance / m</th>
<th>inhomogeneity / ppm</th>
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</thead>
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<td>0</td>
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<tr>
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<td>1.5</td>
</tr>
<tr>
<td>4</td>
<td>2.5</td>
<td>0.8</td>
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</table>
Further (numerical) optimization of correction currents reduces the induced inhomogeneity slightly. The results indicate that a distance of 2 to 2.5 m between inner magnetic shielding walls is needed and sufficient.

**Effects**

Any NSE setup irrespective of the method and setup used is sensitive to magnetic disturbances exceeding a few mGauss (0.1 µT) variation. A magnetic shielding around an NSE spectrometer has been proven to be feasible and effective at the SNS-NSE spectrometer. To provide sufficient attenuation with a limited amount of µ-metal it has to consist of 2 shells that are separated by several decimeters. In practice this gap can be used to take up the material (concrete or heavy concrete) needed from radiation shielding.

As the operation of the older existing NSE spectrometers shows it is possible to do experiments—with some additional effort to compensate static environmental fields by extra coils and current loops—also without shielding. However, ability to perform measurements and even more the data quality is vulnerable and may be hampered by various external magnetic disturbances. These may be monitored by sensitive magnetometers or inferred from other information. If detected the data acquisition of the NSE is paused. Frequent interruption are caused by the use of cranes that distorts the earth-field depending on their position. Further the use of strong magnets at neighbour instruments will in many cases lead to the mutual incompatibility of data collection. Farther field sources may still add to the effective noise of the NSE results, in particular if changes occur during a so-called phase-scan. A compromise between residual extra noise and non-operation must be found and thus determines the thresholds for a halt of NSE-data acquisition.

Besides the interference with NSE operation, in practice, the magnetic sensitivity of any instrument (here NSE) imposes restriction on all neighbours and surrounding technical and building structures. Freedom of crane usage must be restricted and certain magnetic sample environments and installations can only be used at adjacent instruments under the pressure that a blocking of another instrument (here NSE) by this exerts.

Of course it is difficult to predict how frequent situations with relevant interference will occur at the ESS installation. However, crane movements will always be required and magnetic field experiments at other instruments are badly predictable and will largely depend on the drifts and trends the scientific focus will undergo in the coming few decades.

The experience at J-NSE shows that depending on activities at other instruments up to 5% of counting time is blocked due to crane movement, during 5% of the time the instrument is grounded due to scheduled magnetic field experiment at neighbour instruments and another estimated 5% of results have to be questioned or discarded a posteriori due to detected magnetic disturbance. The additional noise on the accepted data is still difficult to assess.
<table>
<thead>
<tr>
<th>effect</th>
<th>advantage</th>
<th>disadvantage</th>
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<tbody>
<tr>
<td>shielding ESSENSE from outer magnetic fields</td>
<td>stable operation, better data quality, less counting time losses</td>
<td>cost, fully compensated coils are mandatory</td>
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<tr>
<td>minimizing restrictions to neighbour instruments</td>
<td>crane operation and use of magnetic sample environments on neighbour instruments does not interfere, no need for <em>mutual exclusive</em> operation.</td>
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<tr>
<td>shielding neighbour instruments form ESSENSE fringe fields</td>
<td>allows operation of magnetically sensitive neighbour instruments even without extra shielding.</td>
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</tr>
<tr>
<td>removing requirements to amagnetic building structures and magnetically quiet installations</td>
<td>effort and <strong>cost savings</strong> on ESS side.</td>
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</table>

*Table 4: Magnetic shielding: pro’s and con’s.*
Other Instruments

In addition to the comparison with IN15 in the main text as standard, here we show $S(Q,t)$ data simulated for SNS-NSE for the same sample scattering functions and using the same detector patch area as in the ESSENSE vs. IN15 juxtaposition. The SNS-NSE instrument is closest to ESSENSE in the sense that it also uses time-of-flight to tag wavelength within a frame. However, due to the higher repetition frequency of 60 Hz the frame width is restricted to $\Delta \lambda < 3.6$ Å. Further the present intensity ratio to ESS is given by a factor 5 in source power and a wavelength depended factor in the range of 5 in moderator brilliance.

![SimRes:Polyethylene Instr:SNS−NSE Mod:SNS−cold runtime/h: 17.11 nphas= 20 24 28 Mw= 10.0000 $\Phi$= 0.9999 d= 0.0005 ctime/s=100.0000 $q= 0.305 \lambda= 3.20 3.92$ $q= 0.256 \lambda= 3.92 4.64$ $q= 0.220 \lambda= 4.64 5.36$ $q= 0.193 \lambda= 5.36 6.08$ $q= 0.171 \lambda= 6.08 6.80$](image1)

![SimRes:Polyethylene Instr:SNS−NSE Mod:SNS−cold runtime/h: 17.11 nphas= 20 24 28 Mw= 10.0000 $\Phi$= 0.9999 d= 0.0005 ctime/s=100.0000 $q= 0.195 \lambda= 5.20 6.10$ $q= 0.169 \lambda= 6.10 7.00$ $q= 0.148 \lambda= 7.00 7.90$ $q= 0.132 \lambda= 7.90 8.80$](image2)

**Figure 29:** Simulations for the SNS-NSE spectrometer. Comparison of the first sample example (incoherent scattering from PE) assuming the same counting times. To cover the same range as ESSENSE at least two wavelength settings are needed. The error bars in both cases are considerably larger than those expected for ESSENSE.
Figure 30: Simulations for the SNS-NSE spectrometer. Left: comparison of the second sample example (coherent scattering from PEO) assuming 10 times longer counting times. To cover the same range as ESSENSE at least two wavelength would be are needed. Here we compare the frame corresponding to the central frame of the ESSENSE example. The error bars still are larger than those expected for ESSENSE. Right: comparison of the second sample example (coherent scattering from PEO) assuming 50 times longer counting times. Instead of 3 curves here all counts are summed to yield one curve. Here we compare the frame corresponding to the central frame of the ESSENSE example.

The highest Fourier time points have large error bars due to the limitation in field integral homogeneity, which is improved by a factor of 2.5 in the ESSENSE design.

Besides that, the ratio of overall efficiency (time needed to collect information on $S(Q,t)$) is determined by the power ratio $\times$ moderator efficiency ratio $\times$ frame width ratio and is of the order of 50 at intermediate wavelength and more for long wavelength.
Costing supplement

Compilation of hardware parts only. 17 Note that this list contains the costs for the optional pulse shaping chopper, which has not yet been included in the global costing tables (section 1.4).

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</tr>
<tr>
<td>current_supply_1</td>
<td>Current supply for longitudinal field coil of spin rotation sector</td>
<td>10</td>
</tr>
<tr>
<td>current_supply_2</td>
<td>Current supply for longitudinal field guide</td>
<td>10</td>
</tr>
<tr>
<td>sensors_guide</td>
<td>Radiation, temperature and vacuum monitors along neutron transport</td>
<td>30</td>
</tr>
<tr>
<td>sensor_interface</td>
<td>Interfacing for sensors_guide</td>
<td>10</td>
</tr>
<tr>
<td>secondary shielding</td>
<td>Radiation shielding walls, enclosure around spectrometer as required for radioprotection</td>
<td>800</td>
</tr>
<tr>
<td>beam stop</td>
<td>Primary beam stop behind the spectrometer</td>
<td>20</td>
</tr>
<tr>
<td>magnetic shielding</td>
<td>Double walled mu-metal enclosure, if needed it has to be integrated into the secondary radiation shielding</td>
<td>2200</td>
</tr>
<tr>
<td>degaussing system</td>
<td>Demagnetisation system for magnetic shielding</td>
<td>60</td>
</tr>
<tr>
<td>tanzboden</td>
<td>Granite floor, enabling motion of the spectrometer arms on air cushions</td>
<td>150</td>
</tr>
<tr>
<td>guide 7 26.5-28m</td>
<td>Last section of guide leading up to the first π/2-flipper, must have a guide field coil wound around it</td>
<td>50</td>
</tr>
<tr>
<td>carrier-structure</td>
<td>Mechanical carrier structure of the spectrometer comprising first and second arm and sample platform, all on air pads</td>
<td>100</td>
</tr>
<tr>
<td>sample stage carrier</td>
<td>Sample column, height variation, attached rotateable ring to hold n sample field coils</td>
<td>120</td>
</tr>
<tr>
<td>pressurized air control</td>
<td>Tubing, control valves, sensors for the pressurized air to operate the air pads and beam attenuators etc.</td>
<td>20</td>
</tr>
<tr>
<td>entrance diaphragm</td>
<td>Variable entrance diaphragm behind the neutron guide exit and before the main monitor</td>
<td>15</td>
</tr>
<tr>
<td>beam attenuator</td>
<td>Beam attenuator (different factors), behind the main monitor</td>
<td>10</td>
</tr>
<tr>
<td>sample-diaphragm</td>
<td>Variable diaphragm in front of the sample</td>
<td>15</td>
</tr>
<tr>
<td>detector-diaphragm</td>
<td>Variable diaphragm controlling the illuminated detector area, especially the low-Q side, alternative: floor fixed beam stop</td>
<td>15</td>
</tr>
<tr>
<td>collimator</td>
<td>Collimator in front of the analyzer detector, (with motorized adjustment)</td>
<td>60</td>
</tr>
</tbody>
</table>

17Items that were left without price tag require the material cost quoted for the group (flippers, solenoids ..) and mainly internal workshop hours (staff costs, not included in this table) and some amount of the consumables.
<table>
<thead>
<tr>
<th>Component</th>
<th>Description</th>
<th>Current Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>curr-flip1</td>
<td>current supply for flipper_1, rampable</td>
<td>15</td>
</tr>
<tr>
<td>curr-flip2</td>
<td>current supply for flipper_2, rampable</td>
<td>15</td>
</tr>
<tr>
<td>curr-flip3</td>
<td>current supply for flipper_3, rampable</td>
<td>15</td>
</tr>
<tr>
<td>curr-flip4</td>
<td>current supply for flipper_4, rampable</td>
<td>15</td>
</tr>
<tr>
<td>curr-flip5</td>
<td>current supply for flipper_5, rampable</td>
<td>15</td>
</tr>
<tr>
<td>curr-flip6</td>
<td>current supply for flipper_6, rampable</td>
<td>15</td>
</tr>
<tr>
<td>curr-flip7</td>
<td>current supply for flipper_7, rampable</td>
<td>15</td>
</tr>
<tr>
<td>corrector_3.1</td>
<td>correction element at entrance of first coil</td>
<td>40</td>
</tr>
<tr>
<td>corrector_1.1</td>
<td>correction element at sample side of first coil</td>
<td>20</td>
</tr>
<tr>
<td>corrector_1.2</td>
<td>correction element at sample side of second coil</td>
<td>20</td>
</tr>
<tr>
<td>corrector_3.2</td>
<td>correction element at detector side of second main coil</td>
<td>40</td>
</tr>
<tr>
<td>curr_lcc3.1</td>
<td>current supply for corrector_3.1</td>
<td>15</td>
</tr>
<tr>
<td>curr_lcc3.2</td>
<td>current supply for corrector_3.2</td>
<td>15</td>
</tr>
<tr>
<td>curr_lcc1.1</td>
<td>current supply for corrector_1.1</td>
<td>15</td>
</tr>
<tr>
<td>curr_lcc1.2</td>
<td>current supply for corrector_1.2</td>
<td>15</td>
</tr>
<tr>
<td>yz-stage_3.1</td>
<td>yz-adjustment stage for corrector_3.1</td>
<td>20</td>
</tr>
<tr>
<td>yz-stage_3.2</td>
<td>yz-adjustment stage for corrector_3.2</td>
<td>20</td>
</tr>
<tr>
<td>yz-stage_1.1</td>
<td>yz-adjustment stage for corrector_1.1</td>
<td>20</td>
</tr>
<tr>
<td>yz-stage_1.2</td>
<td>yz-adjustment stage for corrector_1.2</td>
<td>20</td>
</tr>
<tr>
<td>yz-controller_1</td>
<td>ye-motion controller for 1st arm and interface</td>
<td>20</td>
</tr>
<tr>
<td>yz-controller_2</td>
<td>ye-motion controller for 2nd arm and interface</td>
<td>20</td>
</tr>
<tr>
<td>SHTERS</td>
<td>material for z-shifters</td>
<td>5</td>
</tr>
<tr>
<td>zcurr-shift3.1</td>
<td>current sheet for z-shift at 3.1 correction (option?)</td>
<td>15</td>
</tr>
<tr>
<td>zcurr-shift1.1</td>
<td>current sheet for z-shift at 1.1 correction (option?)</td>
<td>15</td>
</tr>
<tr>
<td>zcurr-shift3.2</td>
<td>current sheet for z-shift at 3.2 correction (option?)</td>
<td>15</td>
</tr>
<tr>
<td>zcurr-shift1.2</td>
<td>current sheet for z-shift at 1.2 correction (option?)</td>
<td>15</td>
</tr>
<tr>
<td>curr_shift3.1</td>
<td>current supply (rampable) for curr_shift3.1</td>
<td>15</td>
</tr>
<tr>
<td>curr_shift1.1</td>
<td>current supply (rampable) for curr_shift1.1</td>
<td>15</td>
</tr>
<tr>
<td>curr_shift3.2</td>
<td>current supply (rampable) for curr_shift3.2</td>
<td>15</td>
</tr>
<tr>
<td>curr_shift1.2</td>
<td>current supply (rampable) for curr_shift1.2</td>
<td>15</td>
</tr>
<tr>
<td>curr_phacomp</td>
<td>current supply for phase-comp</td>
<td>15</td>
</tr>
<tr>
<td>curr_phase1</td>
<td>current supply for phase coil 1</td>
<td>15</td>
</tr>
<tr>
<td>curr_phase2</td>
<td>current supply for phase coil 2</td>
<td>15</td>
</tr>
<tr>
<td>main-coil-set pair</td>
<td>system consisting of 2 cryostats that each contain a set of superconducting coils</td>
<td>2500</td>
</tr>
<tr>
<td>curr_sample1</td>
<td>current supply for main coils (4 quadrant, with quench protection)</td>
<td>130</td>
</tr>
<tr>
<td>sec_cooling system</td>
<td>piping, valves, filters, flowmeters, 50 -60 KW heat exchanger</td>
<td>60</td>
</tr>
<tr>
<td>SOLENOIDS</td>
<td>material (Cu-wire, supports, etc. for all normal conducting auxiliary solenoids</td>
<td>65</td>
</tr>
<tr>
<td>phase-comp</td>
<td>phase compensating coil (in warm box) for asymmetric cc3 correctors</td>
<td></td>
</tr>
<tr>
<td>phase-coil1</td>
<td>phase coil in warm bore of solenoid 1</td>
<td></td>
</tr>
<tr>
<td>phase-coil2</td>
<td>phase coil in warm bore of solenoid 2</td>
<td></td>
</tr>
<tr>
<td>solpi2.1</td>
<td>ring coil, part of the field control at the first $\pi/2$-flipper position</td>
<td></td>
</tr>
<tr>
<td>solpi2.2</td>
<td>ring coil, part of the field control at the last $\pi/2$-flipper position</td>
<td></td>
</tr>
<tr>
<td>solpi2.3</td>
<td>ring coil, part of the field control at the last $\pi/2$-flipper position</td>
<td></td>
</tr>
<tr>
<td>solpi2.1.2</td>
<td>ring coil, part of the field control at the last $\pi/2$-flipper position</td>
<td></td>
</tr>
<tr>
<td>solpi2.2.2</td>
<td>ring coil, part of the field control at the last $\pi/2$-flipper position</td>
<td></td>
</tr>
<tr>
<td>solpi2.3.2</td>
<td>ring coil, part of the field control at the last $\pi/2$-flipper position</td>
<td></td>
</tr>
<tr>
<td>solsample1</td>
<td>ring coil in sample region to control the field at the sample position at arm1</td>
<td></td>
</tr>
<tr>
<td>solsample2</td>
<td>ring coil in sample region to control the field at the sample position at arm2</td>
<td></td>
</tr>
<tr>
<td>solplz</td>
<td>ring coil around sample stage below scattering plane</td>
<td></td>
</tr>
<tr>
<td>solplh</td>
<td>ring coil around sample stage above scattering plane</td>
<td></td>
</tr>
<tr>
<td>solsample_z_y.a</td>
<td>ring coil rotating around sample position to set horizontal field at sample</td>
<td></td>
</tr>
<tr>
<td>solsample_z_y.b</td>
<td>ring coil rotating around sample position to set horizontal field at sample</td>
<td></td>
</tr>
<tr>
<td>currpi2.1</td>
<td>current supply for circuit solpi2.1.1-solpi2.1.2</td>
<td>10</td>
</tr>
<tr>
<td>currpi2.2</td>
<td>current supply for circuit solpi2.2.1-solpi2.2.2</td>
<td>10</td>
</tr>
<tr>
<td>currpi2.3</td>
<td>current supply for circuit solpi2.3.1-solpi2.3.2</td>
<td>10</td>
</tr>
<tr>
<td>currpic</td>
<td>current supply for circuit solpic</td>
<td></td>
</tr>
<tr>
<td>currsample_z</td>
<td>current supply for circuit solsample_z_x.low-solsample_z_x.high</td>
<td></td>
</tr>
<tr>
<td>currsample_xy</td>
<td>current supply for circuit solsample_x_y.a-solsample_x_y.b</td>
<td></td>
</tr>
<tr>
<td>solpic2.1</td>
<td>ring coil close to inner $\pi/2$-flipper for shorty/ferro operation 1st arm</td>
<td></td>
</tr>
<tr>
<td>solpic2.2</td>
<td>ring coil close to inner $\pi/2$-flipper for shorty/ferro operation 2nd arm</td>
<td></td>
</tr>
<tr>
<td>solshrt1</td>
<td>compensated ring coil set for shorty operation in the sample region 1st arm</td>
<td></td>
</tr>
<tr>
<td>solshrt2</td>
<td>compensated ring coil set for shorty operation in the sample region 2nd arm</td>
<td></td>
</tr>
<tr>
<td>Description</td>
<td>Quantity</td>
<td></td>
</tr>
<tr>
<td>-------------------------------------------------</td>
<td>----------</td>
<td></td>
</tr>
<tr>
<td>currpic2 1 current supply for solpic2.1-solpic2.2</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>currshrt.1 current supply for solshrt.1</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>currshrt.2 current supply for solshrt.2 (phase=diff currshrt1-currshrt2)</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>solpic2.1 ring coil at the π/2 side of main solenoid set for π-operation in shorty2 mode, 1st arm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>solpic2.2 ring coil at the π/2 side of main solenoid set for π-operation in shorty2 mode, 2nd arm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>solshrt2.1 compensated ring coil set close to outer π/2 flipper for shorty 2 mode, 1st arm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>solshrt2.2 compensated ring coil set close to outer π/2 flipper for shorty 2 mode, 2nd arm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>solextra2.1 ring coil to reduce inhomogeneities at the π/2-flipper position when shorty2 mode, 1st arm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>solextra2.2 ring coil to reduce inhomogeneities at the π/2-flipper position when shorty2 mode, 2nd arm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>solpic22 1 current supply for circuit solpic22.1-solpic22.2</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>solpic22 2 current supply for circuit solpic22.1-solpic22.2</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>curextra.1 current supply for solextra2.1</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>curextra.2 current supply for solextra2.2</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>solanalyzer set of coils for the analyzer field</td>
<td></td>
<td></td>
</tr>
<tr>
<td>curranalyzer current supply for analyzer</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>curranalyzer+ short-term (low accuracy) high current supply for magnetization of analyzer</td>
<td>15</td>
<td></td>
</tr>
<tr>
<td>analyzer drive</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>analyzer housing</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>analyzer multilayer analyzer (either FeSi m=4.5 or FeCoTiV m=3..3.5)</td>
<td>475</td>
<td></td>
</tr>
<tr>
<td>monitor 1 monitor for entering beam intensity, eventually prompt gammas from Al window</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>detector 300 or 400 mm area detector 100-200 single 2x2..3x3 cm counting tubes</td>
<td>450</td>
<td></td>
</tr>
<tr>
<td>flight path atmosphere windows, flight tubes and enclosures for collimator, analyzer etc to hold a He atmosphere</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>He-circuit He supply, circulating pumps, heat exchanger, purity sensors etc.</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>background shielding detector enclosure from B4C, beam catcher at sample stage for high scattering angles, enclosure of beam path</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>electronics control computers with interfaces, motor controllers, power supply interfaces, sensor inputs, air pad control, auxil</td>
<td>150</td>
<td></td>
</tr>
<tr>
<td>UPS online, redundant, 2 x 10 KW or 2 x 20 KW</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>safety shutter control, control of atmosphere, etc.</td>
<td>25</td>
<td></td>
</tr>
<tr>
<td>safety IPTS with all panels, sensors and dedicated cabling</td>
<td>75</td>
<td></td>
</tr>
<tr>
<td>electrica General electrical distribution, fusing, emergency shut down, light and plugs in enclosures</td>
<td>100</td>
<td></td>
</tr>
<tr>
<td>cable a considerable amount of cables is necessary</td>
<td>50</td>
<td></td>
</tr>
<tr>
<td>cooling water cooling water manifold, surveillance, eventually heat exchangers</td>
<td>40</td>
<td></td>
</tr>
<tr>
<td>pressurized air pressurized air manifold, surveillance (compressor?)</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>cabin cabin for users, computers, image plate equipment etc.</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>aircondition for cabin</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>aircondition for experiment enclosure (if really closed, probable)</td>
<td>25</td>
<td></td>
</tr>
<tr>
<td>turbo pumps vacuum pumps, vacuum hoses, valves, connectors</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>tools hand tools, power tools, test equipment (oscilloscope, multimeter, counter, arbitrary waveform generator etc)</td>
<td>25</td>
<td></td>
</tr>
<tr>
<td>installation tools lifting fixtures, chopper test stands, crane for the instrument cave etc.</td>
<td>40</td>
<td></td>
</tr>
<tr>
<td>sample stage special amagnetic sample goniometers, changers etc.</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>sample environment - Bio-oven, water-bath thermostat, gas handling, vacuum pump</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>sample environment - humidity cell</td>
<td>40</td>
<td></td>
</tr>
<tr>
<td>sample environment - cryo-oven: closed cycle cryostat, high T sample stick, temperature controller</td>
<td>100</td>
<td></td>
</tr>
<tr>
<td>sample environment - simple oven</td>
<td>50</td>
<td></td>
</tr>
<tr>
<td>sample environment - high temperature oven, vacuum pump, temperature controller</td>
<td>150</td>
<td></td>
</tr>
<tr>
<td>sample environment - pressure cell, CO2-pressure pump, controller</td>
<td>100</td>
<td></td>
</tr>
<tr>
<td>Consumables (eg. travel costs, installation work from others, materials etc.)</td>
<td>2200</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>15050</td>
<td></td>
</tr>
</tbody>
</table>

**Costing Options**

Here we describe the influence of possible choices of the used technology on the costs and performance of the instrument. In particular the role of magnetic shielding and the choice
normal-conducting versus superconducting main solenoids are considered. Further possible future staging would be the addition of the pulse shaping chopper.

**Superconducting versus water-cooled copper coils**

<table>
<thead>
<tr>
<th>Parameter / Coil type</th>
<th>superconducting</th>
<th>water-cooled copper</th>
</tr>
</thead>
<tbody>
<tr>
<td>direct investment</td>
<td>2.5 M€</td>
<td>1.5 M€</td>
</tr>
<tr>
<td>indirect investment (installation of power and cooling)</td>
<td>0.1 M€</td>
<td>1 M€</td>
</tr>
<tr>
<td>maximum power consumption</td>
<td>0.05 MW</td>
<td>1.0 MW</td>
</tr>
<tr>
<td>average operation cost (power &amp; cooling)</td>
<td>90 K€ &amp; M€</td>
<td>320 K€ &amp; M€</td>
</tr>
<tr>
<td></td>
<td>Full power used at 100% of time.</td>
<td>Average power assumed 1/3 of full power used during 200 days/year.</td>
</tr>
<tr>
<td>max field integral</td>
<td>≥ 1.5 Tm</td>
<td>≤ 1 Tm</td>
</tr>
<tr>
<td>residual intrinsic inhomogeneity</td>
<td>~300 ppm</td>
<td>~300 ppm</td>
</tr>
<tr>
<td>field-integral ramp rate</td>
<td>0.1…0.2 Tm/min</td>
<td>1…2 Tm/min</td>
</tr>
<tr>
<td>hysteresis</td>
<td>type II superconductor shows a limited hysteresis but computation and operation at SNS-NSE yield no adverse effects.</td>
<td>none</td>
</tr>
<tr>
<td>winding accuracy</td>
<td>sub-mm</td>
<td>mm to cm</td>
</tr>
<tr>
<td>maximum scattering angle (geometry only)</td>
<td>90°</td>
<td>~80°</td>
</tr>
<tr>
<td>maximum stray field at 4 m distance from coil center for 1 Tm field integral</td>
<td>0.06 Gauss (0.006 mT)</td>
<td>4 Gauss (0.4 mT)</td>
</tr>
<tr>
<td>maximum stray field at 4 m distance from coil center for 1 Tm field integral WITH MAGNETIC SHIELINGING</td>
<td>&lt;=0.001 Gauss (0.1 µT)</td>
<td>N.A. → 4 Gauss (0.4 mT)</td>
</tr>
<tr>
<td>magnetic shielding possible ?</td>
<td>YES</td>
<td>NO</td>
</tr>
</tbody>
</table>

Table 6: *Comparison superconducting vs. normal coils.*
Magnetic shielding yes or no?

The magnetic shielding is an extra investment of 2 to 2.5 M€, it requires also the mandatory use of fully compensated, i.e. superconducting main solenoids. Retrofitting of a magnetic shielding would cause considerable extra-costs in terms of money and loss of operation time.

<table>
<thead>
<tr>
<th>Effect</th>
<th>Advantage</th>
<th>Disadvantage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shielding ESSENSE from outer magnetic fields</td>
<td>Stable operation, better data quality, less counting time losses</td>
<td>Cost, fully compensated coils are mandatory</td>
</tr>
<tr>
<td>Minimizing restrictions to neighbour instruments</td>
<td>Crane operation and use of magnetic sample environments on neighbour instruments does not interfere, no need for mutual exclusive operation.</td>
<td>None.</td>
</tr>
<tr>
<td>Shielding neighbour instruments from ESSENSE fringe fields</td>
<td>Allows operation of magnetically sensitive neighbour instruments even without extra shielding.</td>
<td>None.</td>
</tr>
<tr>
<td>Removing requirements to amagnetic building structures and magnetically quiet installations</td>
<td>Effort and cost savings on ESS side.</td>
<td>None.</td>
</tr>
</tbody>
</table>

Table 7: Magnetic shielding: pro’s and con’s.
Remark: Pulse shaping chopper

The optional pulse shaping chopper allows to reduce the intrinsic wavelength spread by a variable factor up to 10.

The assumed pulse shaping chopper would be located at a distance of $6 \cdots 7$ m. It consists of two closely spaced synchronously co-rotating disks each with two symmetrically placed $90^\circ$ sectors. By phasing of the two disk any effective sector width between $0^\circ$ and $90^\circ$ can be set. The chopper opens twice per revolution, its frequency range is between $n \times 7$ Hz $\rightarrow$ $7 - 168$ Hz with $n = 1, 2, \cdots 24$.

The basic consideration is that a short opening at the distance $L_p = 6$ m will transmit intensity from a $\tau_p = 3$ ms long source pulse such that neutrons (with varying wavelength) will arrive at the detector distance $L_D = 35 \cdots 36$ m during a time interval $\tau_d = \tau_p(L_D - L_p)/L_p = 15$ ms. Thus we need about 4 (5) pulse-openings in the frame time-window projected to the distance $L_p$, i.e. in a time interval of $(1/f) \times L_p/L_D \simeq 71 \times 1/6 \simeq 12$ ms the pulse chopper should open 4 to 5 times in order to use as much neutron flux as possible. Further the frequency must be an integer multiple $n$ of 14 Hz. Thus an opening frequency of e.g. $336$ Hz ($n = 24$) equivalent to a rotation frequency of $168$ Hz for the pulse chopper is required. To improve separation between subframes $n$ may be somewhat reduced. In order to open the pulse window for $0.3$ ms (i.e. a nearly 10 fold reduction) then requires an opening sector of $9^\circ$ and just a 3 times improvement of wavelength resolution would be obtained with a $27^\circ$ opening.

In case of “normal” operation the pulse shaping chopper may be stopped in an open position.

Examples

Combination of the 4 frame overlap chopper system with a pulse chopper

First we show how the combination of the pulse shaping chopper works in combination with the 4-chopper frame overlap system starting at $14$ m.
Table 8: Parameters for chopper system including pulse-shaping chopper. Here: first chopper in pulse shaping mode. Pulse chopper **frequency 140 Hz**. \( L \) is the moderator distance and \( f \) the fraction of sector opening compared to the default sector.

<table>
<thead>
<tr>
<th>pulse chopper</th>
<th>chopper 1</th>
<th>chopper 2</th>
<th>chopper 3</th>
<th>chopper 4</th>
<th>detector</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L )</td>
<td>6 m</td>
<td>14 m</td>
<td>16.7 m</td>
<td>20.12 m</td>
<td>23 m</td>
</tr>
<tr>
<td>( f )</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.98</td>
</tr>
<tr>
<td>( \Delta T )</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-0.6 ms</td>
</tr>
<tr>
<td>sector</td>
<td>2 ( \times X )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The loss of intensity after reduction of the wavelength spread through the pulse shaping chopper is shown in figure 32.
Figure 32: Monte Carlo simulation of the 4-chopper frame overlap system with the pulse shaping chopper, the latter rotating at a frequency of $24 \times 7$ Hz and with an aperture of $90^\circ$ each sector.
Letters of Interest
Letter of Interest for the high resolution NSE Project at ESS

Dear panel members:

With this letter, we, Arantxa Arbe and Juan Colmenero, want to express our highest interest for the construction of the high resolution NSE instrument at the ESS. We are Research Professor and University Professor respectively at the Materials Physics Center (Joint center of the National Research Council CSIC-University of the Basque Country). The research in our Group is focused on the investigation of the structure and dynamics of soft materials based on polymers. For this we use a very successful methodology that combines experimental approaches including relaxation and scattering techniques and molecular dynamics simulations. Neutron scattering is one of the bases of this methodology; and, in particular, NSE is an extremely powerful tool. We just mention that we were coauthors —together with D. Richter and M. Mokenbusch— of the book ‘Neutron Spin Echo in Polymer Systems’ of the prestigious series ‘Advances in Polymer Science’ (Springer Verlag, Berlin Heidelberg New York) published in 2005. In this full book the crucial importance of the NSE technique to investigate the dynamical processes of polymer-based materials was highlighted and illustrated with tens of real examples. Since then the technique has been successfully applied to many other problems in systems of increasing...
complexity. We would state that indeed high resolution NSE is THE neutron scattering technique for disentangling dynamical processes in soft matter and this instrument is a must in the ESS. Of particular importance is the achievement of the microsecond range. This would allow a good overlap with relaxation techniques, a very important issue to fully understand dynamical properties in these systems.

San Sebastián, October 22, 2013

Arantxa Arbe  
Research Professor  
Tel.: + 34 943 018802  
Email: a.arbe@ehu.es

Juan Colmenero  
University Professor  
Tel.: + 34 943 018791  
Email: juan.colmenero@ehu.es
To whom it may concern,

Letter of interest for a neutron spin-echo spectrometer at the ESS

With this letter we express most strongly our interest in the development of a high resolution, high intensity, spin-echo spectrometer for the ESS. The combination of high resolution, expressed in terms of a maximum Fourier time range of the order of 1000 ns, combined with a high intensity, will allow to address challenging and exciting problems related to materials science, which are not within reach with other methods. In our field of research, which focuses primarily on studies of hydrogen dynamics in energy relevant materials, such as proton conducting oxides, an enhancement in instrumental performance in relation to present-day neutron spin-echo spectrometers will have a considerable impact. In particular, the high resolution is needed in order to study the relatively slow proton diffusion mechanisms in these systems, whereas higher intensity will allow measurements of thinner samples than those ~5-10 mm thick proton conducting oxide samples that are needed in today's measurements due to the relatively low proton concentration and suppression of incoherent scattering (Karlsson et al., Chem. Mater. 22 (2010) 740). The possibility of studying much thinner samples, combined with a reduced data collection time, further opens up unique possibilities in relation to studies under the illumination of light, which may only penetrate a few micrometers in the sample, for example.

Yours sincerely,

Maths Karlsson

Maths Karlsson, Assistant Professor
DEPARTMENT OF APPLIED PHYSICS
Chalmers University of Technology
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CHALMERS tekniska högskola AB
Reg.No: 556479-5598 VAT No: SE556479559801
Dr. Michael Monkenbusch,
Jülich Centre for Neutron Science & Institute for Complex Systems
Forschungszentrum Jülich
D-52425 Jülich

October 24, 2013

Dear Dr. Monkenbusch,

I express my strongest support for your proposal of building a neutron spin-echo (NSE) instrument at the ESS. Extending the accessible timescale to the μs and offering a dynamical range of 6 decades would make this NSE spectrometer unique in the world.

Molecules of interest for applications, such as branched alkanes, aromatics, or drugs, have slow diffusion rates in nanoporous materials when the size of the molecule is comparable to the pore size. We used the spin-echo method in several cases (e.g. Angew. Chem. Int. Ed. Vol. 43, 2004, p. 364), but we often have to increase the temperature of the sample to unrealistic values to observe diffusion. An improved resolution and a significant gain in intensity would allow us to study totally new systems in strategic domains such as catalysis, separation, or drug delivery.

I wish you success for your application.

Yours sincerely,

Hervé Jobic
Directeur de Recherche au CNRS
To whom it may concern

Berlin, 15.10.2013

Letter of interest: Neutron Spin Echo

Dear ladies and gentlemen,

with this letter we express our strong interest in the facilities of an advanced neutron-spin-echo spectrometer at the ESS. The significantly enhanced efficiency due to increase in flux at the sample, exploiting the pulsed nature of the source by multiplexing of several wavelength bands in a frame and the enhanced resolution properties of the new magnetic layout, will become essential for our research projects requiring very high resolution neutron spectroscopy.

Present projects like studies of the dynamics within microgel particles could be extended towards extensive coverage of parameters with increased data quality and resolution.

New experimentally still hardly feasible more difficult topics like dynamics at close to interface e.g. of adsorbed microgels or of confined complex fluids will first become possible to tackle.

Therefore we emphasize the importance to include the high resolution neutron spin-echo spectrometer in the ESS instrument suite.

Kind regards,

R.v. Keim
To whom it may concern

Dr. Reidar Lund  
Dept. of Chemistry, 
University of Oslo  
Postboks 1033 Blindern  
0315 Oslo  
Norway  
Email: reidar.lund@kjemi.uio.no  
Phone: +47 22 85 55 08  
20 Oct. 2013

Support for the NSE spectrometer at ESS, Lund, Sweden.

With this letter we would like to express our strong interest in an advanced neutron-spin-echo spectrometer at the ESS. The significantly enhanced efficiency due to increase in flux at the sample, exploiting the pulsed nature of the source by multiplexing of several wavelength bands in a frame and the enhanced resolution properties of the new magnetic layout, will become essential for our research projects requiring very high resolution neutron spectroscopy.

Present projects like “dynamics in block copolymer melts” or “chain dynamics in hydrogel systems” would benefit greatly from a more powerful NSE with broader dynamic range. This particularly concern slower processes such as various activated diffusion processes that is hard to resolve experimentally. Capabilities to extend the dynamic range towards microseconds would also allow NSE to close the gap to time resolved synchrotron/neutron scattering techniques. This would greatly enhance the understanding of kinetic/dynamic processes in self-assembled systems. In addition, the higher flux would allow investigations in systems where limited amount of sample is a severe issue, such as in bio-hybrids or biological systems.

Therefore we emphasize the importance to include the high-resolution neutron spin-echo spectrometer in the ESS instrument suite.

Yours sincerely,

[Signature]

Reidar Lund
To: Whom it may concern.

Subject: An advanced neutron-spin-echo spectrometer at the ESS.

With this letter I express my strong interest in the availability of an advanced neutron spin-echo spectrometer at the ESS.

A state of the art new magnetic layout on a machine designed for fully exploiting the pulsed nature of the source by multiplexing several wavelength bands in a frame will result in an unprecedented enhanced time resolution and will therefore push the NSE technique to its best. Also, the significant increase in flux will become essential for my research projects requiring very high resolution neutron spectroscopy.

I am currently working on the dynamics of polymer electrolytes. These systems are used as electrolytes for lithium batteries for car propulsion. Present projects like the dynamics of these polymer electrolytes in bulk or under confinement could be extended towards extensive coverage of parameters with increased data quality and resolution. But even more importantly, new experiments like following the dynamics of such electrolyte after an electrical excitation ("Pump-Probe" experiments) would become feasible. Such a new way of using a neutron spin-echo spectroscopy would open a brand new field of knowledge at the cross-road of Basic Science and Technology.

I therefore emphasize the importance to include the high resolution neutron spin-echo spectrometer in the ESS instrument suite.

Yours sincerely,

J.-Marc Zanotti
To whom it may concern,

with this letter we express our strong interest in the facilities of an advanced neutron-spin-echo spectrometer at the ESS. The significantly enhanced efficiency due to increase in flux at the sample, exploiting the pulsed nature of the source by multiplexing of several wavelength bands in a frame and the enhanced resolution properties of the new magnetic layout, will become essential for our research projects requiring very high resolution neutron spectroscopy.

Present projects like: **Dynamics of Water Confined in Periodic Mesoporous Organosilica** could be extended towards extensive coverage of parameters with increased data quality and resolution.

New experimentally still hardly feasible more difficult topics like: **Dynamic Properties of Low-temperature Surface Water in Mesoporous Systems, Logarithmic decay in coherent relaxations of hydrated deuterated protein powder** will first become possible to tackle.

Therefore we emphasize the importance to include the high resolution neutron spin-echo spectrometer in the ESS instrument suite.

Marie-Claire Bellissent-Funel  
Laboratoire Léon Brillouin  
CEA Saclay  
91191-Gif-sur-Yvette-Cedex
To whom it may concern,

With this letter I express my strong interest in the facilities of an advanced neutron-spin-echo spectrometer at the ESS. The significantly enhanced efficiency due to increase in flux at the sample, exploiting the pulsed nature of the source by multiplexing of several wavelength bands in a frame and the enhanced resolution properties of the new magnetic layout, will become essential for our research projects requiring very high resolution neutron spectroscopy.

Present projects like measuring the protein diffusion in crowded solutions or high concentration will be extended towards extensive coverage of parameters with increased data quality and resolution. It is especially interesting to notice that the simultaneous broad wavelength band measurement covering huge spectral domain will allow measurements of short living sample like cells. This new experimentally still hardly feasible more difficult topics like protein motions measurements in cytoplasmic environment will first become possible to tackle. Such measurements will significantly improve our understanding of the kinetics of chemical and biochemical reactions in cells.

Therefore I emphasize the importance to include the high resolution neutron spin-echo spectrometer in the ESS instrument suite.
ESS spin-echo: call for letters of interest

Dear Dr. Monkenbusch

We are writing this letter to express our interest in a spin-echo instrument at the ESS. Our group is studying, inter alia, structure & interactions in protein solutions and their dynamics (see, e.g., Roosen-Runge et al., PNAS (2011)), and we would strongly benefit from the availability of a spin echo spectrometer with a high energy resolution and a broad dynamical range at the ESS.

Yours sincerely

[Signature]

Frank Schreiber and Fajun Zhang
TO WHOM IT MAY CONCERN

Letter of Support for a high-resolution Neutron Spin Echo (NSE) instrument at ESS

Neutron scattering experiments allow to deduce information about structure and dynamics on the microscopic and mesoscopic level. This is particularly important for the investigation of soft-matter systems, as they are encountered in smart synthetic materials or biological systems. This field has seen an enormous development in recent years, where an enhanced understanding of the principles of such systems has allowed to develop increasingly complex materials with functional properties as they are required for addressing questions from the ranges of: tailored drug delivery, materials for fuel cells and energy storage, smart membranes, responsive systems, etc. Similarly our understanding of biological systems and the interactions of pharmaceutically active materials with them have been improved substantially – and this development in general is expected to be significantly further extended and to be one of the cornerstones of 21st century science.

However, this means that already now and increasingly more in the future an important part of the scientific community will study systems from the realm of soft-matter that are composed of different constituent components, encompass relevant size ranges of 1-500 nm, and will often be structured in a hierarchical way. Their detailed understanding is a challenging task and requires state-of-the-art experiments, which requires developing our experimental methods to improved levels. Here an essential technique for gaining insights into the dynamic behavior of such materials is the method of neutron spin echo (NSE), that allows to obtain information on the dynamics taking place in the size range of 1-200 nm with an unparalleled energy resolution. Such experiments are possible by the design offered by the High Resolution Neutron Spin Echo (ESSENSE), as it has been proposed to be built within the first instrument suite of ESS. The planned ESSENSE instrument would be tailored at reducing the amount of sample required (often very important for biological samples) and going to long Fourier-times (necessary to cover longer scale dynamics and to make the bridge for instance to DLS experiments), while with the high flux available at ESS being able to reduce measurement times for a given experiment quality substantially. Only a fully dedicated NSE instrument like ESSENSE could really deliver all these features, which are required to move NSE experiments into the next generation.

In my opinion such an instrument should be having highest priority as it allows to address important questions on the above mentioned systems in a unique fashion, for instance internal movements of polymer chains, nanoparticle or protein dynamics in composite
In particular, the option of contrast variation available in neutron scattering is highly important for the investigation of complex soft-matter systems as it allows to obtain information on the dynamic behavior of the individual components in a separate fashion. This is the key for understanding the properties of such systems and it can not be obtained in any comparable fashion from other methods like dynamic light scattering (DLS), x-ray photon correlation spectroscopy (XPCS), or fluorescence correlation spectroscopy (FCS). In that respect NSE is not only complementary to these above methods by covering a different q- and t-space of the dynamic information, but it is fully original as it allows to deduce information on individual components in a unique way – and this will become increasingly important in future research. Accordingly the NSE technique is absolutely essential in order to enhance our understanding of such materials important for health, energy and with innovative new properties (self-healing systems, T-responsive, etc.) further. As it can yield experimental data not to be obtained by any other methods it is also essential for providing such information to be compared to theoretical predictions and simulations, in order to advance our knowledge and understanding of such more complex systems on a sound and systematic basis.

The main shortcomings of NSE are in general that it requires a high neutron flux and it is difficult to advance it into the range long Fourier-times (and thereby normally also further into the larger size range important for the understanding of more complex materials). Here ESS with its predicted high flux and the optimized configuration of ESSENSE would offer outstanding options to advance NSE studies on complex materials onto a new level of quality and thereby also to ensure ESS world-leadership in this important field. In contrast, without this instrument ESS would not be able to position itself in this research field and leave this strategically important science area to other neutron centers, with the consequence that major developments will be done elsewhere and similarly the corresponding scientific community will work and contribute elsewhere.

This is something that ESS should strongly try to avoid as it risks ESS competitiveness in a highly important science area that is going to contribute increasingly importantly to essential areas in the fields of bringing innovative materials to work in areas of pharmaceutical delivery, materials for energy, membrane technology, catalysis etc.. Therefore I do strongly recommend to consider having a highest resolution NSE instrument in the initial instrument suite of ESS.

With best regards,

Michael Gradzielski

1. August 2014
Dear Madam/Sir

I am writing this letter in support of the neutron spectroscopy efforts at the ESS. Our group is performing, inter alia, neutron scattering experiments on proteins in solution, in many cases under crowding and pre-crystallisation conditions. Typical results are found, e.g., in F. Roosen-Runge, M. Hennig, F. Zhang, R. M.J. Jacobs, M. Sztucki, H. Schober, T. Seydel, and F. Schreiber. Protein self-diffusion in crowded solutions PNAS 108 (2011) 11815

The dynamics of the proteins under these conditions is a crucial ingredient in the understanding of these systems, in particular given that typical conditions also in biological environments are characterised, inter alia, by crowding.

I therefore very strongly support assigning high priority to high-resolution neutron spectroscopy, including in particular spin-echo and backscattering spectrometers at the ESS. Complementary use of high-resolution neutron spectroscopy, in particular with the extension of the spectroscopic energy / time scales such as proposed for the NSE instrument, is vital for an improved understanding of these complex systems. It is also important for testing advanced theoretical and simulation ideas, for which the dynamical behaviour is a key aspect, in addition to the (time-averaged) structure determined by scattering techniques without energy resolution.

Yours sincerely

Frank Schreiber
July 22, 2014

Dear Prof. Richter,

You requested some comments regarding your document entitled “The High Resolution Challenge” addressing the need for neutron spin echo (NSE) at the European Spallation Source.

At the Center for Molecular Biophysics we undertake a variety of simulation-based research, about a quarter of which is concerned with neutron scattering. We also have sizeable efforts in biofuel development, environmental biogeochemistry, supercomputing and drug design. Concerning neutron scattering we participate in the design and analysis of crystallographic, SANS, inelastic, quasielastic and spin echo experiments on biological systems.

In my opinion in the biological sciences NSE is *the most important* neutron technique to develop in the future, and, if signal-to-noise problems can be overcome, is likely to have a greater impact than any other structural or dynamic neutron scattering technique.

The reason for this opinion stems from the increasing awareness in the biological community of the critical role that slow motions play in the function of biological systems. Whereas, until recently, most of molecular biology was discussed in terms of structure, and particularly structures derived using X-ray crystallography, there is now near universal recognition that the next major advances in molecular biology will arise from understanding disorder and correlated dynamics. Some of the critical areas that need to be researched are mentioned in the report you sent. However, I would like to emphasize that the characterization of intrinsically disordered proteins and the relative motions of domains with flexible linkers have been identified as of critical importance in several biological and biomedical fields. The time-scales and length-scales relevant to biological function are those probed by NSE; not quasielastic or inelastic scattering.

To illustrate the importance of slow dynamics it suffices to describe recent trends in one field in which I specialize; that is, drug design. Whereas in the 1990s drugs, such as Tamiflu and HIV protease inhibitors, were designed using static crystallographic structures and the lock-and-key principle, within the last 10 years the state-of-the-art has come to involve ‘ensemble docking’, meaning that metastable protein states identified in molecular dynamics (MD) simulation are individually targeted. This dynamic view led to Merck’s last blockbuster, raltegravir, and has now become a standard approach in the USA. Drugs designed to be allosteric inhibitors for GPCRs function in a similar way.

Critical to the furtherance of ensemble docking will be a detailed characterization of the motions between the metastable states targeted. No experimental technique other than NSE can *directly* measure these correlated motions; X-rays cannot, NMR cannot, and single-molecule spectroscopies cannot.

The fact that recent work spearheaded by your group and others has demonstrated unequivocally that inter-domain motions can indeed be characterized using NSE is, in my opinion, the most significant technical advance in biological or soft-matter neutron scattering of the last ten years. Considerable hurdles exist before NSE becomes standard in the way that, for example, SAXS has become. The major problems are signal-to-noise and the unambiguous interpretation of the results, which will require detailed MD studies. However, if these can be overcome NSE will prove to be truly unique, and not just in a niche way. Neutron crystallography and SANS have not garnered the attention of mainstream biologists, as they have been outplayed by their X-ray counterparts. X-ray scientists have no such technique that can compete with NSE.
ESS would be remiss to not develop NSE, the neutron technique that has the potential to make the single largest impact in biology in the future.

Please do not hesitate to contact me if you wish to discuss this matter further,

Yours sincerely,

Prof. Jeremy C. Smith
UT Governor's Chair
Director, UT/ORNL Center for Molecular Biophysics
San Sebastian, July 21, 2014

Ref: Workshop on NSE-ESS

Letter of support for the Project ESSENSE

Dear organizers of the workshop NSE-ESS:

First of all I would like to thank you for inviting me to participate in the workshop about neutron spin echo in the context of ESS. I apologize very much for not attending personally the workshop. It is absolutely impossible for me to travel to Copenhagen for the scheduled date. However, I would like to contribute to the discussion with the present letter.

In my opinion the scientific case for a high-resolution NSE spectrometer at the ESS like ESSENSE is straightforward. Pushing the instrumental capabilities toward high resolution is fundamental for resolving the dynamical features of large structural units. Such big molecules or aggregates of molecules compose the field of soft matter and biological materials, and it is out of question the relevance that such kind of systems have from both, a scientific and a technological point of view. I would like to highlight in particular the importance of (i) disentangling the slow motions in proteins and bio-mimetic materials, which are fundamental for understanding the functionality of these systems and (ii) characterizing the chain dynamics in polymer-based systems, which will provide the fundamental knowledge to design tailor-made materials.

In my opinion, accessing larger Fourier times will have –at least— two important impacts for the investigation of soft-matter and biological systems: (i) to provide a good overlap with other experimental techniques as, for instance, broadband dielectric spectroscopy and NMR; (ii) to facilitate a source of validation for...
molecular dynamics simulations, not only fully atomistic, but also coarse-grained. I would like to emphasize here that the combination of neutron scattering with both, other experimental techniques and molecular dynamics simulations, has always guided my personal work in the field of polymers & soft matter. Let me focus here on the last issue, which, in my opinion, is becoming crucial. Nowadays it has become evident that the combination of neutron scattering and molecular dynamics simulations is a powerful tool for investigating soft materials, including e.g. polymers and bio-molecules. It is worthy of remark that the strategy plan of all current neutron scattering facilities contemplates this synergetic combination as one of the corner stones for future development. In particular, NSE is very well suited for this combination thanks to its large dynamic range, to the possibility of simple "deconvolution" from the instrumental resolution and to operate in the time-domain. Up to date most of the works applying such a methodology are using wide angle NSE and fully atomistic molecular dynamics simulations. Such studies have indeed demonstrated to be highly successful to address the structure and dynamics at relatively small length scales and time scales. Investigations at large length scales and long times –fundamental for soft materials and biological systems-- are limited for fully atomistic simulations, that for such goal would require constructing huge cells with many millions of atoms and running the dynamics over many computational steps with atomic discrimination. Although the future development of computing capabilities will certainly allows overcoming by “brute force” some of these difficulties, it is obvious that using coarse-grained systems will also allow exploring ‘a new world’ where the atomic details are not important, but universal properties like e.g. those depending on chain connectivity in the case of polymers, play the fundamental role. These simulations allow thus ‘increasing the effective size’ and ‘improving the time resolution’ of the investigation. Here is where the development of high-resolution NSE instruments becomes essential in my opinion. Experiments on real systems, exploring the large-scale dynamics, can provide the right validation tool to check the ‘realism’ of the coarse-grained simulations and to map the simulations results to the real world. Once the simulated system has been validated, one can calculate magnitudes that might
not be experimentally accessible like e.g. other correlation functions or mean squared displacements of molecular centers of mass, contributing in this way to a better understanding of the neutron scattering results. It is noteworthy that applying this kind of strategy opens a wide range of possibilities, including e.g. checking the validity of scaling laws and theories related with polymer dynamics or characterizing the dynamical behavior of macromolecules of different complex architectures and bio-molecules.

I thus believe that the future research of soft materials and biological systems will enormously benefit from ESSENS and thereby I am recommending upgrading this project to enter the engineering design phase as soon as possible. ESS would certainly be incomplete without this kind of instrument.

Professor Juan Colmenero
Head of the Research Line “Polymers & Soft Matter”
Materials Physics Center (CSIC-UPV/EHU)
Letter of Support for the High-Resolution Project ESSENSE

Dear Organizers of the Workshop on Neutron Spin Echo at ESS,

First, I would like to state that I am really surprised –and disappointed-- by the decision of the SAC of not recommending ESSENSE for entering the engineering design phase. On the other hand, I thank the organizers of the ‘Workshop on Neutron Spin Echo at ESS’ for inviting me to the scientific discussion about this question.

In the report, the SAC asks to strengthen the science case. In my opinion, the science case document presented ‘The high Resolution Challenge_ESSENSE’ is well structured, convincing and, being general and broad enough, also provides a large number of examples on specific systems and situations of high scientific and/or technological impact that would certainly profit from the capabilities of ESSENSE. In the following, I will try to emphasize some of the points I consider as crucial and provide a couple of examples of my particular scientific interest.

ESSENSE’s performance is summarized in two concepts (i) large length scales (big structures) and (ii) wide dynamic range emphasizing high resolution (slow motions). These are also the two key concepts involved in the extremely wide field of materials comprised under the general term ‘soft matter’ including also biological systems. This makes from ESSENSE
the natural tool to approach dynamical processes in soft- and biomaterials. Some particular examples like the cases of batteries, electrolyte membranes, encapsulated microgel particles, microemulsions, polymers in nanopores, oil recovery, planar interfaces, proteins, enzymes, drugs or macromolecular machines in biological processes have been mentioned in the science case to emphasize the huge diversity of applications. I would like to present another particular kind of systems I am currently addressing in my investigations: bio-mimetic single-chain nano-particles. These nano-particles are obtained by internal cross-link of isolated macromolecules through different synthesis routes, leading to nano-objects exhibiting diverse functionalities as e. g. drug carriers or enzymatic activity. Obviously, the slow dynamical motions of these particles are one of the key ingredient defining the type of functionality developed by them. This is of course extensible to all kinds of macromolecular systems and complexes with biological activity. Another focus of my current research is the influence of nano-objects of different nature on the chain dynamics of polymeric materials. NSE at low scattering angles and high resolution allows the characterization of the confinement of the macromolecules in diverse composites. All these studies require high resolution NSE techniques and thereby the development of ESSENSE would be of utmost interest. It is also worth mentioning here that a crucial advantage of increasing the resolution is to facilitate the overlap of the dynamic range explored by neutron scattering with that accessible by other techniques like dielectric spectroscopy. In this way, different techniques may be used in a complementary way allowing the coverage of a huge dynamic range (from pico-seconds to hundreds of seconds) over which some of the macromolecular motions usually take place.

Another requirement of the SAC is to provide arguments in favor of ESSENSE if a choice has to be made between two NSE options (high
resolution vs wide angle). I first want to state that the largest part of my research has been realized by using wide angle NSE (in the following, WANSE) and I thus know and appreciate it very much. WANSE is the most appropriate technique to investigate the dynamic structure factor in fully deuterated samples, addressing the dynamics of the structural relaxation (following the decay of correlations at the inter-molecular peak) and sometimes of other more localized processes like those involved in the secondary relaxations. Though I consider this kind of problems of high scientific interest—as I said, I devoted many years of my career to them—I honestly think that they only conform a very small fraction of the prominent questions in the general field of soft matter. Conversely, WANSE has a rather limited applicability for soft materials compared with high-resolution NSE, in the sense I will explain in the following. It is clear that one of the advantages of neutron scattering, specially for soft materials and biological systems, is the H/D labeling. WANSE studies on such labeled samples are technically very difficult due to the huge incoherent contribution from H, which kills the NSE signal at high Qs. On the contrary, the contrast between protonated and deuterated molecules originates at small angles the overwhelming coherent contribution, which analysis allows accessing the large-scale molecular motions by NSE instruments like ESSENSE—and these motions are very slow, requiring high resolution! Thus, as a soft matter researcher, my choice is very clear: ESSENSE is by far more versatile and appropriate than WANSE for the general investigations in the soft matter field.

Finally, I do not fully understand the meaning of the point ‘Develop a strategy for spin-echo instrumentation and spin-echo add-ons within the context of a wider spectroscopy suite that includes chopper and backscattering spectrometers’, but I will try to address it. Large length scales and high resolution (the two essential concepts implicitly involved in ESSENSE) are
also the two singular characteristics differentiating this instrument from the rest of the neutron scattering spectrometers. Therefore, for complementarity, I consider that it should be naturally part of the suite of instruments at the ESS. In this direction, it is also worth emphasizing that compared with BS and TOF instruments—which usually address self-dynamics of hydrogens at more or less local length scales—ESSENSE would access collective dynamics at large length scales. This means, another correlation function and thereby additional and complementary information.

I hope that the outcome of this workshop is convincing enough to reconsider ESSENSE as a candidate for entering the engineering design phase.

Yours sincerely

San Sebastián, July 21, 2014

Arantxa Arbe
Research Professor

Tel.: + 34 943 018802
Email: a.arbe@ehu.es
The main outcomes of the workshop can be summarized as follows.

https://indico.esss.lu.se/indico/conferenceDisplay.py?confId=199

The main outcomes of the workshop can be summarized as follows.
Goal 1: To inform the ESS on the choice between the high-resolution and the wide-angle spin-echo spectrometer, if only a single spin-echo instrument could be built as part of the ESS construction project.

- The high-resolution instrument will extend the ESS capabilities into the µs regime, while the wide-angle instrument will be limited to a few 10s of ns. This is somewhat better than the backscattering instrument which covers times up to about 2ns, but not at all decisive.
- ESSENSE will outperform the current best-in-class instruments by 5-20 times in flux over the wavelength range of 7-20Å, corresponding to a performance gain of 10-15 times for an average experiment on a standard setting.
- The flux gain factor is important in itself, as spin-echo is often a strongly flux-limited technique, particularly for the measurement of incoherent scattering.
- The current flux calculations do not take into account the additional gains expected from the pancake moderators, which may increase the flux on sample by up to an additional factor of two.
- The currently world-leading instruments for high-resolution NSE are IN15 (ILL), JNSE (MLZ) and SNS-NSE (SNS). IN15 and JNSE are about to be upgraded to reach longer Fourier times. ESSENSE can be expected to reach even longer Fourier times. The coil design will provide a similar field inhomogeneity per unit beam area, but the higher flux on ESSENSE will allow measurements to be performed with smaller beams and thus longer spin-echo times.
- Lessons from both the IN15 and JNSE upgrades will emerge in the coming 1-2 years, sufficiently early to feed into the ESSENSE design.
- ILL is currently building a dedicated wide-angle spin-echo instrument, WASP. An ESS wide-angle NSE instrument is expected to outperform WASP by up to a factor of 5 or so. The gain factor is less than for the high-resolution instrument, because WASP will have a better optimized guide than IN15 with a larger cross section of 55 mm x 120 mm.
- WASP will come online in 2016. The detailed study of a wide-angle NSE instrument for ESS needs to wait for the lessons from the WASP project, which will take a number of years. In particular, there are some unresolved issues relating to the correction coils for any WANSE with field integrals beyond 0.05..0.1 Tm. JCNS is investing in the WASP project and will benefit from lessons learned.
- All of the measurements enabled by a wide-angle NSE instrument at ESS can also be covered by ESSENSE, albeit with a reduced detector solid angle. ESSENSE is the obvious first NSE instrument to build, significantly extending the dynamic range of the whole facility.
ESSENSE will be able to access larger angles than existing high-resolution NSE instruments, due to the use of compensated superconducting coils minimizing the crosstalk of the fringe fields. Combined with its ability to use neutron wavelengths as low as 3-4 Å while accessing effective field integrals that span Fourier times from a few ps to \( \mu s \), this opens up a new high-Q, long-t regime, inaccessible by current instrumentation.

**Conclusion**: the high-resolution instrument is clearly the first NSE instrument to build. The wide-angle instrument is more specialized, does not significantly extend the \( q-\omega \) range of the instrument suite and has unresolved technical issues.
**Goal 2:** To strengthen the case for the ESSENSE proposal by identifying compelling science that can only be achieved by the new capabilities that it can offer.

The science case for NSE is strong and wide-ranging, covering polymers, biological materials, magnetism as well as functional and energy materials. A common feature of many such systems is the complexity of their hierarchical nature: covering length and time scales spanning many decades and requiring a detailed probing and understanding at each level. A number of essential science cases were raised some of which are mentioned below, starting with three highlights:

**Life science, protein dynamics and drug design:** understanding molecular micromechanics and dynamics in proteins to enable rational computer aided drug design. Whereas, until recently, most of molecular biology was discussed in terms of structure, and particularly structures were derived using X-ray crystallography, there is now near universal recognition that the next major advances in molecular biology will arise from understanding disorder and correlated dynamics. The characterization of intrinsically disordered proteins and the relative motions of domains with flexible linkers have been identified as of critical importance in several biological and biomedical fields. The time- scales and length-scales relevant to biological function are those probed by ESSENSE. Whereas in the 1990s drugs, such as Tamiflu and HIV protease inhibitors, were designed using static crystallographic structures and the lock-and-key principle, within the last 10 years the state-of-the-art has come to involve 'ensemble docking', meaning that metastable protein states identified in molecular dynamics (MD) simulation are individually targeted. This dynamic view led to Merck's last blockbuster, raltegravir, and has now become a standard approach in the USA. Drugs designed to be allosteric inhibitors for G protein-coupled receptors (GPCRs) function in a similar way. Critical to the furtherance of ensemble docking will be a detailed characterization of the motions between the metastable states targeted. No experimental technique other than NSE can directly measure these correlated motions; X-rays cannot, NMR cannot, and single-molecule spectroscopies cannot. In opening this window ESSENSE will be THE tool for calibration tuning and verification of state-of-the art MD-methods in general and in particular for computer aided drug design.

**Interface and surface dynamics, tribology and lubrication:** Wear and friction are ubiquitous in machines and vehicles, where they cause huge economical losses. Friction and drag are responsible for about 1/3 of the total energy needed to run machines. Proper lubrication is essential and must work over large ranges of temperatures, pressures or chemical environments. In biological systems like joints with glycoproteins controlling the friction between cartilages, loss of effectiveness can be painful. Understanding the role of solid-surface fluid boundary on molecular scale is essential to optimize or develop new lubrication systems. Information on the mobility and response of the lubricant molecules close to the surface are vital for understanding the force transmission into the liquid or in the regime of boundary lubrication. Dynamics of such boundary layers are accessible by neutron spectroscopy only in nanoporous systems but also -only recently demonstrated-- at smooth extended flat surfaces due the newly developed grazing incidence NSE technique, which will further gain by a resonator sublayer. Scattering origins from the evanescent neutron
wave function extending a few 100nm into the liquid phase side. With resonator enhancement by more than an order of magnitude and general ESSENSE related gain factors (20) the latter method will allow systematic and routine surface dynamics investigations. Flat surfaces will also allow to apply external fields (flow, pressure, electrical ...) to the boundary layer. Tribology is one example of a huge field which relies strongly on the understanding of surface dynamics, and which could be transformed by joint application ESSENSE and thereby boosted molecular dynamics simulations.

**Functional and self-healing polymers:** Self-healing materials are an emerging class of functional materials with strong potential in technological applications. The healing functionality of such materials enables the recovery of fracture and of barrier properties or improves corrosion resistance under harsh conditions, e.g., in surface materials or in coatings. Self-healing elastomers are the ideal candidates for robust and long lasting dynamic sealings or vibration damping with huge possible economic impact due to mainly longevity, cost-saving seals for vehicles, heavy-duty seals for wind turbines, vibration abatement systems for roads and bridges, noise abatement systems or even asphalt mixtures. The candidate materials with the desired properties essentially consist of dense polymeric networks with flexible linkages that rely on various association mechanisms like reversible H-bonds, reversible polymerization or chain (re)-entanglement. The recovery process is highly dependent on the mobility and diffusion of the polymer chains inside the material. ESSENSE is an ideal tool to investigate the relevant molecular mobilities and diffusion properties that are prerequisites for the healing mechanisms.

**Further hot topics are:**

- **Proton dynamics in fuel cell membranes:** localized proton motions and the nature of proton traps. The study of thin films is critically flux-limited and would be opened up by ESSENSE. Local (jump) motion at lattice spacing distance even with only a few ns time scale needs high resolution NSE due to the small wavelengths imposed by the spatial scales.
- **Relaxation of ion-polymer dynamics in battery electrolytes**
- **The increasingly hierarchical nature of the systems of interest increases the need to properly understand their internal dynamics. Synthetic capabilities are dramatically increasing and allowing the creation of complex architectures with lots of internal degrees of freedom. Tailoring and understanding such systems requires molecular dynamics simulations, which rely on understanding the underlying force fields. HR-NSE is required for validating these force field parameters.**
- **Neutrons can play a big role not only in drug design but also in understanding the molecular basis of disease, underpinning and verifying simulations. Spin-echo is unique placed for that.**
- **The leading edge studies of high-resolution NSE and molecular dynamics simulations are moving in parallel and need each other to progress. MD will soon be routinely going to the microsecond timescale, requiring a concurrent evolution of NSE capability. There is no technique comparable to NSE, which would allow benchmarking the MD calculations.**
Further virtues are:

- NSE gives unique access to the ns-nm regime. No other technique can access this combination of structural and dynamical scale.
- The timescales between 1ns and 1micros are also very poorly covered by other techniques. Neither XPCS nor DLS can adequately cover this region.
- The ESSENSE concept is the only way to reach the tens of ns time regime at high Q (\(\geq 2\text{Å}^{-1}\)), by using short wavelengths and high scattering angles. This will open up new science, not accessible by current instruments, particularly interesting for energy materials and magnetism.

**Conclusion:** There is a vast range of scientific problems, which can be addressed only using high resolution NSE. The large increase in count rate, offered by ESSENSE will be transformative in a number of areas and is needed to validate MD simulations as they evolve to cover larger systems.
Goal 3: To help ESS complete its spectrometer strategy.

- NSE fills a unique momentum transfer-time regime, extending the accessible dynamic regime of the ESS instrument suite by up to 3 orders of magnitude towards slower processes, making it an essential part of the ESS instrument suite.
- A suite of instruments covering many decades in time/energy is required to properly address the complexity of the increasingly hierarchical systems being studied. This suite should consist of high-resolution NSE - backscattering spectroscopy - cold chopper spectroscopy. These three instrument types are necessary to cover the full time window of interest.
- Molecular dynamics simulations combine synergistically with neutron spectroscopy to provide full understanding of the complex systems.
- One of the main current advantages of NSE over backscattering for the study of magnetism is the ability to separate nuclear from magnetic scattering using polarization analysis. This is a good argument for implementing polarization analysis on the ESS backscattering instrument.

Conclusion: NSE is an essential part of the ESS spectrometer strategy.