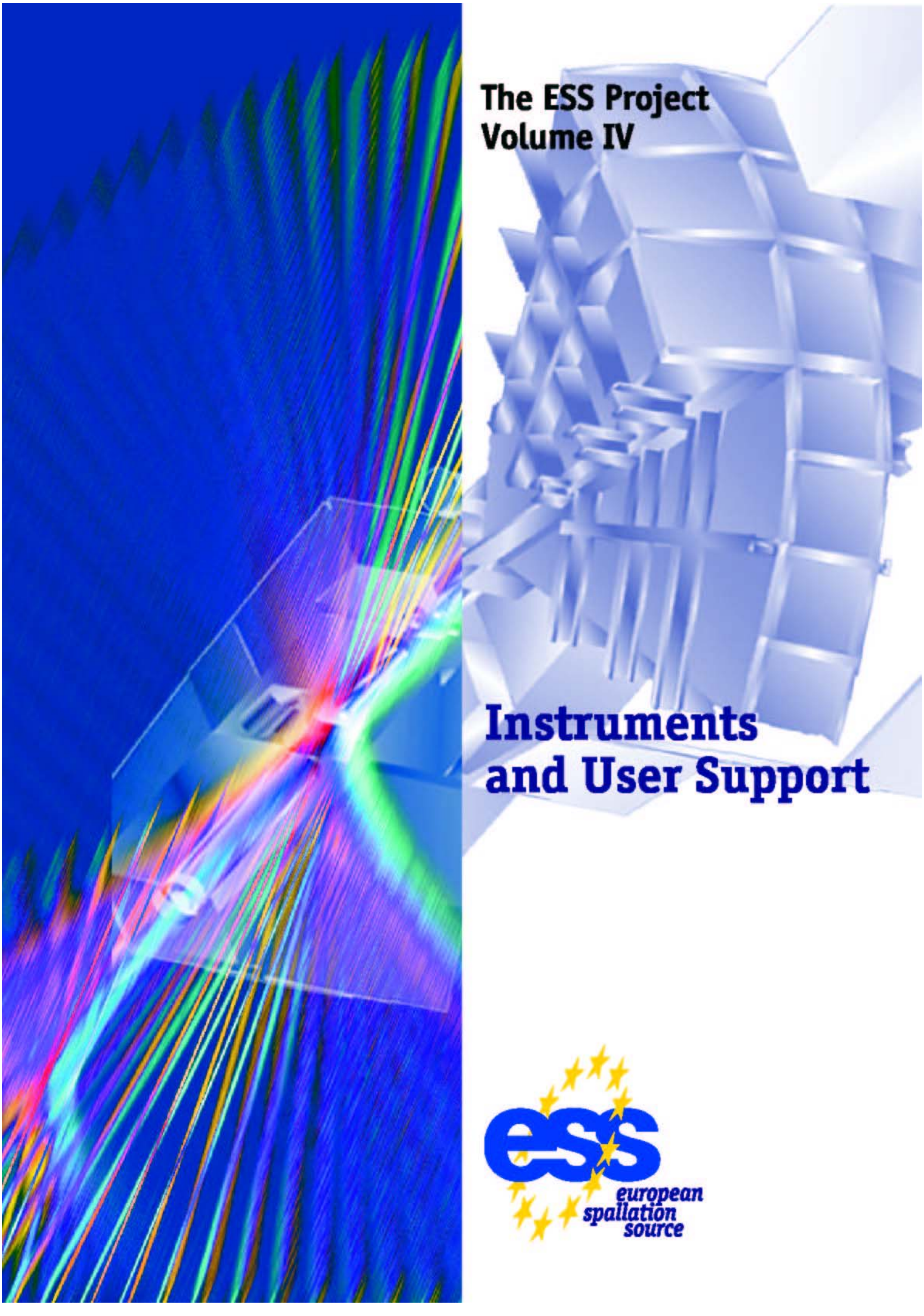

The ESS Project
Volume IV

Instruments and User Support

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The European Spallation Source Project

The ESS Project

Volume IV

Instruments and User Support

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The ESS Project

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Technical Report

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Instruments and User Support

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INTRODUCTION

I INTRODUCTION

This volume of ESS Project 2002 aims at giving a preliminary taste of the first ESS "user guide" that the neutron research community will be provided with in about 10 years from now in order to help to prepare their first research proposals to do experiments at ESS. Of course, the chapter on important practicalities, such as where to submit the proposals, travel information how to reach the ESS site and guest facilities is missing – for the obvious reason that the decision on site preference is not yet made. It is also obvious, furthermore, that the first half of the ESS instruments, which will gradually come on line for full user operation by 2013, with commissioning (at first without neutrons) starting in 2010, will mostly be refined versions of what can be conceived today – and is described in this provisional user guide. Nevertheless with the detail design work to start for the first batch of about 10 instruments around 2005, we can have a reasonable first idea of how these instruments will look.

Within the construction phase of ESS, planned to last until the end of 2011, about 20 neutron scattering instruments and beam facilities will be in more or less advanced stage of manufacturing and installation, following a carefully staggered time schedule. This timeline foresees the technical completion of on average 5 instruments a year between mid 2010 and mid 2014. After this date 3 instruments will come on line each year to achieve a total of 40 to be built and operated by ESS. Further 8 beam lines are envisaged for instruments to be built and run by external co-operating research groups. The scope of ESS project construction phase includes funding of the costs incurring before 2012 for the building of the first neutron scattering instruments. These will amount according to the above schedule to the equivalent of 15 instruments fully completed, while more than 20 will have been started, at least with detailed design, by this date. Further funding for completion of the full instrument suite, as well as modernising and rebuilding on longer term will be part of ESS operational budget.

The selection of the suite of instruments described in this volume is based on the recommendations of the ESS Scientific Advisory Council (SAC) as compiled in November 2001 as a results of a statistical evaluation of the priority research needs expressed by the various science groups of the SAC. A subsequent workshop of the SAC in March 2002 was specifically dedicated to review the outstanding opportunities offered by ESS for applied research, health care and technology development missions and the corresponding instrumental needs. It was found that these overwhelmingly coincide with the experimental priorities defined in November 2001 on the basis of the evaluation of basic scientific opportunities.

The instrumental capabilities detailed in this guide convincingly fulfil the ESS project goal to decisively advance the power of neutron scattering as a versatile research tool in all areas of condensed matter science and technology, compared to that currently available at the most advanced continuous and/or pulsed neutron sources. Achieving this goal will also make ESS provide the community with unique, unprecedented research opportunities, complementary to other important foreseeable advances in large-scale facilities for condensed matter science. These two aspects of ESS based science can be illustrated by the following examples.

Small angle neutron scattering (SANS) is currently one of the main strengths of continuous reactor sources, which thus provide unique potentials in the study of nano-scale structures in solid-state physics, polymer and material research and life sciences. SANS is a very important area in neutron science where pulsed spallation sources are by now in general dominated by continuous ones and it was therefore one of the particular priorities in ESS design optimisation. Indeed, as much as by its enhanced accelerator power as by its innovative target configuration ESS will offer an order of magnitude gain in sensitivity in this crucial research field not only compared to the currently leading reactor sources but also relative to the 2 MW SNS pulsed spallation source facility now being built in Oak Ridge, Tennessee (cf. Fig. I-1).

Another representative and crucial application of neutron scattering is to explore the atomic and molecular dynamics on the mesoscopic time scale $10^{-12} – 10^{-7}$ s, characteristic for many fundamental phenomena in soft and complex matter. Here ESS will offer 3 orders of magnitude enhanced sensitivity as a result of combining source power and innovative beam delivery and instrument design (cf. the description of cold neutron spectrometers in chapter 2 of this volume). This will make possible to study many to date inaccessible phenomena, for example exploring the endemically small dynamic signals in all kinds of non-crystalline matter.

Neutron and X-ray scattering experiments are primarily complementary by the information they deliver due to the different properties of the two kinds of radiation. For example neutrons offer uniquely high sensitivity for observing light elements in the presence of heavy ones, magnetic disorder and dynamics, isotopically labelled parts of large molecules, etc. In addition, with the power of ESS in many experiments the data collection rates will also be superior to those attainable at advanced synchrotron radiation facilities, notorious for their high beam intensities. In particular, in the kind of inelastic spectroscopy mentioned in the previous paragraph, the sheer beam intensity of ESS will be orders of magnitude superior to that of the most brilliant synchrotron sources today and also superior to the projected, most powerful X-ray free electron lasers (X-FEL). Indeed, the spectral density of the neutron beam over the typically 10 cm^2 beam

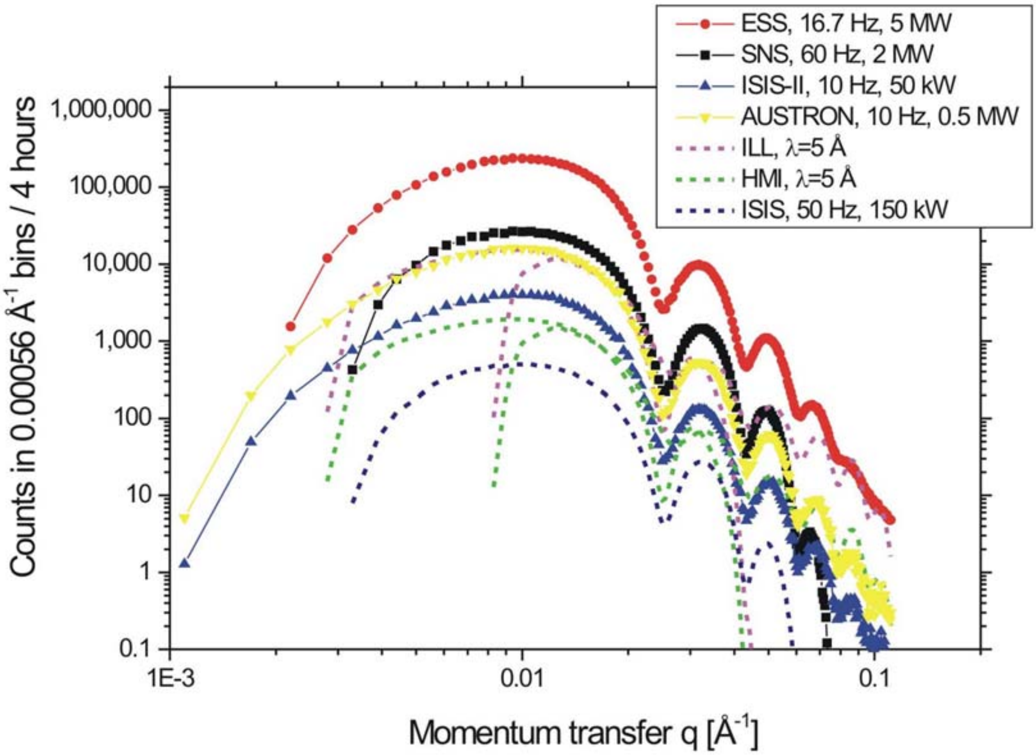

Figure I-1: *Simulated data collected on a isotropic colloidal model sample by virtual SANS instruments of equal angular resolution, sample size, detector area and detector pixel size at various existing (dashed lines) and projected (symbols) neutron sources. The settings are chosen to optimally explore the q range 0.005 to 0.05 $Å^{-1}$. For the two reactor sources, ILL and HMI two settings with different collimations and sample to detector distances were assumed (12 m +12 m for 90 % of the data collection time and 4 m + 4 m for 10 %), in order to cover a q domain similarly broad to that at the spallation sources in a single setting (12 m + 12 m, single source frame data collection).*

area will reach at ESS peak values of $2*10^{11}$ neutrons/s/meV (the relevant intensity parameter in neutron time-of-flight spectroscopy with repetition rate multiplication) compared to 10^8 – 10^9 photons/s/meV at ESRF and 10^{10} – 10^{11} photons/s/meV expected at the most powerful X-FEL. Of course, the some 0.1 mm^2 beam cross section of these X-ray sources is a major advantage for very small samples, but many samples, in particular in soft matter research can be produced in sufficient quantity to take full advantage of the large beam cross sections typical for neutron scattering instruments. In the 10^{-9} eV resolution range (corresponding to about 10^{-7} s in time) the beam intensity advantage of neutrons is even bigger: The ESS high resolution neutron spin echo instrument will deliver 10^8 neutrons/s to typical samples compared to 10^{5-6} photons/s at the X-FEL (using γ resonance techniques).

In contrast to the study of dynamics by inelastic scattering experiments, in elastic diffraction work the advanced X-ray sources deliver orders of magnitude higher beam intensities than any thinkable neutron source. However, the high X-ray intensities over a very small beam cross section can actually lead to the rapid deterioration of the sample, in contrast to the fundamentally non-destructive character of the neutron radiation in diffraction studies even at sources as powerful as ESS. Indeed, for samples of substantial size in the several cm^2 range the number of neutrons impinging in an experimental run of about an hour will reach as much as 10^{15} at ESS without any damage to the sample. This is about the same as the number of photons which are expected to impinge on a sample in one single pulse on a projected X-FEL instrument, before the sample is fully destroyed.

In order to help to better appreciate the performance and hence the scientific capabilities of the first ESS instruments, comparisons to neutron intensities on similar, top of the line, popular user instruments currently in operation are included in this provisional ESS user guide. Such information, of course, will be by no means part of the real user guide to come at a time, when thousands of users will be given the chance to experience first hand and make their scientific work benefit from the unprecedented opportunities ESS will bring to the broadest research and development community.

Ferenc Mezei
ESS Instrumentation Task Leader

Chapter 1

ESS NEUTRON INSTRUMENT SUITE AND LAYOUT

1. ESS NEUTRON INSTRUMENT SUITE AND LAYOUT

In this volume a first set of 21 first priority neutron scattering instruments and beam facilities are described in detail. The ESS Scientific Advisory Council has selected them on the basis of an evaluation of the broad scientific impact. The two target stations, however, will accommodate 48 beam lines (or a few more if it is found feasible during the detailed engineering design to diminish the angle of neighbouring beam lines). In order to establish a reference instrument layout which better represents the completed status of ESS for the purpose of facility planning, the list of the priority instruments has been extended by another 16 spectrometers, which reflect the current state-of-the-art in neutron scattering for a fairly full coverage of the broadest experimental needs. This extended suite (see Table 1-1 and 1-2, below), with particular weight on the requirements of the priority set, has been used as reference to choose the types and number of moderators for each target station and to establish a reference lay-out of the target stations and their environment.

The reference geometry of the moderators for both the short and long pulse target stations (cf. Vol III, chapter 4) consists of two large size moderator positions (~ 20 x 12 cm^2), each viewed from both sides, i.e. four extended viewing fans per target station with different moderator characteristics:

a) short pulse target station (SPTS):
    - a conventional thin decoupled cold H_2 moderator viewed from one side, back-to-back to a decoupled thermal H_2O moderator viewed from the opposite side,
    - a novel type, so-called multi-spectral moderator with the combined spectra of a coupled thermal H_2O and a coupled cold H_2 moderator placed side by side to one another. At the SPTS, one viewing fan faces the multi-spectral side, while the opposite viewing fan faces the coupled cold part of the moderator, only,
    - the use of advanced cold moderators (solid methane like) is being considered. A decision to replace some of the above moderators at a later stage by such an advanced one will eventually be made after detailed studies of feasibility, performance, stability and maintenance.

b) long pulse target station (LPTS):
  - a coupled cold H_2 moderator viewed from both sides,
  - a novel type, so-called multi-spectral moderator with the combined spectra of a coupled thermal H_2O and a coupled cold H_2 moderator placed side by side to one another and viewed from both sides
  - the use of advanced cold moderators (solid methane like) is being considered, as the SPTS.

Common features both target stations:

- straight viewing fans with opening angles of ~60 deg each
- the total number of beam-lines at each target station is 24 at minimum, i.e. 6 per viewing fan,
- angular separation of the beam-lines: 11 deg or less (space for additional beam lines),
- each beam-line will have its own individual shutter and no bundled guides are foreseen (splitting of guides possible)
- the distance between the moderators and neutron guides front-end is ~1.5m,
- net open cross-section for the neutron guide inserts in the 2.8 m diameter shutter wheels is 23 x 17 cm² to give sufficient space for curved guides, beam splitters and multi-spectral beam extraction.

Figs. 1-1 and 1-2 illustrate the schematic geometries of the short pulse target station (SPTS) of the ESS:

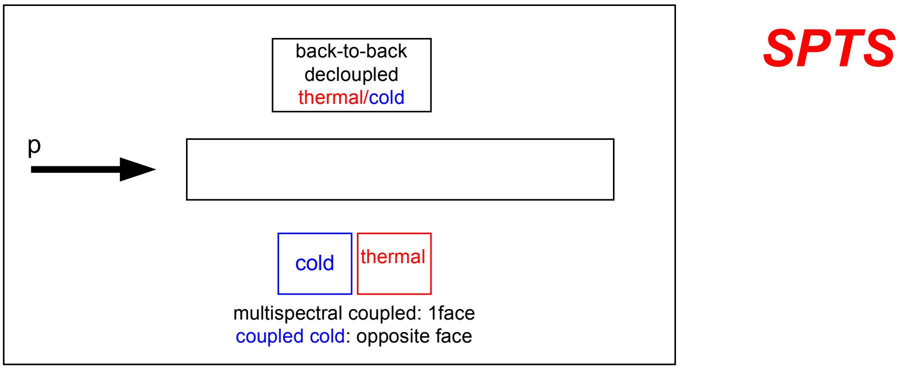

Figure 1-1: *Short pulse target station: schematic cross section*

For the reference design conventional, established moderators technique have been adopted. The replacement of conventional moderators by advanced cold moderators will be considered once they become established, technologically proven and extensively tested for performance and stability. The fairly short pulse moderator with a decoupled thermal H_2O side and a decoupled cold (20K) liquid hydrogen side placed back-to-back with a Cd-decoupler sheet in between is located on the top of the lq. Hg-target. Spectral and pulse width properties are described in detail in Vol. III, chapter 4. Thus, one viewing fan of 6 beam ports provides a thermal neutron spectrum, whereas the opposite side serves for the short pulsed cold moderator (see Fig. 1-2). There will be no poisoned moderator at the SPTS because of too short burn-out times of the poison at the high beam intensity of ESS. The newly conceived multi-spectral moderator with combined spectral properties of both a thermal and a cold coupled moderator [Mezei, 2002] is placed below the lq. Hg-target. At the short pulse station, however, the multi-spectral beam will be extracted on one side only. The viewing fan on the other side will face a purely coupled cold moderator, which provides rather short pulses in the thermal energy range. The top and bottom moderators can be exchanged according to engineering demands if requested. The footprint of the SPTS geometry is sketched in Fig. 1-2.

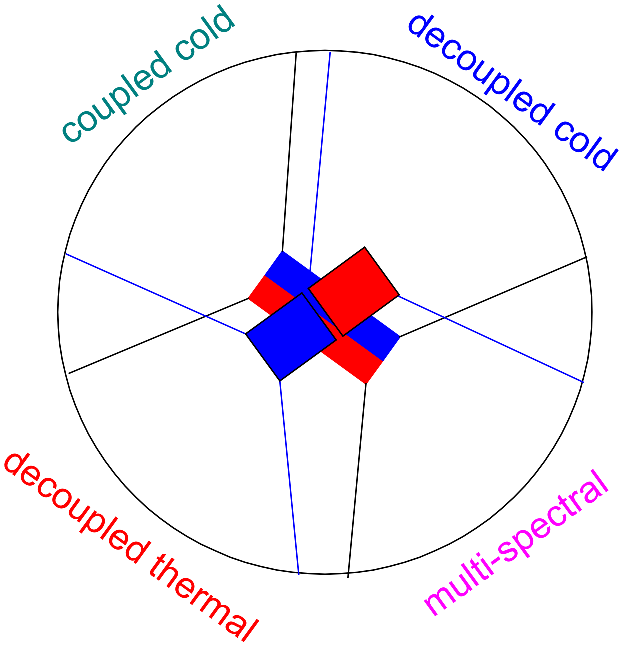

Figure 1-2: *SPTS footprint and neutron fan spectral properties*

The geometry of the LPTS is similar to that of the SPTS. Only the back-to-back moderators are replaced by a conventional pre-moderated and fully coupled, super-critical liquid H_2-moderator, optimized for high neutron current leakage. The multi-spectral moderator at the bottom of the lq. Hg-target is viewed from both sides (Fig. 1-3).

The neutron spectrum requirements of the instruments, the target station geometries and moderator constraints allow for a number of possibilities to shuffle the instruments around one or the other target station. Fig. 1-4 shows a scaled draft of the long and short pulse target stations with all the neutron

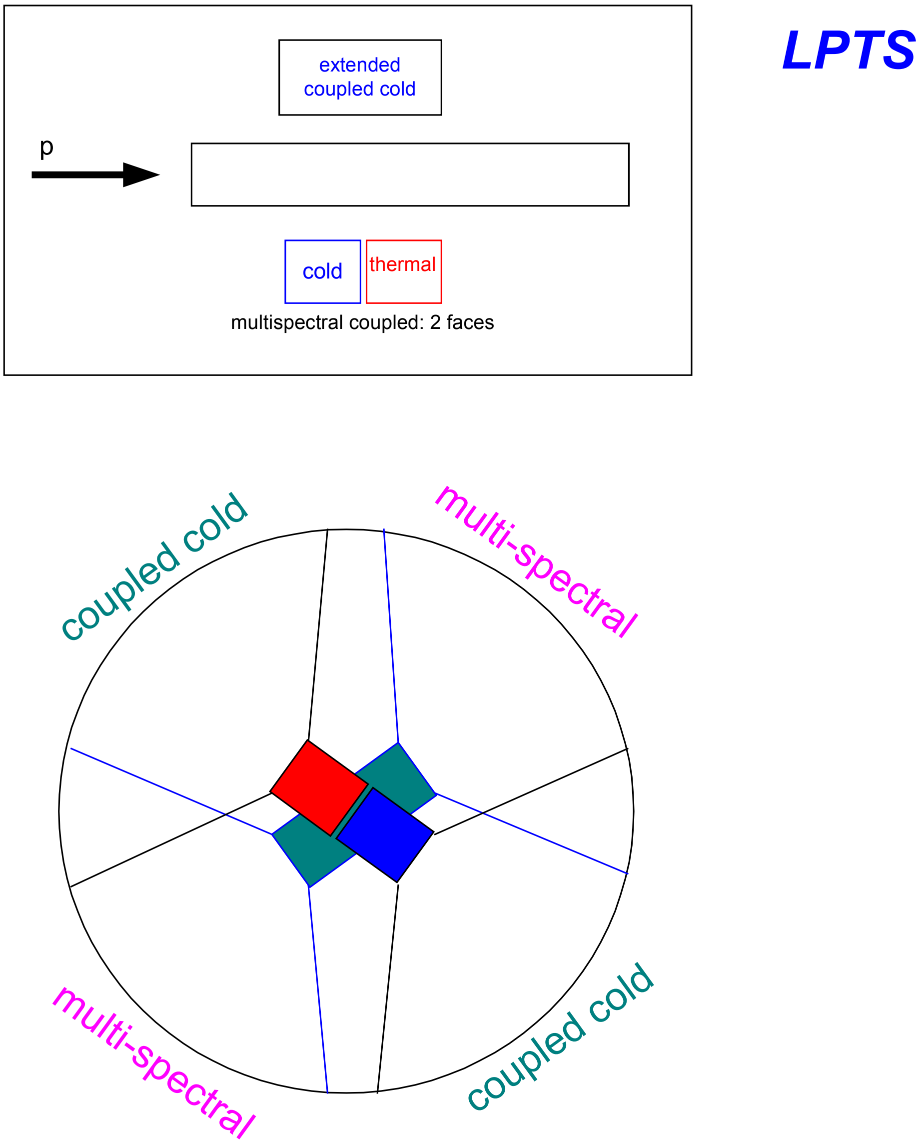

Figure 1-3: *LPTS geometry and spectral properties of neutron beam extraction fans*

beam ports named and numbered throughout. The inner circle is scaled to the real size of the reflector, all 24 of the 2.8 m diameter wheel shutters are drawn at a separation angle of 11 deg. All the beam-line front-ends start 1.5 m from the moderators. The outer circle at a radius of 6 m illustrates the approx. size of the target shielding. The beam port number comprises the type of the target station, S or L, respectively. The second character stands for the moderator type followed by a consecutive port no. This number links the neutron beam port with a specific neutron instrument identified in Tab. 1-1 or Tab. 1-2, respectively.

Several geometrical constraints must be satisfied to fit the instrument suite into the anticipated angular sectors and a given moderator beam-port fan. The individual footprints of the instruments need to be accommodated in accordance with the optimised layout of all neutron instruments. The result of this instrument shuffle is compiled in Tab. 1-1 for the SPTS and Tab. 1-2 for the LPTS. The footprint of this arrangement is illustrated in Fig. 1-5. Fig. 1-6 displays the general site layout of the whole ESS facility visualizing the reference instrument placement and space allocation.

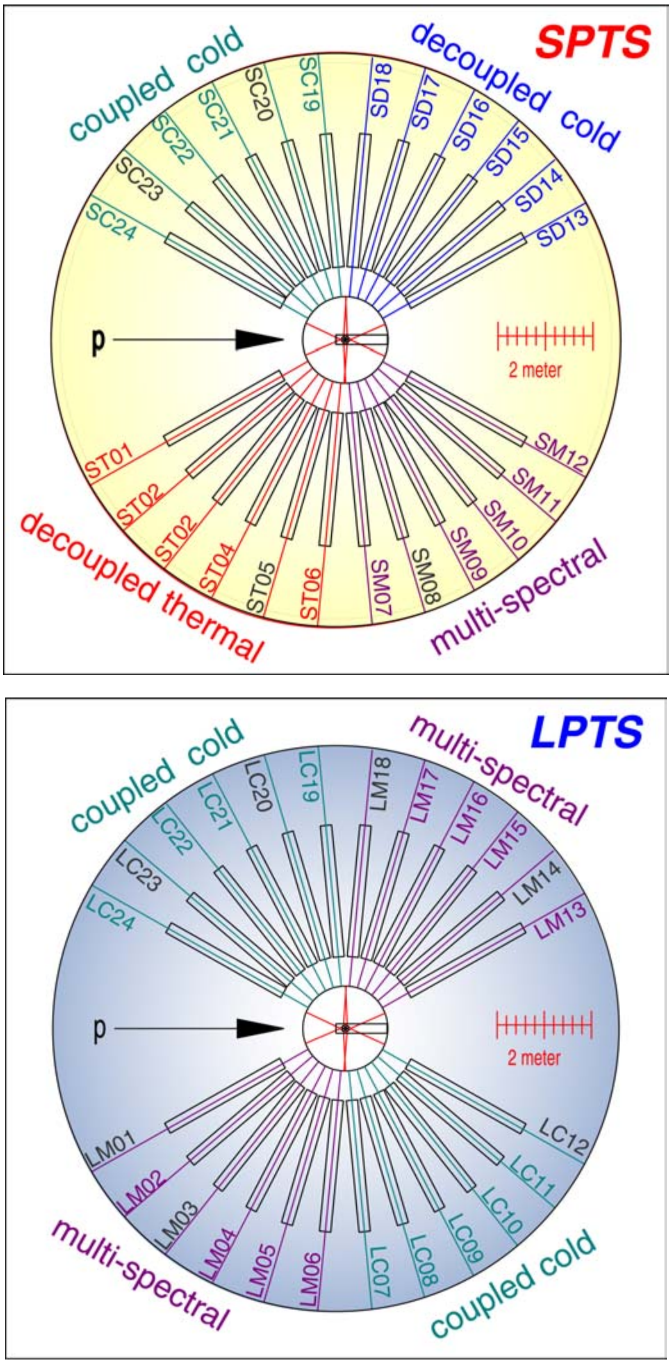

Figure 1-4: *Scaled draft of the short pulse target station SPTS (top) and long pulse target station (bottom: reflector vessel (inner circle), set of 24 beam shutters of 2.8 m diameter with beam front-end 1.5 m from the moderators, beam port no., size of target shielding (outer circle).*

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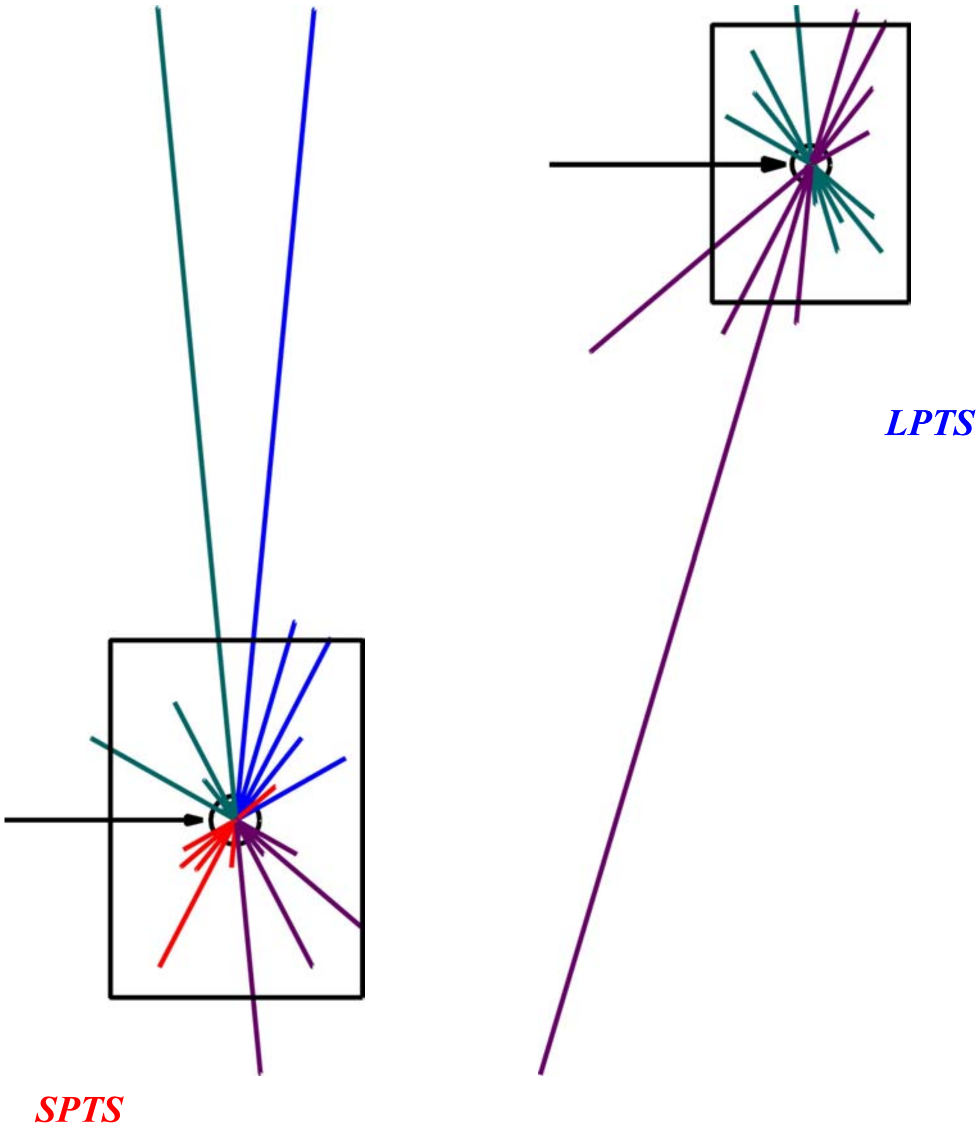

Figure 1-5: *Scaled footprints of the SPTS (left) and LPTS (right) target stations. The proton beam is incident from the left, the rectangle shows the size of the individual target station hall (62 x 88 m²).*

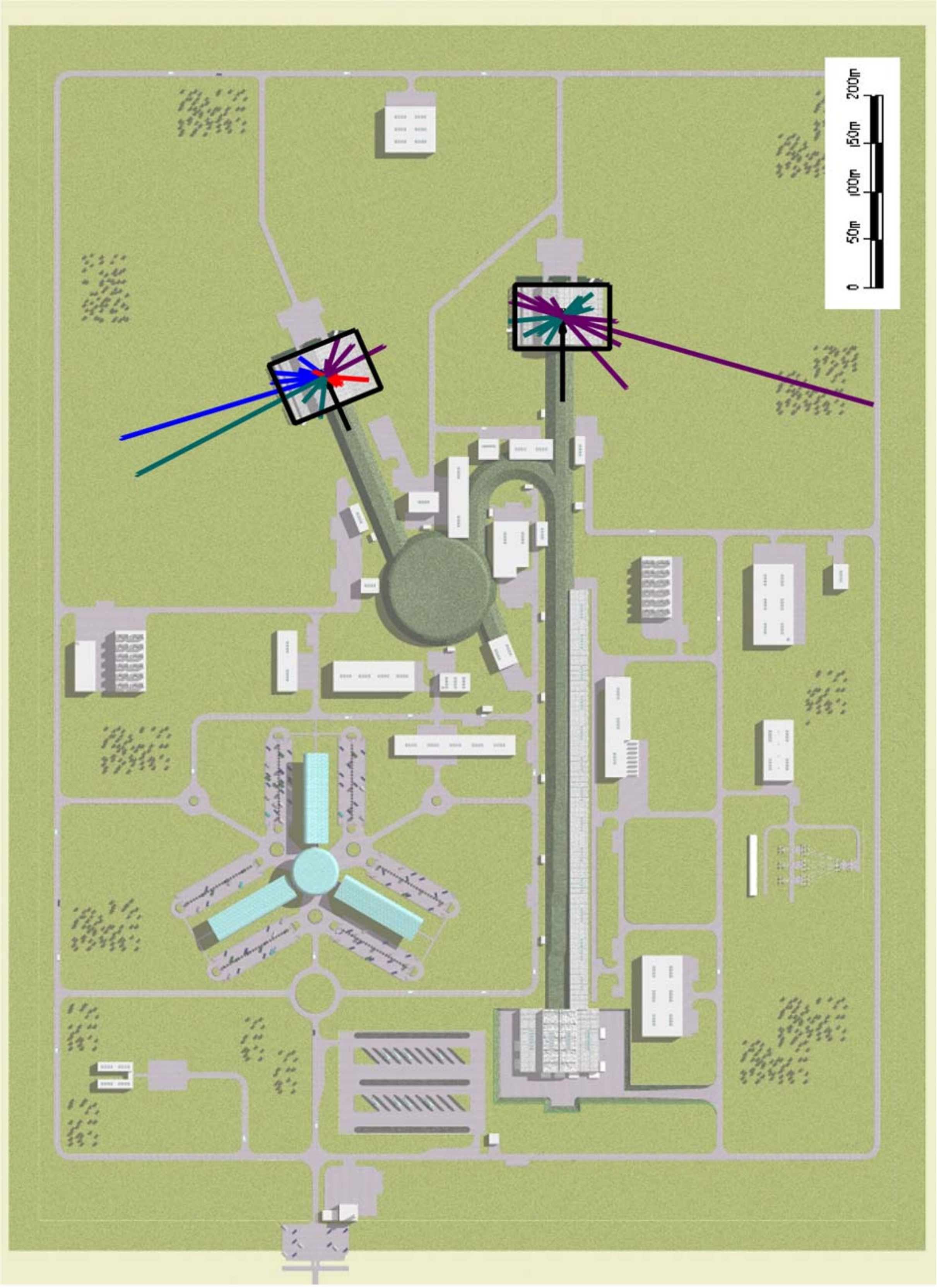

Figure 1-6: *Footprint of the ESS neutron instrument suite and site layout at the short pulse target station (top left) and long pulse target station (top right).*

Tab. 1-1: *Instruments at the Short Pulse Target Station (SPTS)*
Reference instruments are in red.

Port no.	**Instrument**	**Acronym**	**Moderator**	**Flight Path Length (m)** (prim.L_i, sec. L_f)	**Incident Energy (meV)**	**λ-range (Å)**
ST01	**Thermal Chopper Spectrometer (medium resolution)**	MET	TDC	14, 2.5	15-1500	0.23-2.5
ST02	**Molecular Spectroscopy**	TOSCA	TDC	17, 1.5	3-2000	0.2-5
ST03	**High Resolution Single Crystal Diffractometer (chemical crystallogr.)**	CHRSXD	TDC	15, 3	3-1300	0.25-5
ST04	**High Q Powder Diffractometer**	HQP	TDC	40, 2	1-10	3-8
ST05	–	–	–	–	–	–
ST06	**Liquids and Amorphous Materials Diffractometer**	LAD	TDC	11, 6	3-33000	0.05-5
SM07	**Particle Physics Beam Line S**	PPS	MS	40, x	–	–
SM08	–	–	–	–	–	–
SM09	**High Resolution Protein Single Crystal Diffractometer**	HRPSXD	MS	40, 2	3-25	1.8-5
SM10	**Single Pulse Diffractometer**	SPD	MS	10, 2	1-250	0.5-8
SM11	**Medium Resolution Backscattering Spectrometer (5 μeV)**	MRBS	MS	40, 2	1.6-20	2-7
SM12	**High Energy Chopper Spectrometer (high resolution, low Q)**	HET	MS	15, 8	15-1500	0.23-2.5
SD13	**Backscattering Spectrometer (17 μeV)**	LRBS	CDC	30,2	1 – 80	1 - 9
SD14	**eV Spectrometer**	EVS	CDC (hot mod.)	12, 1	5000-64000	0.04-0.11
SD15	**Tomography / Radiography Instr.**	TOMO	CDC	25, 4	1.6-82	1-7
SD16	**Engineering Diffractometer**	ENGIN	CDC	50, 3	1.6-170	0.7-7
SD17	**Magnetic Powder Diffractometer**	MagP	CDC	50, 2	0.1-82	1.0-30
SD18	**High Resolution Powder Diffractometer**	HRPD	CDC	200, 2	0.3-170	0.7-15
SC19	**High Resolution Backscattering Spectrometer (0.8 μeV)**	HRBS	CC	200, 3	1-20	2-10
SC20	–	–	–	–	–	–
SC21	**High λ Resolution SANS Instrument**	HR-SANS	CC	12, 20	0.2-20	2-20
SC22	**High Resolution Reflectometer**	HRRf	CC	12, 3	1.6-20	2-7
SC23	–	–	–	–	–	–
SC24	**Cold Chopper Spectrometer (low resolution)**	LET	CC	40, 3	0.5-80	1-12

Moderator: TDC thermal decoupled, MS multi-spectral, CDC cold decoupled, CC cold coupled

Tab. 1-2: *Instruments at the Long Pulse Target Station (LPTS)*
Reference instruments are in red.

Port no.	Instrument	Acronym	Moderator	Flight Path Length (m) (prim.L_i, sec. L_f)	Incident Energy (meV)	λ-range (Å)
LM01	–	–	–	–	–	–
LM02	**Variable Resolution Cold Neutron Chopper Spectrometer**	VarChop	MS	90,3	0.2-80	1-20
LM03	–	–	–	–	–	–
LM04	**High Intensity SANS Instrument**	HiSANS	MS	21,30	0.2-20	2-20
LM05	**Ultra-high Resolution Powder Diffractometer**	URPD	MS	300,3	1-100	0.9-10
LM06	**High Pressure Diffractometer**	HiPD	MS	40,6	1-300	0.5-10
LC07	**Neutron Depolarisation Instrument**	n-DEPOL	CC	12,2	–	–
LC08	**Grazing Incident SANS Instrument**	GISANS HiRef	CC	20,8	0.2-80	1-20
LC09	**Single Peak Diffractometer (CryoPAD)**	SPAD	CC	20, 2	3-330	0.5-5
LC10	**Very High Intensity SANS Instrument**	SANS	CC	21,15	0.1-20	2-25
LC11	**Fourier Diffractometer**	FourDif	CC	25,2	0.2-80	1-20
LC12	–	–	–	–	–	–
LM13	**Low Resolution Single Crystal Protein Diffractometer**	LRPD	MS	20,2	0.3-3.3	5-15
LM14	–	–	–	–	–	–
LM15	**Coherent Excitation Spectrometer (TAS)**	TAS	MS	30,2	1-170	0.7-10
LM16	**Wide Angle NSE Spectrometer / Diffuse Scattering Instrument**	WanNSE	MS	50,4	0.1-20	2-25
LM17	**High Magnetic Field Instrument**	HiMag	MS	50,2	1- 80	1 - 9
LM18	–	–	–	–	–	–
LC19	**Particle Physics Beam Line L**	PPL	CC	40, x	0.1-20	2-25
LC20	–	–	–	–	–	–
LC21	**High Intensity Reflectometer**	HiRef	CC	37,3	1-20	2-9
LC22	**Focusing Mirror Low Q SANS Instrument**	FocSANS	CC	20,8	0.7-3.3	5-12
LC23	–	–	–	–	–	–
LC24	**High Resolution NSE Spectrometer**	HRNSE	CC	30,6	0.1-20	2-25

Moderator: MS multi-spectral, CC cold coupled