

GERSEMI – Gaining Enhanced Resolution with Spin Echo for Multiscale Investigations

A high-resolution Neutron Spin Echo instrument for the ESS

Community proposal

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1 Executive summary

GERSEMI is a high-resolution neutron spin echo (NSE) spectrometer aiming for novel and promising characteristics for a broad user community from soft matter, life science and hard condensed matter that will combine time-of-flight spin echo with optimised field shape precession coils.

GERSEMI exploits the long-pulse at ESS by its design of a versatile time-of-flight monochromatisation, which allows for a wider simultaneous momentum-transfer q , range at excellent q and time resolution. Due to the high flux at ESS for a wide wavelength band, GERSEMI provides unique potentials for high-quality characterisation across a broad dynamic range, spanning picoseconds to microseconds in time and sub-nanometre to several nanometres in length. This is a broad and relevant time and length scale regime not covered by the current ESS instrument suite, and links neutron spectroscopy to other methods that operate at longer length and time scales. As such, GERSEMI does not only close the high-priority capability gap identified in the ESS suite, but it also provides the capacity for high-resolution neutron spectroscopy essential to grow and consolidate a strong and versatile research program of the neutron user community for the next decades. The conceptual design is fully based on established and proven technology, and backed up by expertise from JCNS, ILL, LLB and NIST.

Future science cases with high societal impact are expected in life science (e.g. lipid drug delivery, functional protein motions, pharmaceutical formulations), soft matter (e.g. advanced polymer materials, glass transition in complex fluids), and material science (e.g. conductivity in energy materials, magnetic relaxations for spintronics). The NSE user community has been highly active in the proposal process, resulting in a widely co-signed support letter to the ESS directorate, and many experts contributing to an instrument workshop and this community proposal.

2 Scientific case

Neutron spin echo spectroscopy is currently used by a community spanning a broad range of material classes. GERSEMI is foreseen as a general-interest and interdisciplinary, high-resolution spectrometer, i.e. targeting not only the more prominent science cases in biological and soft matter, but explicitly accounting for significant potentials of NSE for energy and magnetic materials.

While more detailed accounts of impactful science cases are presented in Section 2.2, the following section provides an overview of the scientific fields with their related societal impact as well as general scientific driving factors for use and development of NSE methodology.

2.1 Key scientific drivers

2.1.1 Societal relevance of NSE science cases

High-resolution neutron spectroscopy provides unique information relevant to understanding the dynamics in advanced materials. NSE instruments suitably probe the broad range of dynamic modes and relaxation processes, from fast, local dynamics to slower and large-scale collective motions and diffusion, which ultimately determine macroscopic behaviour.

In *soft matter* as the most prominent user community, NSE offers detailed insights into structural relaxation in molecular liquids and glasses, polymer systems, and many emerging composite materials of these, which is promising for future conceptual design of new smart materials with tunable structural response and viscoelastic properties.

In *biological matter and life science* as a closely related field, NSE research focuses mainly on the understanding of collective motions of biomembranes and proteins, both of which are essential for biological function of enzymatic reactions and transmembrane transport. NSE is thus an important cornerstone for the understanding of the macromolecular machinery behind biofunction and disease. In addition, NSE provides microscopic unique insights into pharmaceutical formulations and food emulsions, where optimisation and rational design based on mechanistic understanding implies high economic impacts and functionality improvements for the food and health sector.

Within *energy materials*, NSE allows the study of collective and self-motions across a wide range of systems, providing microscopic insight into the mechanisms governing transport and diffusion over relevant length and time scales. In particular, NSE studies have revealed a strong link between dynamics at the local scale and macroscopic functional properties, including transport and conduction mechanisms. This knowledge is essential for the rational design of improved materials with optimized ionic conductivity and storage capacity for batteries and hydrogen technologies.

Magnetic systems present a special case, where interest in low-energetic relaxations is growing, and NSE thus offers potentials for novel physical insights for future spintronics applications. The ability of NSE to differentiate between nuclear and magnetic scattering may prove very valuable in such cases.

GERSEMI will be able to contribute to all these fields in a significant way.

2.1.2 Methodological relevance of NSE in the scientific toolbox

Neutron Spin Echo spectroscopy provides unique information on the dynamics of structures, in biological systems and soft matter as well in hard and magnetic materials. This fact is reflected in the ESS gap analysis classifying high-resolution NSE as highest-priority gap in ESS instrumentation. Three main aspects highlight in particular the high methodological relevance of NSE:

Essential link between nanoscopic and macroscopic scales

The length and time scales accessible by NSE (Fig. 1) close a gap between the nanoscopic to the macroscopic regime. Importantly, structural relaxation in this scale window cannot be studied by other techniques. This lack of insight limits progress in understanding and rational design of materials. Bridging the slow/large to the fast/small limit allows to understand and exploit the emergence of macroscopic properties from molecular building blocks, and as such is of interest to a broad community and versatile applications in food and pharmaceutical products, and advanced polymer and energy materials. In particular, NSE allows to connect results from the microscopic view – as obtained by neutron backscattering and time-of-flight spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, and serial femtosecond crystallography – with mesoscopic and macroscopic accounts from X-ray photon correlation spectroscopy (XPCS), dynamic light scattering (DLS), fluorescence and microscopy techniques, and pulse-field gradient NMR.

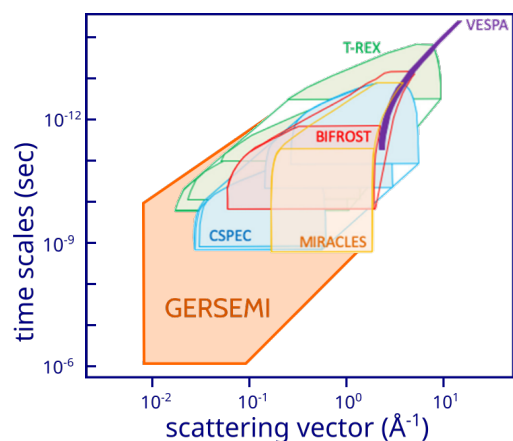


Figure 1: Time and length scales of neutron spectroscopy at ESS.

Essential validation and calibration for computational and analytical modelling of matter The information from NSE on structural relaxation on well-defined length and time scales is essential to validate modelling approaches on the dynamics of structures. Particular examples include neighbour cages in solution, domain structures in macromolecules and membrane undulations. These collective features are intrinsically difficult to validate otherwise, as simulation force fields are typically specified by single-bead properties such as self-diffusion and bead-wise attraction. Given the direct opportunity to calculate the NSE observables from computer simulations, NSE is thus an essential link to characterize emerging collective dynamics in a unique way, and as such validate classical and emerging machine-learning-driven force fields and in general coarse-graining approaches [1, 2]. This fundamental understanding combining experiment and simulation is essential in several application areas: as one challenge for pharmaceuticals, the paradigm shift from purely static structures to ensemble-docking methods combined with de-novo in-silico synthesis requires strongly validated computational models to reach optimized conditions. An analogous pressing challenge in battery electrolytes is the establishment of an experiment-based reliable computational model for the prediction and rational optimisation of transport properties.

Important contributions to polarisation analysis in neutron spectroscopy Polarisation analysis at neutron instruments is of significant interest due to opportunities for novel analysis and insights. NSE, with its intrinsic sensitivity to neutron polarisation, provides a complementary approach to polarisation analysis at other quasielastic neutron scattering (QENS) instruments, enabling direct access to the static coherent and incoherent scattering contributions. Furthermore, intensity modulated NSE [3, 4] could be used to identify self and collective dynamics separately, at the price of reduced intensity. Given the strong interest in polarised QENS, NSE will thus likely be of high importance for a broader understanding how different contributions are connected, with impact on a wide field of research and application areas relying on detailed optimisation of molecular transport processes.

2.2 Potential new science

2.2.1 Enabling factors for new science at GERSEMI

GERSEMI will allow for new and more efficient use of NSE for several overarching challenge areas, which will act as enabling factors for new science.

Time-resolved characterisation of structure formation The mechanistic understanding of non-equilibrium structuring processes requires not only the characterisation of structure and dynamics, but also their kinetic evolution. From such a time-resolved picture, the role and nature of intermediate precursor structures as well as kinetic traps can be studied, and exploited or avoided in applications.

Time-resolved NSE (TR-NSE) allows one to follow how the collective diffusion and correlated motions of building blocks change as assemblies form, reorganize, or solidify. This makes TR-NSE particularly powerful for studying assembly processes in biological and soft matter such as protein crystallization [5, 6], arrest of antibody phase separation [7], and polymer gelation [8]. Established sample environments for NSE in ambient conditions allow for multiple relevant triggering mechanisms, such as temperature changes [7, 9], illumination [10], and chemical sensing [11] to follow how molecular mobility, collective diffusion, and viscoelastic relaxation respond. Furthermore, TR-NSE can be synergistically combined with complementary methods such as DLS [12] and rheology [13], allowing for a multi-scale understanding for ultimate control of hierarchical self-assembly in biologically relevant systems, soft and hybrid materials, and energy-related functional nanostructures. Beyond traditional soft-matter applications, TR-NSE will also benefit emerging areas such as catalytic materials, electrochemical interfaces, or responsive composites, where kinetic changes in nanoscale diffusion underpin performance and function.

GERSEMI will offer optimal conditions for time-resolved scans, given the broad neutron wavelength band from the time-of-light primary optics at world-class instantaneous monochromatisation and excellent flux at all relevant wavelengths. This combination allows to not only study simultaneously a broader q -range at excellent long correlation times with so far inaccessible kinetic frame rate, but also limits the shadowing effects around potential Bragg peaks on neighbouring q -values, which are a common aspect of structure formation.

Dynamics at surfaces The surface-sensitive measurement mode of NSE under grazing incidence conditions (Grazing Incidence NSE spectroscopy, GINSES) opens opportunities for the wide research field of surface science. Access to the solid-liquid interface deep inside the sample is a challenging task per se, and neutron scattering offers unique potentials due to the large penetration power of neutrons. Going beyond structural information to dynamics and fluctuations on molecular length scales at buried interfaces offers a mechanistic understanding of surface processes: The dynamics of buried solid-liquid interfaces is a crucial property for adsorption and adhesion to antifouling coatings, or in functional surfaces for designated and controlled capture and release of cells at the surface. The dynamics also plays an important role for biological membranes in crowded or confined environments such as blood vessels or in microfluidic applications. Variations of structural fluctuations close to rigid flat interfaces have been observed in surfactant membranes in microemulsions [14, 15], lipid membranes and mesophases [16–18]. The polymer dynamics in surface coatings of microgels [19, 20] and polymer brushes [21, 22] provide unique insights into specific adaptation of polymers to one-sided confinement.

GERSEMI provides highly promising conditions to realise GINSES as a fruitful mode with count times of full data sets within a day, given the high neutron flux on a simultaneous broad wavelength band. Importantly, neutron optical components like prisms allow for a uniform depth of the evanescent neutron wave into the surface layer, and use of resonator structures can increase the near-surface intensity [23, 24].

2.2.2 A biomolecular view into biological function and formulations

Understanding and mitigation of disease mechanisms and molecular assembly

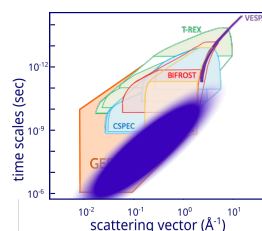
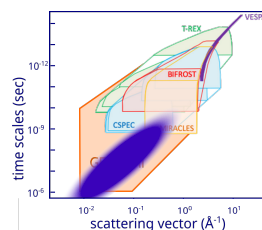
The cellular function is dependent on a well-tuned and functioning interaction network of macromolecules in crowded solutions. The deeper understanding of macromolecular crowding requires a multi-scale and multi-modal characterisation. In this context, NSE plays a specific role, as it delivers information on collective dynamics on the scale of few protein diameters, i.e. where protein interaction starts to affect diffusion and phase behaviour.

As one example, the fluid of eye lens cells has been studied to elucidate and mitigate mechanisms of cataract and presbyopia. Importantly, crystallin proteins in the mammalian eye lens undergo liquid-liquid phase separation and dynamical arrest as potential disease pathways. NSE offers a unique view on short-time cage diffusion as essential complement to larger-scale diffusion which is affected by arrest and critical phenomena [25]. Importantly, this short-time diffusion from NSE proved as an ultimate test for coarse-grained colloid models and paves the way for understanding how specific anisotropic and protein-specific interactions result in emerging dynamical properties [26–28].

As another example, sickle cell disease results from the polymerization of the human hemoglobin variant S (HbS). The HbS polymerization depends highly on concentration and the oxygen partial pressure (i.e. low pO₂), and is inhibited by fetal hemoglobin (HbF). Small-angle scattering and NSE could monitor the structure and the dynamics of HbS during polymerization. The observed strong effect of the pO₂ and the fraction of HbF present in solution lays the ground for using HbF expression as a therapeutic strategy [29].

For GERSEMI, recent developments in neutron spectroscopy using contrast-matched cellular lysate [30] and linking protein diffusion to cellular death [31] promise future NSE studies for essential insights into biological (mis)function in even more realistic systems. As a particular future perspective, GERSEMI will allow a better understanding of transport processes and dynamic arrest in membraneless biomolecular condensates which are increasingly established as integral parts of cellular function.

Understanding of allostery and biofunction via protein dynamics NSE accesses the amplitudes and relaxation times of the internal collective dynamical modes and domain motions in proteins, which is not possible with other techniques in this detail and clarity. Knowing how proteins and protein drugs work at the macromolecular level is essential for rational design of novel treatments of diseases or improvements of protein drugs. In addition, these collective motions of protein domains and chain segments are essential for the allostery of protein function.



For folded proteins, NSE offers insights into functional domain motions with sensitivity to bound substrates [32–34], and effects of functionalisation for drugs [35]. For antibodies as essential part of the immune system and therapeutic drugs, the functional “attack” motions can be investigated even under crowding conditions while rotational motions are suppressed [36]. For these studies, NSE is essential to disentangle distinctive spatial patterns of specific domain motions from translational and rotational diffusion. Even detailed information on cellular function such as the cell-cell adherens junction can be understood via the force sensitivity of an activated domain motion in the cadherin–catenin protein complex [37], and binding to the actin-binding protein vinculin [38]. Direct comparison of experimental data and coarse-grained or all-atom simulations reveals a conclusive molecular picture of modes [34, 39], which is essential for an integrative view on structural dynamics and allostery in biology.

Intrinsic disordered proteins (IDP) play a significant role in various biological processes and diseases. NSE is an essential tool to understand IDP motion in detail, such as the importance of internal friction [40, 41], and influence of environmental changes [42]. NSE also proves important to study more specific biological function: the interaction mode of myelin basic protein with nerve membranes related to multiple sclerosis [43], the dynamics-controlled binding of signalling complexes [44], and detailed dynamics of α -helical and disordered regions of α -synuclein related to Parkinson’s disease outline the potential for future biological science cases with high impact.

GERSEMI will allow to expand these applications to a wide class of biomolecular systems. As an emerging topic, membraneless organelles and biomolecular condensates present highly relevant future perspectives, where protein function is regulated through crowded, dynamic environments in a multi-scale picture [45]. GERSEMI will thus offer enormous potential for fundamental insights into biological function, which otherwise would be missed not only at ESS, but in the entire science community.

Understanding and optimising liquid formulations of macromolecules Viscosity, solution stability and phase behaviour of macromolecular liquids are linked to thermally driven fluctuations, and NSE is thus of high relevance to understand and optimize liquid formulations in the food and pharmacy sector.

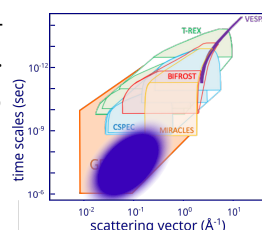
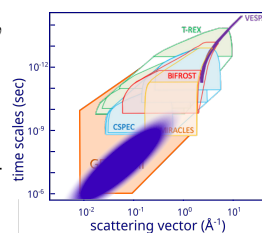
In general, NSE proved essential to evaluate and validate liquid theory interpretations of macromolecular solutions, as the time scale of few picoseconds to close to one microsecond allows us to cover the theoretically important short-time collective diffusion, *i.e.* the initial relaxations of cages and density inhomogeneities. The local dynamical picture from NSE confirmed theoretical predictions and interpretation for protein cluster formation [46–49], the approach to dynamical arrest [25, 27, 46, 50], as well as short-time diffusion under competing interactions [51] and in multicomponent systems [28, 52].

In pharmaceutical formulations of biologics such as antibodies, tunability of the viscosity without inducing aggregation is essential for improved drug quality. NSE evidenced that antibodies even in very dense environments still remain mobile [36, 53]. The formation of small transient clusters in antibody solutions is an important contributor to viscosity increase, and could in detail be characterized in a multi-scale approaches involving NSE [47, 48].

A significant exemplary challenge for sustainable food is to achieve similarly efficient and reliable stabilization of oil-in-water emulsions for plant-based milk analogues as for milk. Recent first experiments on milk proteins [54] and plant-based analogues [55] have achieved unique insights into the protein stabilization layer by exploiting contrast variation and selective deuteration.

GERSEMI will allow to continue these research lines with increased capacity and capability due to the high flux and broad wave length band. The high time resolution allows to study the transition from short-time to long-time diffusion as a central question of dynamic properties in formulations. GERSEMI will offer a more comprehensive understanding of formulation science based on physical principles, enabling novel protocols with tunable and optimized outcomes.

Understanding and adaptation of lipid remodelling The dynamics and mechanical properties of biological membranes are essential for many of their functions. Membranes act as a barrier between the inside of the cell and its surrounding, while selectively permitting and facilitating processes that require deformation of and transport through the membrane. These processes are controlled by an intricate balance of dynamic processes [56, 57], including budding and fusion



[58, 59], molecular transport [60, 61] and reaction to stress and other external stimuli [62, 63]. The cell membrane is also host to membrane proteins. Their function is intimately related to the surrounding membrane [64].

NSE is uniquely suited to study the dynamics of membranes which span many orders of magnitude, up to hundreds of nanoseconds and length scales up to tens of nanometres. So far, mostly model systems with small unilamellar vesicles have been used in NSE to measure bending rigidities with the help of the Zilman-Granek model [65, 66]. However, bending rigidities have been shown to be crucial in a number of systems relevant for the understanding and treatment of diseases. For example, additives in vaping liquids have been shown to soften pulmonary surfactant models and consequently lead to disease [67]. Encapsulating cargo (e.g. proteins) in lipid nanoparticles altered the relative membrane bending rigidity and membrane dynamics dependent on the protein type and concentration [68]. This is highly relevant for further investigation of clinical lipid nanoparticles with cargo. The long term storage of red blood cells has been shown to increase the bending modulus of the plasma membrane [69]. Further, the efficacy of lipid-based drug delivery systems has been shown to be related to their bending rigidity [70] and their bending rigidity relative to their target cells [71, 72].

With recent advances in theory [73, 74] a truly quantitative description of membrane dynamics on the nanometre length scale has become possible. A reliable measurement of the unrelaxed bending rigidity needs a q range from roughly 0.05 to 0.15 $1/\text{\AA}$, which is extremely well-suited for GERSEMI as the time-of-flight-mode allows measurement in only one single configuration. Importantly, the observed membrane dynamics in the NSE time and length scale window are not simply controlled by the unrelaxed bending rigidity but also membrane viscosity [75, 76]. The membrane viscosity determines the time scale of membrane protein diffusion, which in turn influences the cell metabolism [77]. At lower $q < 0.05$ $1/\text{\AA}$ the transition from unrelaxed to relaxed bending rigidity becomes visible. Here, NSE is a cornerstone to motivate and validate a future full theory, which would allow to make the connection to macroscopic measures of the bending rigidity. The transition from unrelaxed to relaxed bending rigidity is governed by the interleaflet friction, and NSE has the potential to become a unique tool to measure this property, which is relevant for any process where the monolayer leaflets need to slide past each other, such as membrane fusion, endocytosis or cell division.

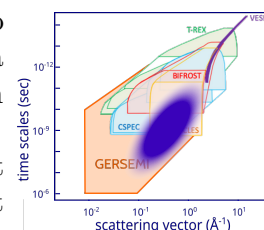
The high flux of GERSEMI at ESS will be helpful for studying fundamental mechanisms in more complex, real-life samples which can be unstable over the extended time spans currently needed for NSE measurements. The possibility of smaller sample volumes is particularly relevant for life sciences and clinical samples, as large quantities might not be available or connected to prohibitive costs (e.g. clinical lipid nanoparticles). In addition, the increased capabilities for lipid deuteration also available at ESS will greatly help to disentangle effects originating from different components in complex many-component systems.

2.2.3 Mechanistic insights into functional materials

Understanding of glass and gel transitions and complex fluids NSE allows to probe collective dynamics and separate coherent and incoherent scattering on a dynamic range highly suitable for complex fluids in general, and the investigation of the glass-transition phenomenon in particular [4, 78].

From a fundamental point of view, the glass-transition and related arrest phenomena in complex liquids are not yet fully understood, despite the great potential for diverse applications, inter alia, as green solvents, in batteries [79], and in the pharmaceutical industry [80].

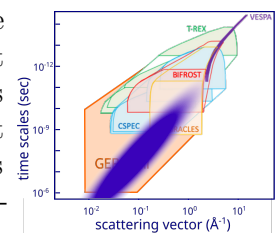
Following the dynamic structure factor at different length scales while cooling toward the glassy state remains the experimental cornerstone for future understanding. In this context, the mesoscale region governed by supramolecular aggregates [81, 82] is a rather unexplored territory [78, 83–85]. Disentangling universal behaviour from features associated to the presence of aggregates in the dynamic structure factor is a challenge that could be faced with NSE, which provides essential information to rationalize observations by other experimental techniques [86]. These supramolecular self-associates arise in H-bonding liquids like alcohols [81] as well as in systems like ionic liquids [82, 87]. Such



mixtures present self-organization at the mesoscale, influencing the dynamics. Self- and coherent dynamics have to be distinguished in order to rationalize transport [88, 89]. On a larger length scale, dynamics of multi-component or multi-domain solutions, containing e.g. surfactants and biomaterials uniquely falls into the length and time scales of NSE [90–92]. Together with selective deuteration, NSE allows to determine the elastic properties of the aggregates, e.g. micelles, membranes. These studies are of interest to the cosmetics and pharmaceuticals industries. Transport in confinement, like porous and heterogeneous systems, is another challenge faced by scientists. Nanoporous solids for separation or catalysis, nanochannels in biology, swelled synthetic or natural polymeric materials are systems where liquids flow with complex mechanisms that need to be modelled to predict their properties at the macroscopic scale. NSE addresses also these questions thanks to the long accessible time scales [16, 79, 93].

GERSEMI will offer great potential for these investigations for several reasons: the wide q range due to the time-of-flight-mode allows easier studies of processes. In addition, GERSEMI will allow to use neutrons with relatively short wavelengths, giving access to higher q than usually available at high-resolution NSE instruments. In the longer term, this field could benefit further from the synergy between GERSEMI and a possible future wide-angle NSE instrument at ESS.

Tuning viscoelastic properties and response in advanced polymer systems The development of functional materials and novel technologies represents a significant challenge in modern science. In this context, the dynamics of polymeric materials represent a primary case study for neutron scattering experiments with significant relevance for industrial applications. Since the 1960s, the fundamental principles governing polymer dynamics have been extensively researched. Modern nano-scaled polymer materials exhibit complex hierarchical architectures and topologies, necessitating enhanced sensitivity and resolution as provided by NSE.



Ring polymers, first identified in biological contexts such as cyclic DNA structures, represent a crucial area of study [94]. Understanding the relationship between the dynamics of ring polymers and their microscopic and macroscopic properties, along with phenomena such as topological glass transitions and liquid-liquid phase separation, is vital for predicting the functional properties of bio-polymers at the chain level [95]. NSE has proven an essential technique to validate and, in some cases, challenge theoretical and computational studies. Many open questions still need to be addressed on pure rings dynamics and ring-linear polymer blends. It has been recently observed by NSE [96] how topological polymer loop structures control mechanical properties in industrially-relevant composites, underlying the importance of polymer-solid interfaces in various industrial adhesives. A fundamental, yet unanswered question is whether the cross-linking structure and dynamics at the interface differ from the bulk, and a GINSES option at GERSEMI at the ESS could enable entirely new perspectives on these issues.

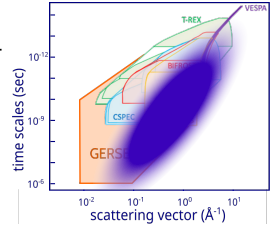
Another class of materials that attracted interest in recent times are polymer nanocomposites (PNCs). These are conventionally synthesized by blending polymers and nanoparticles, the latter typically being either inorganic [96–98] or polymeric [99–101] components. The enhanced mechanical and thermal properties have made PNCs popular e.g. in the rubber and tire industries. Current applications extend to a much wider range, from the energy and environment sector to biomedicine and biosensors. Functional properties of PNCs including mechanical strength, morphology, and dielectric response can be controlled by fine-tuning properties such as polymer chain length, grafting density, and functionalisation. The local arrangement and nanostructuring give rise to dynamic confinement and surface effects that can explain anomalous properties of the material, and are accessible by NSE.

NSE has proven to be an essential technique to investigate the dynamics of polymer transient networks and nanoparticles (e.g. kinetically frozen micelles formed by associative (bio)polymers [20, 102]). In such systems the viscoelastic behaviour is dictated by both kinetic effects, such as transient cross-linking, and dynamics at the microscopic level, such as grafting and “soft” confinement. Microscopic dynamic processes revealed by NSE are crucial to understand functional properties of the material at the macroscopic level, from transport to self-healing. Moreover, NSE can resolve slow collective motions during domain formation, interface fluctuations, and rearrangements in block copolymers, essential for understanding morphology evolution and stability [103]. For systems close

to phase transitions, NSE can access slow density fluctuations and provide insights into early-stage phase separation kinetics [21]. In polymer grafted chains it has been recently observed [104] that the correlations originating from the spatial arrangement of polymer chains give rise to modulations in the NSE intensity. This is a good example of how the possibility to tune *a posteriori* the desired q resolution on GERSEMI would be beneficial.

In summary, GERSEMI will offer novel opportunities to understand and optimize advanced polymer materials, using the excellent characteristics for standard runs, and exploiting novel opportunities becoming available via e.g. GINSES at GERSEMI.

Characterising and optimising energy materials The transition towards more efficient and robust energy technologies places increasing demands on solid-state materials used in fuel cells, electrolyzers, batteries, and hydrogen-related applications. Key examples include liquid electrolytes, proton-conducting oxides and mixed-anion materials, the latter attracting growing attention due to their structural versatility and potential for optimised ionic transport, as well as for their applications in catalysis [105–108].



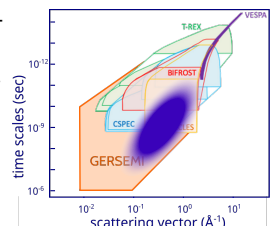
In solid-state ionic conductors relevant for the transition to new solid-state batteries, performance and long-term stability are affected by atomic-scale transport mechanisms that are thermally activated and intrinsically multiscale, spanning fast local motions and slow diffusion processes [109]. Gaining experimental access to the full dynamical range relevant under realistic operating conditions remains a central challenge in energy materials research. A combination of neutron spectroscopy techniques offers a powerful approach to probing conduction mechanisms in these materials, with NSE specifically addressing the slow dynamical regime. In recent years, NSE has been applied, for example, to studies of barium zirconates, oxohydrides, and borohydrides [110–112].

The relatively limited number of NSE investigations compared with INS and QENS reflects in part the experimental complexity of combining high-resolution dynamical measurements with the elevated temperatures required to activate transport processes in these compounds. Moreover, their crystalline structure places stringent requirements on momentum-transfer selectivity. GERSEMI will address these challenges by enabling flexible selection of reciprocal-space regions while remaining compatible with demanding sample environments, thereby opening new opportunities to investigate slow dynamics in next-generation solid-state energy materials. Given the broad dynamical range of these systems, the long Fourier times provided by GERSEMI will enable detailed investigation of the slow dynamics, currently unattainable within the ESS instrument suite. Looking ahead, complementing GERSEMI’s capability with a wide-angle NSE instrument at the ESS, providing access to higher q values and simultaneous q dependence, albeit at shorter time scales, would further extend the accessible dynamical window and advance our understanding of these materials.

Moreover, NSE plays a central role in advancing the understanding of slow dynamics in complex fluids and soft matter relevant in energy applications, such as molten salts, ionic liquids, and battery electrolytes [113, 114]. The potential of NSE spectroscopy to advance liquid electrolytes is linked to the complex connection of macroscopic transport properties and local ion mobility [115], which require detailed understanding to reach rational optimisation. A similar behaviour is observed for polymer electrolytes [116] and in general molten salts [117], which stresses the broad relevance of GERSEMI for novel energy applications.

GERSEMI will offer great potentials for energy materials, in particular by offering high time resolution with variable q resolution to minimize shadowing effects around Bragg peaks. GERSEMI will also ensure the needs for specific sample environments for energy materials.

Understanding magnetic relaxations for spintronics potentials Neutron scattering has established itself as an indispensable tool for elucidating magnetic phenomena. In recent years, NSE has been used successfully in a number of systems, such as spin glasses [118], spin ices [119], skyrmions [120], flux-line lattices or spin waves [121] which all show slow dynamics in the nanosecond range.



In general, NSE can not only measure quasielastic scattering, but can also be used for systems with a finite energy transfer. A high resolution NSE offers access to energy transfers

down to the neV range, which is a capability otherwise missing among the ESS instruments. On a technical level, this can be done either by directly observing oscillations in the intermediate scattering function [121] or by using the phase of the echo signal [122].

NSE offers some unique possibilities for the study of magnetic systems. In paramagnetic echo mode, it is possible to obtain an echo only from the magnetic scattering of the sample, which allows to study a weak magnetic signal on top of a strong nuclear signal, while in ferromagnetic echo mode, at the cost of reducing the maximal echo amplitude to 0.5, it is also possible to apply a magnetic field to the sample, as long as the change in field direction remains adiabatic [123, 124]. The latter may not only be useful for the study of magnetic phenomena but might also be employed for the study of colloidal samples where the magnetic field induces ordering in magnetic particles and NSE is used to study the dynamics of a soft matrix.

Recently, noise spectroscopy has been used to study monopole dynamics in spin ices [125, 126] and spin liquids [127] reaching relatively high frequencies. However, noise spectroscopy lacks resolution in length scales which can be provided by scattering methods. If the specific system can be tuned to show somewhat faster dynamics, NSE and noise spectroscopy could be used as complementary methods where NSE provides otherwise inaccessible information on the length scale sensitivity of dynamics.

NSE could also be instrumental in the study of fast fluctuations in skyrmion domains in thin films [128–130] which display dynamics in the nanosecond time range and have so far been studied using ultrafast X-ray methods [131].

GERSEMI offers specific opportunities for new and unique insights into magnetic phenomena, by integrating the special design needs for different NSE detection modalities from the design phase.

2.3 Potential user community

The primary user community of GERSEMI, and of NSE more broadly, lies in soft matter — understood in a broad sense to include complex fluids — and in biology. Nevertheless, hard condensed matter and magnetism represent scientific areas with clear potential for further growth. As outlined below, GERSEMI is conceived to be primarily optimised for soft matter and life science, while offering the flexibility required to accommodate a broad range of scientific cases across diverse research areas, with the aim of establishing itself as a truly interdisciplinary instrument for high-resolution spectroscopy.

Despite restricted access over the past decade, resulting from extended facility shutdowns and commissioning periods for major upgrades and new instruments, the NSE community has continued to evolve. It has developed impactful new scientific cases and broadened beyond its traditional core of dedicated NSE specialists, encompassing a more diverse user base that includes occasional neutron users, scientists transitioning from other neutron techniques (e.g. SANS), and researchers new to neutron scattering.

GERSEMI therefore has the clear ambition not only to consolidate the established community, but also to further broaden and diversify the user base across multiple scientific domains.

3 Initial technical overview

3.1 Primary Spectrometer

The design of the primary spectrometer follows optimized design ideas for time-of-flight monochromatisation at the ESS long-pulse source, and enables use of the the ideally suited instrument location N01 in D03 (Fig. 2). The central concept for the primary spectrometer has been outlined in detail in a previous NSE proposal (ESSENSE instrument [132]), which has been shared with the current ESS management. The adaptation to slightly changed source specifications and related opportunities will be performed during technical design without any technical risks or severe challenges foreseen.

Main chopper system The frame selection chopper system consists of four disc choppers positioned along the beamline starting from 15 m (out of bunker). The choppers operate at a rotation frequency of 14 Hz with apertures between 110° and 204° , making use of the whole pulse. This configuration allows the selection of wavelength frames with tunable central wavelength and approximately 8 Å frame

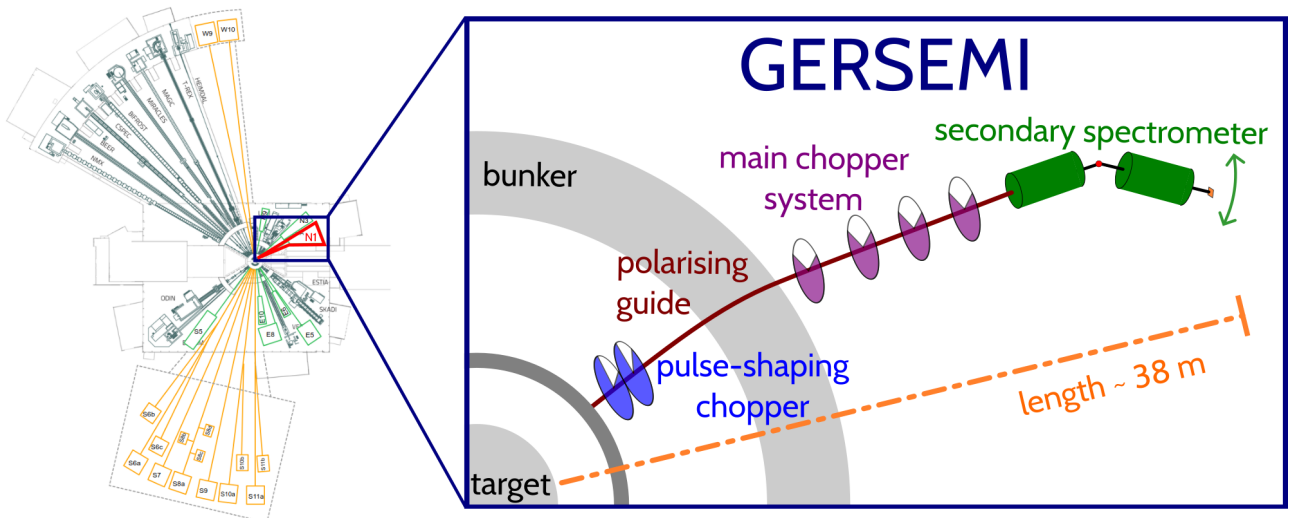


Figure 2: Schematic design of GERSEMI at the foreseen location N1 at ESS in D03. With polarizing guide, chopper system, and secondary spectrometer, GERSEMI has a total length of 30 m.

width within the operational wavelength range of $\lambda = 3 - 25 \text{ \AA}$. Importantly, an efficient background suppression is achieved by proper phasing, avoiding effects of the prompt pulse and contamination of unwanted neutrons with wavelengths shorter than 80 \AA .

Pulse shaping (PS) chopper An additional PS chopper is included to enhance instantaneous wavelength definition. The PS chopper is a double-blade co-rotating disc system located at a distance of 6.5–7 m with symmetric 90° sectors. Operating with a frequency range of 7 – 168 Hz allows to tailor the instantaneous wavelength spread at sample position continuously between 0.035 \AA and 0.3 \AA (Fig. 3). Although the PS chopper can be considered as optional at a first stage, such control enables the suppression of Bragg reflection contamination at a moderate cost in intensity, making it a very important tool to enable more studies in particular in hard condensed matter and magnetism.

Polarising guide In order to cover the planned wide wavelength band, a reflection (kink) polariser and a transmission V polariser will be needed, with an adiabatic flipper in-between.

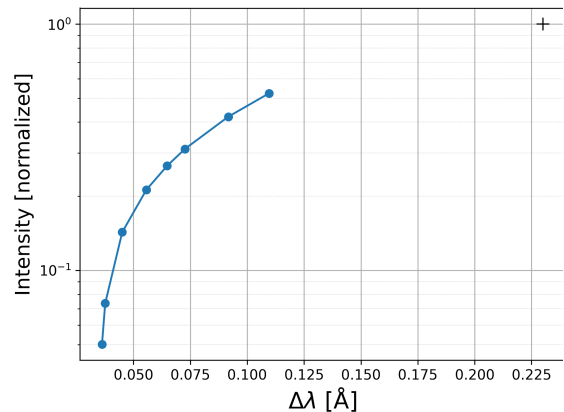


Figure 3: Relative intensity factor with PS choppers as a function of instantaneous wavelength spread $\Delta\lambda$ from dedicated simulations.

3.2 Secondary Spectrometer

Two suitable designs for the secondary spectrometer have been established and proven to deliver the needed scientific requirements of excellent high-resolution NSE also in time-of-flight mode: the J-NSE Phoenix design [133] with superconducting coils, and the IN15 design [134] with classical water-cooled resistive coils. As both designs can be adapted for GERSEMI without specific technical risks, a final decision can be made by the construction team based on an analysis of technological strengths and limitations, in particular technical specifications (e.g. electrical and cooling power), procurement aspects, flexibility of sample environments and efficient implementation of measurements protocols for typical use cases.

4 Adaptation to ESS long-pulse source

The conceptual design of GERSEMI exploits the ESS long-pulse source to reach spectrometer characteristics not achievable at short-pulse or reactor sources. In particular, the long pulse with time-of-flight primary optics allows to have a time-encoded broad wavelength band at the sample, with excellent versatility of the instantaneous monochromatisation by an additional pulse-shaping chopper. While classical wavelength selection at a reactor source would not allow for a broad wavelength band, a short-pulse source does not allow for comparable flexibility regarding the instantaneous monochromatisation. Compared to these two scenarios, GERSEMI will intrinsically perform better for a wide range of science cases. These specific characteristics of GERSEMI are of particular interest for new science cases of time-resolved structuring pathways and hard materials in general, where Bragg peaks typically induce an artificial shadow by q -smearing, which GERSEMI will be able to circumvent.

5 Plans for sample environment and laboratory access

The instrument can benefit from the access to the several laboratories at the ESS for sample preparation and complementary characterisation. Given the planned location (cf. Sec. 6), the most obvious choices are the life science laboratory and the chemical laboratory in D04. Access to laboratories in E04 and D08 will be possible as well. Depending on the type of studied materials, the users can make use of different ancillary equipment offered by the ESS laboratories such as DLS, calorimetry, UV/VIS spectrometer, FTIR, Raman, X-ray fluorescence, ICP-OES, X-ray diffraction (powder and single crystal), Laue camera for single crystal alignment etc.

GERSEMI will be used by different communities with different sample environment requirements. As a first suite of sample environments, we foresee:

- “Bio-oven” with humidity cell: supplying temperature control in the temperature range between $-20\text{ }^{\circ}\text{C}$ and $+120\text{ }^{\circ}\text{C}$ at ambient pressure (suitable for Hellma cells). It will serve the majority of biomolecule dynamics cases, complex fluids and microemulsion, gels, polymer solution and a part of polymer melt investigations. The humidity cell offers controlled humidity (solvent partial pressure).
- Cryofurnace: Temperature range: 2–800 K, routine sample environment for all scientific cases that need low temperature in the range of a few K and/or large temperature range (e.g. polymers, complex fluids, glasses, energy materials, magnetism).
- Dilution insert or ^3He insert, to reach mK temperatures, primarily for magnetism.
- High temperature furnace, temperature range: 300–1300 K for scientific cases that require high temperatures beyond standard cryofurnace, e.g. dynamics of inorganic glasses, energy materials.
- Low-field magnet (2T), can be used in ferromagnetic echo mode (magnetism, magnetic nanoparticles)

The sample environment area will also feature two rotation motors that allow scans for single crystals and other oriented samples. The space for the sample environment area will be also enough to accommodate other more complex equipment such as combined characterisation, e.g. with rheology.

NSE requires low magnetic permeability to avoid beam depolarisation. ESS spectrometers with plans for polarisation analysis (e.g. CSPEC, TREX and MIRACLES) have requirements of low magnetic permeability ($\mu \leq 1.01$) around the sample area, hence GERSEMI can profit from previously acquired knowledge at the ESS and possibly exchange equipment with those instruments, when appropriate.

6 Proposed location at ESS

The preferable beamport is N1 in D03 (Fig. 2). The area has non-magnetic floor with sufficient floor load requirements. The existing instruments in close proximity (LoKI, FREIA and test beamline) are not focused on magnetism, hence reducing the occurrence of magnetic noise from sample environments such as high-field magnets on neighboring instruments. In addition, the location will provide enough space for the desired length of the instrument, a guide design curving out from the line of sight of the moderator in order to lower the background, and the ability to move the instrument arm to reach higher angles, which is an important condition to cater a wide range of impactful experiments.

7 Gap analysis in terms of both capability and capacity

GERSEMI will provide access to a broad and important dynamic range that is not covered by the current ESS instrument suite, thereby addressing a previously identified high-priority gap at ESS.

Within the global neutron landscape, the number of available NSE instruments is very limited and typically heavily oversubscribed. The scarcity of NSE beamtime around the world has been identified as a major obstacle to expanding the user community [135]. By combining high flux, an extended q -range, and versatility across different scientific domains, GERSEMI will enable the development of a strong and sustainable future user base.

More broadly, high energy-resolution spectroscopy is already impacted by the intrinsic limitations for near-backscattering instruments at spallation sources, which cannot achieve the same energy resolution as third-generation backscattering at reactor sources (e.g. $2.5 \mu\text{eV}$ for MIRACLES@ESS vs $0.66 \mu\text{eV}$ for SPHERES@MLZ and IN16B@ILL).

In this context and in light of the ongoing transition towards ESS as Europe’s leading neutron facility, the establishment of GERSEMI is strategically essential to preserve and strengthen the European high-resolution neutron spectroscopy ecosystem, thereby ensuring broad international access to slow dynamical regimes.

8 Comparison to similar instruments in the world

Long Fourier Time, Small-Angle Instruments (CHRNS-NSE@NIST, IN15@ILL, J-NSE-Phoenix@MLZ, SNS-NSE@SNS): All these instruments are equipped with precession coils (electromagnets or superconducting coils) that allow for a maximum field integral between 1 and 1.5 Tm. GERSEMI will have a comparable field integral. The limiting factor for achieving the longest Fourier times is the ability to correct inhomogeneities in the field integral, which are greatly reduced by the use of coils with optimised field shape. The ability to efficiently take advantage of the longest Fourier times depends on a high neutron flux at long wavelengths, where ESS will offer an excellent, highly competitive time-averaged flux. GERSEMI will thus exceed the performance of other NSE spectrometer due to the broad wavelength band, allowing for a broader simultaneous q range at still higher q resolution.

Wide-Angle NSE (SPAN@HZB, WASP@ILL) With the BERII reactor closed and the SNS second target station project on hold, WASP will be the only wide-angle spin echo instrument for the foreseeable future, and in its specific domain (high q , large simultaneous q range, Fourier times up to ~ 10 ns) it provides capabilities that are complementary to those of GERSEMI. However, thanks to GERSEMI being operated in time-of-flight mode and its wavelength band extending to relatively short λ (3 \AA), GERSEMI will still perform better than other high-resolution NSE in this domain and will be able to cover some part of WASP’s science case at least for q up to about 0.6 1/\AA . At high q , where Bragg peaks are often found, the time-of-flight mode with a pulse shaping chopper allows to optimise the q resolution around the peak position, by minimising the smearing of strong peak scattering due to wavelength resolution. As a future outlook, a wide-angle NSE at ESS could provide excellent complementarity and synergy with GERSEMI.

Resonance Spin Echo (Reseda@MLZ, Vin-Rosé@J-Park) Resonance spin echo spectrometers in MIEZE mode are especially suited for measurements of depolarising samples and experiments that require magnetic fields at the sample position, and typically focus on shorter Fourier times than classical IN15-type spectrometers. Thanks to a dedicated ferromagnetic echo mode similar to IN15, GERSEMI will be able to cover most of these science cases (including those with magnetic fields at the sample position) except for samples that need to be measured under depolarising conditions (e.g. ferro-magnets at zero field). However, many of these can still be measured using intensity modulated spin echo, which can be implemented on GERSEMI.

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Appendix

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- support letter: Stephan Förster / Jülich Center for Neutron Science (JCNS)
- support letter: Arnaud Desmedt / Laboratoire Léon Brillouin (LLB)
- support letter: The French Federation for Neutron Scattering (2FDN)
- community support letter for an NSE instrument at ESS
- list of attendees of community workshop for GERSEMI at ESS

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Dr. Daria Noferini - ESS
Odarslövsvägen 113
224 84 Lund, Sweden

DIR/KA/am - 2026/06

Grenoble, 20/03/2026

Letter of Support

Dear Daria,

With the present letter, I would like to express my strong support for your proposal to build the GERSEMI neutron spin echo (NSE) instrument at the ESS. This instrument would significantly extend the time and energy range accessible to ESS users into the μ s and neV regime and would thus significantly enhance the capabilities of the ESS instrument suite.

Complex polymeric materials show long relaxation times inaccessible with any other neutron spectroscopy method, while the study of polymeric materials greatly benefits from the unique possibilities offered by contrast variation in neutron scattering. Increasing the complexity further by the addition of hard materials makes it even more crucial to have access to the high resolution data that GERSEMI would provide. Its flexible design will even allow to study mixed materials with magnetic properties.

If built, this instrument would benefit a community of scientists in Europe, many of whom are currently served by the ILL NSE instruments. ILL provides world-leading capabilities in NSE spectroscopy and could be well placed to support ESS in the design and construction of such an instrument.

With my best regards,



Ken Andersen

To whom it may concern

Ihr Zeichen:
Ihre Nachricht vom:
Unser Zeichen:
Unsere Nachricht vom:

Ansprechpartner:
JCNS-1/JCNS

Tel.: 02461 61-85161
Mobil: 0151 2005 1009
Fax: 02461 61-2610
s.foerster@fz-juelich.de

Jülich, 23.03.2026

Dear ESS instrument selection group

I express my strong support for the proposal of building the neutron spin echo (NSE) instrument, GERSEMI, at the ESS.

The Jülich Centre for Neutron Science (JCNS) has long-standing, internationally recognised expertise in developing, operating and scientifically exploiting neutron spin echo spectroscopy, spanning several decades and including leading contributions at major neutron facilities.

Neutron spin echo spectroscopy provides unparalleled access to dynamics on nanometre length scales and picosecond to microsecond timescales, making it an indispensable tool for addressing fundamental questions in soft matter, biology and materials science. It has enabled breakthroughs in our understanding of polymer and protein dynamics, membrane fluctuations, as well as emerging topics such as energy materials and quantum systems.

The European Spallation Source's combination of high flux, long pulse structure and advanced instrumentation concepts offers an exceptional opportunity to significantly extend the capabilities of neutron spin echo spectroscopy and to fill an important gap in the ESS instrument suite.

Drawing on our extensive experience at JCNS, we strongly recommend the development of the next-generation NSE instrument, GERSEMI, at ESS. This would not only make use of the unique characteristics of the ESS source, but also establish a world-leading platform for studying nanoscale dynamics, enabling transformative science across a broad range of disciplines.

With best regards,





Gif-sur-Yvette, 26th of March 2026

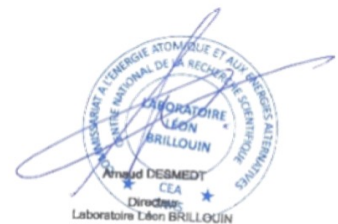
Letter of support for the GERSEMI instrument project.

The Laboratoire Léon Brillouin (LLB), a joint research unit of the CNRS and the CEA, is distinguished by its dual role as both a research laboratory and a national user facility. As the **French Neutron Scattering Center**, it has developed strong expertise in neutron instrumentation and facility operation, including 22 instruments at the Orphée reactor (until 2019), three CRG instruments at the Institut Laue-Langevin (ILL) and Paul Scherrer Institute (PSI), and contributions to five of the first fifteen instruments at the European Spallation Source (ESS) (BIFROST, CSPEC, DREAM, MAGIC and SKADI). It also develops targeted R&D on compact neutron sources (HiCANS), supporting next-generation facilities, with coordination of the development of the future compact neutron source ICONA at Saclay. In parallel, the LLB conducts a **broad in-house research programme** spanning fundamental to applied science, and addressing key challenges in physics, chemistry and biology. These activities are structured around two well-established research themes: (i) soft matter and biologically relevant molecules, and (ii) magnetism, correlated electron systems, and functional materials.

The LLB is firmly convinced of the scientific relevance and strategic importance of the GERSEMI project for the European Spallation Source (ESS). **High-resolution neutron spin-echo** has been identified as one of the most critical missing capabilities in the ESS capability gap analysis, further underlining the importance and timeliness of this development. The implementation of a neutron spin-echo spectrometer would represent a major step forward by significantly extending the kinematic range of the ESS spectrometer suite, in particular by pushing Fourier times up to approximately 1 μ s. As a key instrument for the international spectroscopy community, GERSEMI will connect results from the microscopic view — obtained through neutron backscattering and time-of-flight spectroscopy — to nuclear magnetic resonance (NMR) or photon correlation spectroscopy (XPCS), bridging the gap with mesoscopic and macroscopic techniques.

GERSEMI will substantially enhance the scientific outreach of the ESS instrument portfolio. It is perfectly suited to the ESS long-pulse source, covering a wavelength bandwidth of approximately 8 Å within the operational wavelength range of $\lambda = 3\text{--}25$ Å. Taking advantage of GERSEMI's extensive kinematic range, both in Fourier times and extended Q-range, together with its high Q-resolution and polarization analysis capabilities, this unique capabilities will enable to address key challenges relevant for LLB research activities in **soft matter, biophysics and hard condensed matter sciences**. GERSEMI will contribute to understanding and mitigating disease mechanisms and protein assembly, as well as in studying the dynamics of glasses and complex fluids. The GERSEMI capabilities will enable to investigate magnetic systems such as quantum spin liquids, frustrated magnets, high-temperature superconductors, in particular by providing access to the time scales of slow magnetic fluctuations arising from complex magnetic states and to exotic fractionalized excitations encountered in these systems.

On behalf of the LLB, I would like to express our strong support for the GERSEMI instrument project. I confirm our **full commitment to actively contribute to its scientific and instrumental development**.



Arnaud DESMEDT – LLB Director



Laboratoire Léon Brillouin - LLB

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<http://www-llb.cea.fr>



Montpellier/Saclay, 25th of March 2026

federation.neutron@neel.cnrs.fr

<https://2fdn.cnrs.fr/en>

To the European Spallation Source Instrument Proposal Committee:

The French Federation for Neutron Scattering (2FDN) strongly supports the proposal to develop the neutron spin echo (NSE) instrument GERSEMI as a new instrument for the user community within the upcoming ESS instrument suite.

Owing to its extended Fourier time reaching the microsecond range, GERSEMI will provide an essential link within the hierarchy of dynamical processes, connecting nanoscopic dynamics to mesoscopic and macroscopic behavior. In particular, it enables researchers to bridge microscopic measurements from neutron backscattering and time-of-flight spectroscopy with techniques probing larger length and time scales, such as rheology or optical microscopies.

More generally, NSE is *THE* technique offering a unique combination of spatial and temporal resolution at nanometer and nanosecond-to-microsecond scales, allowing one to probe dynamics spanning from fast local motions to slow relaxation processes. It is highly complementary to techniques such as dynamic light scattering (DLS) or X-ray photon correlation spectroscopy (XPCS), which probe similar time regimes but rely on specific contrast mechanisms, as well as to methods like nuclear magnetic resonance (NMR), muon spectroscopy (μ SR), or broadband dielectric spectroscopy (BDS), which access wide dynamical ranges but with limited or no spatial resolution. NSE obviously conserves one of the key advantages of neutron scattering, i.e. the sensitivity to protons, and the ability to probe both coherent and incoherent motions.

The implementation of GERSEMI will significantly expand the kinematic coverage of the ESS spectrometer portfolio, thereby broadening the scientific capabilities accessible at the facility. As described in the instrument concept paper, GERSEMI will play a central role in advancing investigations across soft matter, biology, functional materials, energy materials, and quantum magnetism. By leveraging the long ESS pulse and operating in time-of-flight (ToF) mode with a pulse-shaping-chopper (PSC), GERSEMI is poised to become a leading NSE instrument on the international stage. It will enhance both the NSE **capacity and capability** by pushing the Fourier time limit up to approximately 1 μ s, offering a broad Q-range, and excellent Q-resolution across the operational wavelength range of $\lambda = 3\text{--}25 \text{ \AA}$, missing on available NSE instruments. . Combined with polarization analysis, NSE is a valuable asset for both soft and hard condensed matter investigations. The instrument will also allow experiments under applied magnetic fields for ferromagnetic spin-echo mode, and proposes a rich sample environment suite.

The research activities of the French neutron community span a broad range of soft matter, biophysics, and hard condensed matter topics, all well matched to capabilities provided by GERSEMI. In soft matter and biophysics, the instrument will allow studies of slow and fast diffusion, collective motions, and dynamics in glasses, complex fluids, proteins and protein assemblies, macromolecules, polymers, membranes, and energy materials. In hard condensed matter, the French community addresses low-dimensional magnets, quantum spin liquids, frustrated magnets, high-temperature superconductors, skyrmion lattices, and other topological textures. In these systems, magnetic anisotropies, exotic magnetic states involving higher-order magnetic multipoles and frustrated interactions produce few μ eV gaps and low lying flat magnetic modes, slow magnetic fluctuations that evade the NMR timescale and appear static at the picosecond neutron diffraction timescale, magnetic fluctuations with small bandwidths and exotic fractionalized excitations and quantized magnon spectra. All of these scientific cases will benefit from the unique capabilities of GERSEMI including

its extensive kinematic range in terms of Fourier times and extended Q-range, its high Q-resolution and polarization analysis.

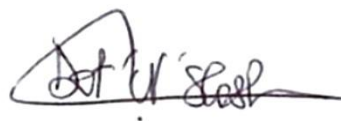
For all these reasons, the 2FDN strongly supports the implementation of GERSEMI in the upcoming ESS instrumental suite.

Sincerely,



Julian Oberdisse

Directors of the French « Fédération Française de Diffusion Neutronique » (2FDN)



Dalila Bounoua



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ESS directorate
Science Director Giovanna Fragneto
Director General Helmut Schober

Lund, May 12, 2024

Community letter of support for a neutron-spin-echo spectrometer at ESS

Dear ESS directors,

During the conference HIRES 2023 at ILL in December 2023, the attendees had a vivid discussion session on future instrumentation at ESS. Without any doubt, the attendees – a significant part of the world-wide QENS/INS community from broad research fields – concluded that a neutron spin-echo instrument at ESS is absolutely necessary to exploit the full potential of neutron science in soft matter and material science.

We are convinced that the opportunities of an NSE instrument adapted to the ESS characteristics will assemble an active user community with a variety of high-quality and high-impact science cases. Without a competitive NSE instrument at ESS, a broad window of time and length scales would remain uncovered, as already noticed in the previous gap analysis at ESS. We stress that without an NSE instrument at the new European flagship facility this situation would result in a severe lack of opportunities and capabilities in the future.

The NSE methodology is a unique and very successful neutron method despite the recent capacity shortage in Europe. Notable developments in the recent years occurred in a broad research field:

- *protein diffusion and internal motion*: NSE has been used to transfer the well-established concepts in polymer physics to biological systems as well as specific polymer systems. Specific results include the characterization of biologically relevant domain motions of proteins¹, the characterization of diffusion and motions of antibodies in the relevant high-concentration dense solutions². This line of research is of utmost importance to understand the onset of biological motions during protein allostery as well as diffusional transport, with strong implication for life science and pharmacy research.

¹B. Sohmen et al. Adv. Sci. 2023,10, 2304262; B. Farago PNAS 2021, 118, e2025012118

²L.R. Stingaciu et al. Sci. Rep. 2016, 6, 22148; A. Girelli et al. Mol. Pharm. 2021 18 (11), 4162–4169

- *polymer dynamics*: NSE proves essential to develop our understanding of complex polymer melts beyond the simple reptation model and beyond simple monodisperse linear melts³. This detailed knowledge opens unique potentials for rationally choosing process and composition conditions to meet desired specifications of polymer materials.
- *lipid membrane dynamics*: NSE is increasingly used to understand membrane undulations by using the Zilman-Granek analysis. Initial work on model lipids has been consolidated and transferred to systems with conditions relevant for biological (mis)function⁴ or drug delivery⁵ as well as artificial membrane analogues⁶. Ongoing research combines these approaches with cofactors, which will open unique potentials to understand mechanisms of membrane fusion and buckling relevant for cellular and viral pathways with apparent potentials for pharmacology and biomedicine.
- *relaxation in complex liquids*: NSE with the opportunity to distinguish incoherent from coherent scattering presents a very important complement to (polarized) backscattering and TOF techniques. NSE presents an essential technique to bridge the molecular scale from QENS and inelastic X-ray scattering to mesoscopic scales from X-ray photon correlation spectroscopy. First examples of these potentials were realized e.g. for battery electrolytes⁷ and deep eutectic solvents⁸, with significant implications for sustainability in materials science.
- *magnetism and correlated systems*: NSE in its different facets has continuously made important contributions to the understanding of the dynamics of magnetic and correlated systems. Recent impactful examples include characterization of low-energy excitations and magnon band structure of the skyrmion state⁹. These findings prepare the ground for more advanced applications within spintronics and quantum technologies.

Moreover, NSE instrumentation has further developed and diversified during the last years with construction, commissioning and successful performance of new NSE spectrometers at ILL and SNS as well as upgrades for existing instruments at NIST and MLZ. We feel that these new experiences provide very promising perspectives to design a world-class instrument at ESS as part of the next generation of beamlines with a call opening in 2024.

NSE is one of the most pressing gaps in the ESS portfolio with huge potential for future impactful operation. As a broad community of QENS users we are confident that an NSE spectrometer will find strong community support and a large and active user community.

³M. Kruteva et al. Phys. Rev. Lett. 2020, 125, 238004; M. Zamponi et al. Phys. Rev. Lett., 2021, 126, 187801

⁴S. Gupta et al. Curr. Opin. Coll. Interf. Sci. 42 (2019) 121–136; S. Chakraborty et al. PNAS 2020, 117, 21896-21905; B. Krugmann et al. Sci. Rep. 2020, 10, 16691; A. Santamaria et al. J. Am. Chem. Soc. 144, 2968-2979 (2022)

⁵J. Gilbert et al. Nanoscale, 2022, 14, 6990-7002

⁶L. Chiappisi et al. J. Coll. Interf. Sci 2022, 627, 160-167

⁷F. Lundin et al. J. Phys. Chem. C 2022, 126, 16262–16271

⁸A. Faraone et al. J. Phys. Chem. B 2018, 122, 1261–1267

⁹M. Soda et al. Nat. Physics 2023, 19, 1476–1481; T. Weber et al. Science 2022, 375,1025-1030

We are looking forward to entering a dialogue within the community and with ESS how to best enable a competitive proposal for a world-leading NSE instrument at ESS.

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ESS NSE Workshop

16 September 2025

European Spallation Source ERIC (+ online via zoom)

Europe/Stockholm timezone

Confirmed speakers:

- Arantxa Arbe, *EHU*
- Bela Farago, *ILL*
- Elizabeth Blackburn, *Lund University*
- Elizabeth Kelley, *NIST*
- Hanna Barriga, *SciLifeLab/KTH*
- Johanna Jochum, *TUM*
- Margarita Kruteva, *Forschungszentrum Jülich*
- Maths Karlsson, *Chalmers University*
- Max Wolff, *Uppsala University*
- Olaf Holderer, *Forschungszentrum Jülich*
- Ralf Biehl, *Forschungszentrum Jülich*
- Stéphane Longeville, *LLB*

Organising committee:

Benedetta Rosi, *ESS*
Daria Noferini, *ESS*
Felix Roosen-Runge, *Lund University*
Ingo Hoffmann, *ILL*
Mads Bertelsen, *ESS*

59 registered participants

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Firoz Malayil kalathil	Jan Swenson
Frank Schreiber	Jason Gardner
Fernando Yamil Moreira	Jonathan Leiner
Masatoshi Arai	Juan Colmenero
Mo Aouane	Luigi Paduano
Pascale Deen	Marie Plazanet
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