Technical Report

A twenty years forward look at neutron scattering facilities in the OECD countries and Russia

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Contents

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Foreword

by Professor Enric Banda, ESF Secretary General

As the need of science for access to larger, more sophisticated research facilities and the costs of establishing and maintaining them both increase, European collaboration becomes even more essential – for Europe's scientific community as well as for the research funding agencies, the Member Organisations of ESF. By making optimum use of the continent's research facilities, we will not only be able to use our existing resources more effectively but also enhance our decision-making on future research investments. In line with its mission to strengthen fundamental science in Europe, the European Science Foundation (ESF) undertakes 'to facilitate cooperation in the use of existing facilities and in the planning and provision of new facilities'. Increasingly, ESF provides a multi-disciplinary scientific focus in Europe for a range of issues related to large research facilities (LRFs). It is able to provide scientific advice and assessment, and serves as an independent European forum to discuss LRF issues, bringing together both the users of LRFs (the science communities) and the operators/owners of LRFs (which in most cases are related to Member Organisations of the ESF).

Before agreeing to coordinate the trans-national use or to share the large financial costs of existing or projected facilities, it is imperative that the users' scientific case is investigated and proven. Ensuring that there is a critical mass of challenging science and research problems, and, even more importantly, a critical mass of committed researchers in Europe, who are capable of moving science and research forward, must be the *sine qua non* for any facility of excellence.

Within this framework, the ESF Standing Committee for Physical and Engineering Sciences (PESC) has initiated and coordinated a series of 'European Neutron Source Studies (ENS Studies)', in order to investigate the scientific case for neutron sources for future research in Europe in the natural and life sciences, and the technical sciences. A comprehensive ESF Exploratory Workshop (Autrans, 1996) was undertaken in collaboration with the European Neutron Scattering Association (ENSA), on the "Scientific Prospects for Neutron Scattering with Present and Future Sources". In addition, specific ESF investigations have targeted the scientific case for a next-generation European (spallation) neutron source (i.e. the ESS Project) and for a medium-scale regional source (i.e. the Austrian project proposal AUSTRON).

On several aspects of these studies into large research facilities at the

Foreword

European level, the ESF has worked in liaison with the OECD Megascience Forum, which pursues related and complementary studies at an international (global) and inter-governmental level. As a result of such cooperation, ESF and OECD jointly initiated the present report on the European and global outlook for neutron sources.

I welcome the joint publication of this survey, which has been undertaken by Professor Richter and Professor Springer. In the context of its own 'European Neutron Source Studies', ESF recognises this expert survey as an important technical report. While the results and opinions given in the document do not necessarily, at this stage, reflect the views of the ESF or its Member Organisations, its publication will certainly broaden the basis for discussion, assessment and planning of future research with neutron sources at the national, European, and international level.

Professor Enric Banda
ESF Secretary General

Foreword
by P.A.J. Tindemans, Chairman, OECD Megascience Forum

On behalf of the Member Delegations of the OECD Megascience Forum, I am pleased to put into the hands of the public this comprehensive report on the projected supply of research neutrons in the OECD countries and Russia. This study, carried out by two eminent scientists - Professors Dieter Richter and Tasso Springer - was commissioned by the Megascience Forum's Neutron Sources Working Group. At various stages of the work, the authors benefitted from interaction with ongoing studies being carried out under the aegis of the European Science Foundation and, therefore, the report is being published jointly by the Forum and the Foundation.

The Megascience Forum is an intergovernmental body whose members are the most economically-advanced democratic countries of Europe, North America and the Asia/ Pacific Region. The Forum brings together senior government science policy officials to discuss ways of strengthening international co-operation on very large scientific projects and programmes. At a time when research budgets are under strain in many countries, the Forum's goals are to preserve vital funding resources by encouraging co-operative efforts and by finding ways of removing barriers to international scientific co-operation. The Forum's deliberations can also be instrumental in defining the international frameworks for vital national decisions on major new scientific projects, such as neutron sources. Governments can use the Forum to strengthen their own decision-making processes by making sure that the priorities, plans and funding decisions of other countries are taken into account when national or regional plans are made. Through the Forum, countries can identify, at an early stage, attractive opportunities and partnerships for international cooperation, as well as realistic constraints on such opportunities.

The Forum's interest in the future of neutron scattering goes back to 1993, when a meeting of representatives of 18 countries was organized at Denmark's Risö National Laboratory. A follow-on meeting took place at the Oak Ridge National Laboratory in 1994. Many of the discussions centered on the question of how nations could deal in a coordinated way with the threatened "neutron gap" - a foreseen decline in the supply of neutrons caused by the shutdowns of research reactors at the end of their normal period of exploitation. To better understand the extent of this "gap", the Forum arranged for a quantitative study by the distinguished Norwegian neutron scientist, Tormod Riste. His analysis was published by the Megascience Forum in 1994. Two years later, Forum delegates established a special-purpose Working Group, composed of senior program managers, charged with exploring specific opportunities for international cooperation in the development of new neutron sources, and the more efficient exploitation and upgrading of existing facilities. The Group was very ably chaired by Paul Williams, Chairman and Chief Executive of the Council for the Central Laboratory of the Research Councils (U.K.). At its first meeting, the Working Group decided to sponsor a new quantitative study of the future neutron supply, taking into account the latest plans and proposals for new and existing sources. Sadly, the original study could not be followed-up by Riste, who died tragically in 1995.

The Neutron Sources Working Group has completed its work, and its final report is available to the public (www.oecd.org/dsti/mega). It strongly endorses the development of new, advanced regional spallation sources, and it recommends various ways in which interested countries could co-operate in order to save money, reduce technical risks and speed up the research and development process. Throughout its deliberations, the Working Group was able to take advantage of the ongoing analysis by Richter and Springer, who developed an original and sophisticated methodology for gauging the impact of proposed new sources (and upgrades of existing sources) on the most important techniques for the study of condensed matter, and the associated scientific disciplines. The report succeeds by linking the highly technical parameters of accelerator- and reactor-based neutron sources with the real-life requirements for pure and applied research in areas of great importance to science and technology policy administrations in OECD countries. These areas include health, environmental protection, economic competitiveness, national security, and many others. Thus, the authors have created a document that can serve as a model of scientifically rigorous and independent analysis that is timely, policy-relevant, and comprehensible to all persons (including non-scientists) who care about the future of this important field.

P.A.J. Tindemans
Chairman, OECD Megascience Forum

Principal Conclusions and Findings

Neutron scattering is an important scientific and technological resource that provides essential information about the fundamental properties of living and non-living materials. An ever-growing scientific community (currently of the order of 6000 scientists) uses neutrons for research in physics and chemistry and, more recently, in materials science, engineering, earth sciences and biology. In the OECD countries and in Russia, currently-active sources of neutrons will not be able to supply the future demand. In fact, some time between the years 2010 and 2020, the presently-installed capacity of neutron sources for beam research will decrease to a level *below one-third of that of today*.

New neutron sources, currently being planned in different regions of the world, can ensure the continuity of the supply of research neutrons, provided that the necessary political and funding decisions are taken between now and 2005 at the latest. When accompanied by the development of advanced instrumentation, the construction of these new sources will bring about significant increases in performance and efficiency. Increases in total scientific output can be anticipated, along with dramatic improvements in the quality and utility of the research.

The following findings of our study support the above conclusions:

- The basic understanding of physical materials (metals, alloys, ceramics, polymers, liquids, glasses, etc.) and of biological matter, requires the detailed knowledge of *the arrangement and the dynamics of their atoms or molecules.* The relation between the characteristics of materials at the atomic level, and their macroscopic and technological properties, is of great scientific interest and forms the basis of modern materials research and development. Similarly, biological function is related to the molecular structure and motion in living matter. Atomic properties are probed mainly by the *interaction* of various kinds of *radiation* (neutrons, photons, electrons, ions) with these materials. Among the different classes of radiation, neutrons play a unique and important role.

- The interaction between radiation (in this case, neutrons), and a sample material is known as *scattering.* In an actual experiment, a neutron beam with a well-defined direction and velocity is incident on a sample. Due to interaction with the nuclei or atoms, the neutrons leave the sample, distributed over many directions and velocities. The detailed analysis of these distributions leads to the desired information on structure and dynamics of the atoms in the sample. In some cases, instead of scattering, the interactions are investigated via the reflection of neutrons from the surface. The type of scattering that leads to the information on atomic positions is called *diffraction*, whereas atomic motion is observed via *spectroscopy*.

- Presently, in the OECD countries and in Russia, about 26 major neutron sources are available for research. Most of the sources incorporate nuclear reactors that were built in the 1950s and 1960s. For technical reasons, the majority of these reactors will reach the end of their useful lives between the years 2005 and 2015. The study shows that less than *one third of the present* neutron sources will be available in the year 2015 (this includes non-reactor spallation sources). Given the size of the neutron scattering community (over 6000 scientists), and the increasing interest in this technique, determined government actions will be needed to compensate for the decline in the number of sources.

- Though neutrons for scattering experiments are produced by large (so-called "megascience") facilities, neutron scattering experiments at these facilities are typically carried out by small research groups, doing the kind of work that is sometimes called "small science". The majority of users need short-term access to the facilities, often no more than a few days. These small research teams do not necessarily use the same source on a long-term basis. In contrast to high energy physics, where large research teams cooperate over periods of years on a single experiment, this kind of utilisation cannot be ensured by one or two "global sources".

- This study analyses the future evolution both of sources and instruments. In view of the pattern of utilisation described above, projections for individual *classes of instruments* will be made for specific *geographical regions*: Europe, North America, and the Pacific region. To quote just a few sample results: in the year 2017, in the absence of new sources, the number of available small angle scattering instruments (which are essential for polymer studies, material science and biological research) in *Europe* will decrease to less than one fourth of the present level. In *North America,* the starting level in general is lower than in Europe, and the decline is less pronounced. In the *Pacific* region, the starting profile is low, and in 2017 almost all of the current installations will simply have shut down.

- This study also analyses the likely *future development of the scientific demand* for neutron sources and instruments. Growth in traditional fields of neutron research is predicted, for example, in solid state physics, and many branches of chemistry. This will involve an increase in the complexity and sophistication of the work, rather than a mere growth of the number of studies. Higher demand is also likely in disciplines that have not made extensive use of neutrons in the past, such as materials research, engineering and earth sciences. In addition, novel methods and creative thinking can, in the future, generate entirely new research fields, leading to important progress in unanticipated ways.

- At this time, *new sources are being planned* in all three world regions and some new sources are under construction. For Europe, the study shows that even the realisation of several new projects would do no more than simply compensate for the predicted decline in current capacity. The increased quality of some of the planned sources may, however, lead to an expansion into new areas of neutron research. In North America, the construction of a new pulsed source would significantly strengthen the research capacity. In the Pacific region, the realisation of the planned sources would approach or even exceed the present capabilities of the other regions even within the next decade.

- Taking into account the long lead time between a formal decision in favour of a project and its completion, *decisions on the proposed projects have to be taken between now and 2005* to avert the threatened shortage of neutrons. Otherwise, a significant period of decline has to be faced.

- While keeping the number of available instruments roughly constant (in Europe) or increasing it considerably (in the Pacific region), the new sources will also enhance the *instrument performance* significantly. This is in particular true for powder diffractometers that are needed for structural research, and for time-of-flight (TOF) spectrometers that provide dynamical information. In general, *to fully exploit the potential of existing and planned sources, new innovative experimental devices and techniques are needed.* Therefore, a significant fraction of the money provided for the projected sources should be spent for the development of their instrumentation. This is especially true for new techniques at pulsed sources.

This study demonstrates that the areas in which a significant increase in demand can be expected are strongly associated with TOF measurements. This correlates well with the current trend towards planning *pulsed* spallation sources. On the other hand, there are also important techniques that require *high average intensities*, such as triple axis, single crystal, and small angle scattering instruments. For these purposes, sufficient intensities are provided by high-flux reactors, or by spallation sources whose beam power is one megawatt or more. For isotope production or materials testing, *multipurpose reactors*, with beam holes and large irradiation volumes, will continue to play a unique and important role.

1. The importance of neutron scattering for materials research and for the study of condensed matter

Modern materials research, together with the traditional scientific interest in understanding condensed matter at the atomic scale, require a complete knowledge of the arrangement and the dynamics of the atoms or molecules, and of their magnetic properties as well. This information can be obtained by investigating the interactions of the material in question with various kinds of radiation, such as visible light, X-rays or synchrotron radiation, electrons, ions, and neutrons. Neutrons play a unique role due to their inherent properties:

- their magnetic dipole moment allows the investigation of the magnetic properties of materials;

- their large mass leads to a simultaneous sensitivity to the spatial and temporal scales that are characteristic of atomic distances and motions.

Thus, while X-ray photons can provide information about the positions of atoms, neutrons can indicate not only where the atoms are, but also the direction and speed of their motions. Neutrons interact differently with the different isotopes of the same atomic species. This allows an experimenter to "paint" selected atoms or molecules by isotope replacement, to highlight these atoms or molecules via neutron scattering, in contrast to the other species. Neutrons can easily penetrate a thick material - an important advantage for materials testing. The interaction of the neutron with a nucleus has a simple form, which facilitates the direct, unambiguous theoretical interpretation of experimental data.

For certain investigations neutron scattering is the only choice, or the most advantageous method compared to the alternatives; in other cases, neutrons are a complementary method, and only a sophisticated analysis allows one to choose the best technique on a case-by-case basis.

The quality and precision of neutron scattering experiments is primarily determined by the counting rate and, therefore, essentially, by the strength of the source. Thus, the usefulness of a research reactor is given by its thermal *neutron flux,* quoted in units of neutrons per square centimetre per second. The first research reactors reached criticality in the 1940s with fluxes of 10^{11} to 10^{12} n/cm^2 s. The "medium-flux reactors" (such as DIDO at Juelich) became operational in the 1950s and 1960s, with fluxes of approximately 10^{14}, and, finally about 10^{15} was obtained in the "high-flux reactors" of the 1960s and 1970s at Brookhaven, Oak Ridge and Grenoble. Fluxes significantly beyond 10^{15} (as in the proposed ANS project at the Oak Ridge National Laboratory) will only be achieved if the formidable technical difficulties can be overcome, and if the considerable financial resources can be procured. So far, no such project has been realised.

Since the first research reactors went into operation, an increase of approximately four orders of magnitude has been achieved in source strength (flux). However, what finally counts is the data collection rate at the detectors. Through the development of improved instrumentation (e.g. analysers, polarizers, detectors) the available effective intensities have been augmented by further orders of magnitude.

The neutrons in a reactor are normally thermal, i.e., their velocity distribution corresponds to the temperature of the moderator. For research with high resolution, it is advantageous to cool the neutrons below the moderator temperature. This is achieved by so-called *cold sources*, consisting of a container of liquid hydrogen or deuterium embedded in the moderator of the reactor.

1. The importance of neutron scattering for materials research and for the study of condensed matter

This technique increases the flux by an additional factor of ten to twenty. *Hot sources*, on the other hand (e.g., a heated graphite moderator), shift the neutron spectrum to higher energies to make better use of certain types of diffractometers and spectrometers.

During the last 10 to 15 years, an alternative way of producing neutrons has become increasingly important. In the process of *spallation*, neutrons are evaporated from heavy nuclei by the impact of protons (with energies in the GeV range) from a high-current accelerator. In general, such spallation sources are pulsed, with pulse lengths of several microseconds, and with peak fluxes that are from ten to several hundred times higher than those of steady-state neutron sources. Spallation sources also have the advantage that different moderators can be installed, tailoring the neutron spectra to the needs of the experiments. Since the majority of condensed matter experiments benefit from the pulsing of the flux, the development of high-power spallation sources will be a key advantage of the next generation of high-flux sources.

The demand for high neutron fluxes leads to large, costly sources. We emphasise, however, that *smaller neutron sources*, with a relatively lower flux, play an important role, in fulfilling national measurement needs and in developing and testing novel methods of neutron scattering.

Modern high-flux sources, such as the reactor at the ILL in Grenoble or the ISIS spallation source in the UK, are *"big science"* machines, like accelerators in high-energy physics. In contrast to high-energy physics which is big science *in toto*, the instrumentation and the experiments at a neutron source have the characteristics of *laboratory work*, carried out by many groups or even single individuals. As an example, we consider the Grenoble reactor, which provides neutrons to over 40 instruments placed around the source. Between 1000 and 1200 scientists per year perform experiments with these instruments and they come from a wide range of laboratories specialising in solid state physics, chemistry, biology, etc. The measurements they perform last for days or weeks. *In this way, a single large neutron source provides an enormous concentration of a wide variety of research equipment that would otherwise be distributed over dozens of university laboratories. Therefore, closing down a high-quality neutron source can deprive hundreds of scientists of their primary research tool.* The unexpected shutdown of the ILL reactor for repairs from 1991 to 1995 was a painful experience for a large user community and a severe drought for European condensed matter science. Such high-intensity sources are "regional" in a literal sense: for instance, there is the "high-flux reactor" at the ILL in Europe, and there are two in the United States. In addition, a larger number of medium-flux reactors are distributed at national research centres throughout the OECD countries.

2. Goal and procedure of this study

The study presents a forward look at the availability of sources from the present to twenty years from now, with detailed consideration of projects which are under construction, under technical study, or awaiting a political decision. This study investigates the impact of these new sources, taking into account the likely shutdowns of many of the existing facilities during the next decades. Specifically, it focuses on the consequences for the relevant scientific disciplines. The study covers the OECD countries and Russia, and it projects the neutron supply for condensed matter research in the fields of solid state physics, chemistry, materials research, engineering, geology, and molecular biology. There are other applications, such as nuclear and particle physics, radio-chemistry, materials testing, and isotope production, which are not subjects of this study. The strategy was as follows.

A survey performed by the authors during March 1997 provided statistical information on the status of existing neutron sources, funded projects, and projects which have not yet been authorised. A questionnaire was sent to the managers of all major neutron sources that are being used for condensed matter science in the OECD countries and Russia. Thirty-five questionnaires were sent out and all were returned except one (a sample questionnaire is attached in Appendix 4). For all of these facilities, an inquiry was also made regarding the number of various types of instruments (diffractometers, spectrometers, etc.). In addition, on the basis of the information from representative sources like the ILL, ISIS, and NIST, an estimate was made of how the utilisation of these instruments is distributed among various scientific disciplines.

To perform the forward projection, *a characteristic lifetime* for the existing sources has to be postulated. As in the earlier Megascience Forum report [1] by Tormod Riste, this study assumes a reactor lifetime of 40 years after first criticality, and of twenty years after a major upgrade. For spallation sources, an indefinite lifetime is assumed, since they have all been built relatively recently and consist of components (ion source, accelerator, target, etc.) that can be independently and consecutively replaced. For the expected lifetime of the instruments at the sources, the same value is used as for the sources themselves. Thus, for example, a diffractometer survives as an instrument type, undergoing periodic improvement and being partly or entirely renewed from time to time. Major innovations in instrumentation technology may alter this picture in an unforeseeable fashion but, naturally, we could not include such eventualities in our study. Based on the above assumptions, the supply of neutrons can be predicted for the coming twenty years. Sources under construction or in the planning stage are included in the analysis. The results can then be related to the estimated demand for research neutrons as evaluated in a recent report of the European Science Foundation ("Scientific Prospects for Neutron Scattering with Present and Future Sources", also known as the Autrans Report, 1996) [2].

Though the inquiry was carried out globally, supply and demand were analysed on a *regional basis*. *North America*, *Europe* and the *Pacific* were chosen as reference regions. As stated above, the regional analysis is appropriate since the majority of users need rapid access to their facilities, with many experiments being performed during short periods of time by small research groups. Such a mode of operation cannot be ensured on a global scale. Also, the impact on the surrounding scientific community is deeper for a regional than it would be for a large global source.

3. Status and time evolution of neutron sources

The results of the survey are listed in Tables 1 and 2 for existing continuous and pulsed sources. Tables 3 and 4 show the data on reactor and spallation source projects which are presently under consideration. Entirely new projects as well as upgrades are included. In each case, we note the status of the project, the anticipated date of a political decision, and the starting date as provided by the advocates of the project.

At present, none of the pulsed sources have been approved, but several upgrades of existing spallation sources are expected.

Table 1: Existing continuous sources

Source	Location	Weight factor	First operation	Power [MW]	Thermal flux [10^{14} n/cm²s]	Special moderators cold	Special moderators hot	Operating time [days/y]	Number of users intern.	Number of users extern.
Australia										
HIFAR	Lucas Heights	2.2	1958	10	1.4	0	0	300	10	62
Canada										
NRU	Chalk River	2.8	1957	120	3.0	0	0	300	10	100
Denmark										
DR3	Risø	2.3	1960	10	1.5	1	0	286	20	120
France										
HFR	Grenoble	4.2	1972	58	12.0	2	1	225	50	1200
Orphée	Saclay	2.8	1980	14	3.0	2	1	240	60	500
Germany										
BER-2	Berlin	2.5	1973	10	2.0	1	0	240	70	300
FRJ-2	Juelich	2.5	1962	23	2.0	1	0	200	50	150
FRG	Geesthacht	1.9	1958	5	0.8	1	0	200	27	68
Hungary										
BNC	Budapest	2.3	1959	10	1.6	1	0	200	20	60
Japan										
JRR-3	Tokai	2.5	1962	20	2.0	1	0	182	192	387
Korea										
Hanaro	Taejon	2.7	1996	30	2.8	0	0	252	16	not yet open
Netherlands										
HOR	Delft	1.2	1963	2	0.2	0	0	160	25	15
Norway										
JEEP2	Kjeller	1.3	1966	2	0.22	1	0	269	8	7
Russia										
IR8	Moscow	2.3	1957	8	1.5	0	0	100	35	10
IWW-2M	Ekaterinburg	2.0	1966	15	1.0	0	0	250	50	-
WWR-M	Gatchina	2.2	1960	18	1.4	1	0	200	60	13
Sweden										
R-2	Studsvik	2.0	1960	50	1.0	0	0	187	10	60
Switzerland										
SINQ	Villigen	2.5	1996	1000 KW Spall. Source	2.0	1	0	250	30	?
USA										
HFBR	Brookhaven	3.0	1965	30	4.0	1	0	260	54	223
HFIR	Oak Ridge	4.2	1966	85	12.0	1	0	210	37	139
NBSR	Gaithersburg	2.5	1969	20	2.0	1	0	250	36	650

Table 2: Existing pulsed sources

Source	Location	Weight factor	First operation	Beam power [KW]	Pulse length [µs] (Proton pulse)	Rep. rate [Hz]	Thermal peak flux [10^{14} n/cm^{2}s]	Moderators cold	Moderators thermal	Operating time [days/y]	Number of users int.	Number of users ext.
Japan												
KENS/KEK	Tsukuba	1.3	1980	3	0.1	20	3	1	1	80	14	400
Russia												
IBR2	Dubna	2.9	1984	2000 fission	305 (therma n)	5	100	1	3	104	50	150
UK												
ISIS	Abingdon	3.4	1985	160	0.4	50	20-100	2	2	168	30	1200
USA												
LANSCE	Los Alamos	3.0	1985	56	0.27	20	34	1	3	100	21	41
IPNS	Argonne	1.5	1981	7	0.1	30	5	3	0	175	58	143

Table 3: Planned research reactors and upgrades

Project	Location	Weight factor	Status	Decision date	Anticipated starting date	Power [MW]	Thermal flux [10^{14}n/cm^{2}s]	Special moderators cold	Special moderators hot
Australia									
HIFAR1	Lucas Heights	2.8	Preproject	1998	unknown	13- 20	3	1	1
Canada									
IRF	?	2.8	Preproject	1998	2006	40	3	1	–
Germany									
FRM II	München	3.6	under constr.	-	2001	20	7	1	1
Russia									
PIK	St. Petersburg	4.2	under constr.	-	2000	100	12	1	1
USA									
HFBR (upgrade)	Brookhaven	3.7	Preproject	1998 or later	2005	60	8	1	0
HFIR (upgrade I)	Oak Ridge	4.2	under constr.	-	2000	100	12	1	0
HFIR (upgrade II)	Oak Ridge	4.2	Calcul.	1998	2001	100	12	1	0

The European ESS, the SNS in the USA, and the Japanese NSRP and JHF projects belong to a category of sources aiming for the very highest fluxes. All proposed spallation sources are characterised by proton pulses in the microsecond range, to fully exploit the scientific value of TOF spectrometers and diffractometers. The NSRP project will have a dual use: scattering research, and studies on actinide (nuclear waste) transmutation. The IBR2 source (which will be upgraded) is the world's only pulsed research reactor, with pulses of 305 ms. Among the reactor projects, only the new FRM II reactor in

Table 4: Planned pulsed sources and upgrades

Project	Location	Weight factor	Status	Decision date	Anticipated starting date	Beam power [KW]	Pulse length [µs] (Proton pulse)	Rep. rate [Hz]	Thermal peak flux [10^{14}n/cm^{2}s]	Moderators cold	thermal
Austria											
Austron	?	4.8	preproject	1998	2005	500	0.44	50	75	2	2
Europe											
ESS	not yet decided	8.9	R+D Phase	2000	2010	4000/1000	1	50/10	2000	4	2
Japan											
JHP	Tsukuba	5.9	Eng.Design	1997	2003	600	<1	25	600	2	2
NSRP	Tokai	9.5	R+D/Eng.	1998	2005/08	5000	<1	50	2600	2	2
Russia											
INR	Troitsk	2.0	under constr.	–	1997	30	1 ?	50	3.5		1
IBR2 (upgrade)*	Dubna	2.9	under constr.	–	2005	2000 fission	305 (neutrons)	5	100	1	3
UK											
ISIS I*	Abingdon	3.8	R+D	1998	2000	240	0.4	50	30-150	2	2
ISIS II*	Chilton	3.9	R+D	2000	2003	240/80	0.4	50/12.5	30-150/10-50	4	2
USA											
LANSCE*	Los Alamos	3.8	under constr.	–	1999	160	0.27	30	64	2	4
SNS	Oak Ridge	5.7	Eng. Proj.	1998	2004	1000	1	60	200	2	2

*replaces existing source

Munich is under construction. The world's only steady-state spallation source, SINQ (in Villigen, Switzerland), started operations in 1996.

Figure 1 displays the likely time development of the number of neutron sources, including existing continuous and pulsed sources, and proposed sources in both categories. As of 1997, twenty-one continuous sources are in operation within the OECD countries. Without major upgrades, only four of them are expected to be operational in 2017. Of the five currently-operating pulsed sources, four will still exist in 2017. Clearly, even the totality of proposed continuous and pulsed sources will not suffice to compensate, in sheer numbers, for the expected shut-down of existing facilities.

Numbers of sources alone, however, do not tell the whole story. To quantify the scientific impact of the different sources, we must introduce weight factors. For continuous sources, the *weight factors* are a function of the available neutron flux, which determines the performance of the totality of the neutron scattering instruments. For pulsed sources, the analysis is more

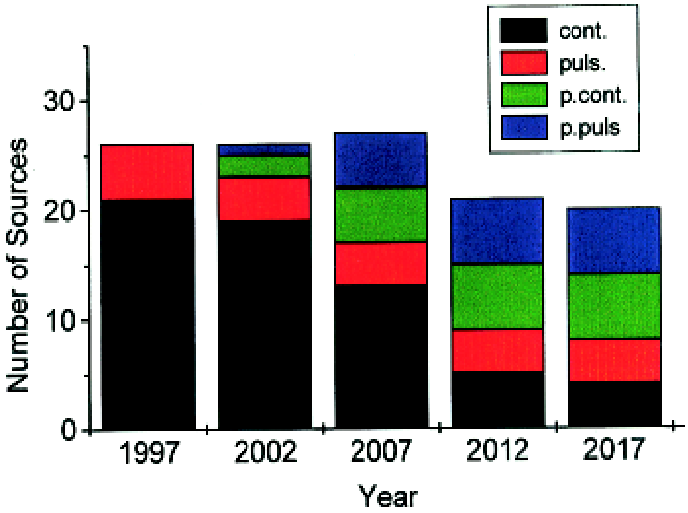


Fig. 1:
Availability of existing continuous and pulsed neutron sources for the next twenty years. The columns present the projected availabilities, in five year steps, commencing with 1997. The black areas display the lifetime projection of existing continuous sources, the red areas relate to existing pulsed sources, while the green and blue areas stand for reactor and spallation source projects. Only those sources which are to be used for beam hole research are shown.

complex, since the efficiency of individual instruments depends on pulse intensity, repetition rate, and average flux. The weighting of these sources (and, in particular, their comparison with continuous sources) cannot be done without a detailed analysis at the associated instrumentation.

In this section, the weighting of continuous sources will be introduced, and figures of merit for these sources will be developed. For pulsed sources, a detailed discussion will follow in the next section, which deals explicitly with instrumentation, but the results will be quoted here in advance to provide a consolidated presentation of continuous and pulsed facilities.

The continuous sources listed in Table 1 span more than two orders of magnitude in neutron flux. At first sight, the utility of each source could be weighted in proportion to its flux, but this would heavily underestimate the importance of smaller sources, which play a unique and valuable role, as outlined in the first section.

Another extreme would be a weighting of the sources on a logarithmic flux scale, but this, in turn, would underestimate the great scientific value of high-flux sources. We chose a procedure in between the two extremes, and introduced a power law source weighting factor:

$$W = 2^{\log\phi} \qquad (1)$$

where the flux ϕ, is in units of 10^{13} n/cm^{2}s.

Thus, low-flux reactors with $\phi = 10^{13}$ n/cm^{2}s have a weight of one; medium-flux reactors with $\phi = 10^{14}$ n/cm^{2}s, a weight of two; and high-flux reactors with $\phi = 10^{15}$ n/cm^{2}s have a weight of four. The weighting of pulsed sources is fully explained in the next section, and Tables 1 to 4 anticipate the results. Although this weighting scheme may seem to be somewhat arbitrary, it represents not only our assessment but also that of number of eminent neutron experts both from continuous and pulsed sources who endorsed the approach as correctly emphasising the relative significance of sources of different flux.

Source strength and degree of exploitation determine the scientific importance of a source. Thus, in order to compare different sources (continuous as well as pulsed), we introduce a figure of merit, *M*. It is the product of the inherent strength of a source (measured by the weighting factor, *W*) and the number of available neutron scattering instruments, *n*:

$$M = W \cdot n \quad (2)$$

For pulsed sources, different weighting factors for different instrument classes must be applied (see section 4) and in Equation (2) an average value is used.

Figure 2 displays the accumulated figures of merit for present and planned sources for the period 1997-2017. For existing sources, the accumulated figure of merit will decline from about 800 in 1997 to 280 in 2017, i.e., a *reduction by about a factor of* 3, in approximate agreement with the reduction in the number of sources from 26 to 8. While all of the planned reactor sources together could not compensate for this decline, the construction of the planned spallation sources would lead to a significant increase in the accumulated figure of merit. In this regard, the large spallation source projects (ESS in Europe, JHF and NSRP in Japan, and SNS in the USA) assume the greatest prominence.

We wish to emphasise that these increases would not just result in more experiments being undertaken, but would greatly enhance the variety and quality of research. This was already observed during the transition from medium- to high-flux reactors, which made it possible to perform experiments that were previously not feasible, and made neutron scattering available to an entirely new, multidisciplinary community of scientists. Future high power spallation sources are again likely to lead to new methods and to unexpected, exciting discoveries.

Tables 1 and 2 also include the numbers of internal and external users. Internal users are those originating from the laboratory which operates the source, e.g.,

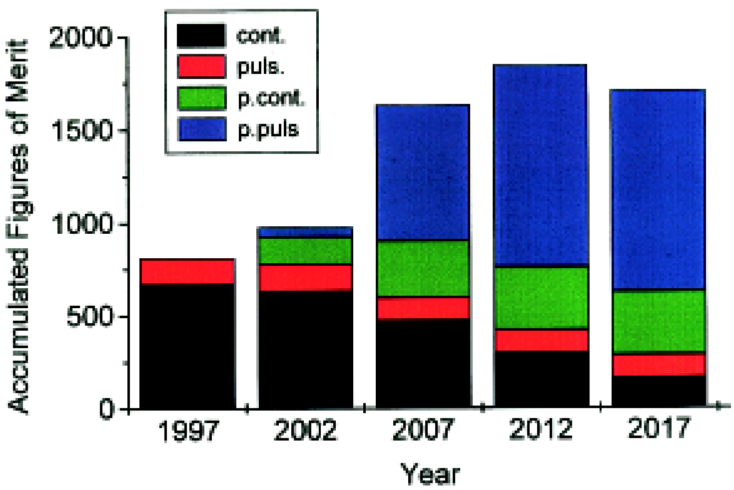


Fig. 2:
Accumulated figures of merit following Eq. (2). The color coding is: *black*: existing continuous sources; *red*: existing pulsed sources; *green*: projected continuous sources; *blue*: projected pulsed sources.

scientists from the Brookhaven National Laboratory are considered to be internal users of the HFBR. External users come from universities, industry, or other research laboratories. The total number is about 7000 (this may be an over-estimate, since some researchers use more than one source). This is consistent with the recent estimate of about 4000 neutron users in Europe based on a user inquiry by the European Neutron Scattering Association (ENSA) [3], and the often-quoted estimates of 1000 users in North America, and about 1000 in Japan.

These 6000 scientists depend on the presently existing neutron facilities, and will be strongly affected if the predicted decline is not compensated by the implementation of the new projects. Given the long lead time from conceptual design to commissioning of a new source (at least 10 years), political decisions on these new facilities are necessary in the next few years, and certainly before the year 2005. *Otherwise, most of these scientists will be deprived of a very important (and, in some cases, unique) research tool*. In this context we quote a recent assessment from the European Science Foundation:

"Neutron scattering techniques remain a vital resource for the structural investigation of condensed matter, including the solution of structural problems in the technical sciences and industrial developments." And: "Synchrotron radiation techniques and radiation sources cannot abrogate neutron techniques and neutron sources (which would have been an appealing hope at financially constrained times with regard to the much lower specific costs of soft X-photon beams compared to neutron beams)." [2]

4. Present state and evolution of instrumentation

The existence of neutron sources is one of the preconditions for neutron beam research; the other is instrumentation. Therefore, in the survey of sources, we inquired about the status of existing and planned neutron instruments, classifying them into four main groups: diffractometers; small angle neutron scattering (SANS) and reflectivity instruments; spectrometers for inelastic scattering; and polarized neutron instruments. Each group was split into subgroups to obtain a detailed picture of the present situation, and of plans for the future.

Table 5 provides information about the existing instrumentation at continuous sources, while Table 6 presents the instruments at pulsed sources, and also shows the planned instrumentation at future spallation sources.

Table 5: Existing instruments on continuous sources

Source	Weight factor	Scatt. Instr.	Fig. of merit	Type of Instruments											
				Diffractometers				SANS + Reflect.		Inelastic Instr.				Polarised Instr.	Others
				Powder	Single crystal	Diffuse	Engi-neering	SANS	Reflect.	TOF	Triple axis	Back-scattering	Spin echo		
Australia															
HIFAR	2.2	7	15.4	2	2			1			1.0			1	2
Canada															
NRU	2.8	6	16.8	1			1		1		2.0			1	1
Denmark															
DR3	2.3	8	18.4	1	1		1	1	1		3.0				
France															
HFR	4.2	32	134.4	4	6	0.5		2	3	3	3.0	2	2	6	11
Orphée	2.8	25	70.0	3	2	2.0	2	3	3	1	5.0		2	2	3
Germany															
BER-2	2.5	16	40.0	1	4	1.0	1	2	1	1	3.0		2	4*	8
FRJ-2	2.5	16	40.0	1	3	1.0		4	1	2	2.0	1	1	1*	3
FRG	1.9	8	15.2				2	3	2	1				5*	5
Hungary															
BNC	2.3	7	16.1	1	1		1	1	1		2.0				6
Japan															
JRR-3	2.5	23	57.5	2	3		2	3	1	2	8.0	1	1	3*	5
Korea															
Hanaro	2.7	6	16.2	1	1	1.0*	1*	1	1		1.0			1	
Netherlands															
HOR	1.2	5	6.0			1.0			1	1				2	
Norway															
JEEP2	1.3	5	6.5	2				1		1	1.0				2
Russia															
IR8	2.3	4	9.2	1	1					1	1.0				
IWW-2M	2.0	7	14.0	4	1			1			1.0				
WWR-M	2.2	12	26.4	2	1	1.0		1	1		1.0		1	4	10
Sweden															
R2	2.0	5	10.0	1	1	1.0	1			1					1
Switzerland															
SINQ	2.5	13	32.5	2	1		1	1	1	2	2.0	1	1	1	3
USA															
HFBR	3.0	14	42.0	2	3	1.0	1	1	1		4.0			1	
HFIR	4.2	9	37.8	1	1	1.0	1*	1	1		4.0			1*	2
NBSR	2.5	17	42.5	1	1*		1	4	2	2	4.0	1	1	1	6
SUM		**245**	**666.9**	**33**	**32**	**9.5**	**14**	**31**	**22**	**18**	**48.5**	**6**	**11**	**20 (14)**	**68**

*instruments already counted in another category

Table 6: Existing and planned instruments on pulsed sources

Source	Scatt. Instr.	Fig. of merit	Type of Instruments														
			Diffractometers					SANS + Reflect.			Inelastic Instr.				Polarised	weight	Others
			Weight factor	Powder	Single crystal	Diffuse	Engi-neering	Weight factor	SANS	Reflect	Weight factor	TOF	Back-scattering	Spin echo	Instr.	av.flux	
Japan																	
KENS/KEK	16.0	20.0	2.8	3.0	1.0	1.0		0.7	2.0	1.0	1.1	5.0	1.0		2.0	0.4	1.0
Russia																	
IBR2	11.0	31.7	5.3	3.0	1.0		1.0	3.0	1.0	1.0	2.1	3.0			1.0	1.1	
UK																	
ISIS	15.5	52.7	7.0	3.3	0.8	2.4	0.5	1.5	1.0	1.6	3.7	4.6	0.9		0.4	1.2	0.5
USA																	
LANSCE	7.0	21.0	6.7	2.0	1.0			1.7	1.0	1.0	2.7	2.0			1/2 ◊	0.9	4.0
IPNS	13.0	19.5	3.2	3.0	1.0	1.0		0.8	2.0	2.0	1.5	4.0				0.5	
SUM	**62.5**	**144.9**		**14.3**	**4.8**	**4.4**	**1.5**		**7.0**	**6.6**		**18.6**	**1.9**		**3.4**		**5.5**
PROJECTS																	
Europe																	
Austron	13.0	62.4	9.9	1.0	1.0	1.0	1.0	3.2	2.0	1.0	5.3	5.0				1.7	
ESS	40.0	356.0	18.4	6.0	5.0	2.0	2.0	4.2	4.0	3.0	9.9	8.0	3.0	1.0	6.0	3.2	4.0
Japan																	
JHP	23.0	135.0	12.8	3.0	1.0	1.0		2.7	2.0	2.0	5.6	10.0			4.0	1.8	1.0
NSRP	37.0	350.0	19.7	4.0	2.0	3.0	2.0	4.2	5.0	3.0	10.5	13.0	1.0	1.0	3.0	3.4	6.0
Russia																	
IBR2* upgrade	14.0	40.6	4.0	3.0	1.0		2.0	3.9	1.0	3.0	2.1	3.0			1.0	1.5	
INR	2.0	4.0	4.2	1.0				0.9			2.3	1.0				0.7	
UK																	
ISIS I*	18.5	70.3	7.9	3.8	0.8	2.1	0.5	1.7	1.0	1.6	4.2	5.6	1.4		1.7	1.4	0.5
ISIS II*	37.5	146.3	7.9	8.5	2.8	3.1	1.5	2.2	3.0	3.0	4.2	8.6	1.0	1.0	5.0	1.4	2.5
USA								2.0									
LANSCE upg.*	14.0	52.5	8.0	7 new instruments not yet specified							3.7	1.2					
NSNS	10.0	57.0	11.5	2.0	1.0	1.0	1.0	2.9	1.0	1.0	6.5	3.0				2.1	

*replaces existing instrument set-up ◊ instruments already counted in another category

Table 7 contains information for new reactor sources. We note that overlaps may occur between the category "polarized instruments" and other classes.

The reactors listed in the tables, even if they have comparable flux levels, are not being exploited for neutron scattering to the same degree. For example, HFR (a high-flux reactor) at the ILL supports 43 instruments, but HFIR in Oak Ridge (which has approximately the same flux) serves only 11. A similar observation holds true for

Table 7: Instruments of planned continuous sources and upgrades

Source	Weight factor	Scatt. Instr.	Fig. of merit	Type of Instruments											
				Diffractometers				SANS + Reflect.		Inelastic Instr.				Polarised Instr.	Others
				Powder	Single crystal	Diffuse	Engi-neering	SANS	Reflect.	TOF	Triple axis	Back-scattering	Spin echo		
Australia															
HIFAR 1	2.8	11	30.8	3	2	1		1			2			2	
Canada															
IRF	2.8	8	22.4	1	1	1*	1	1	0.01		1	1		1	2
Germany															
FRM II	3.6	17	61.2	1	2	2	1	2	2.0	2	2	1	2	5*	6
Russia															
PIK	4.2	21	88.2	4	3	1		3	3.0	2	3	1	1	6*	30
USA															
HFBR upgrade*	3.7	21	77.7	2	3	1	1	3	2.0	2	5	1	1*	1+1*	4
HFIR upgrade*	4.2	12	50.4	1	1	1	1*	2	1.0		5			1	2
HFIR upgradeII*		14	58.8	3	2	1	2.				6				

*replaces existing instruments

national medium-flux reactors: Orphée at Saclay is utilised by 28 instruments, while DR3 in Risø serves only 8. This variation is partly a consequence of the nature of the reactors - HFIR, for example, is a high-flux isotope reactor, with neutron scattering beamlines as an add-on. But limited funding can also prevent the optimum utilisation of a reactor. Thus, we assert that there is a reserve of research neutrons, which could be exploited if funding for additional beamlines and instruments were available. We do not, however, have the detailed information that would allow us to quantify this statement.

To fully assess the information on instrumentation, and to compare projections with the present status, we must confront the challenge of quantitatively *comparing instruments at spallation sources with those at continuous sources*. This is a controversial subject, whose difficulty stems from the essentially different ability of the various instrument classes to utilise the peak flux of a pulsed source. At least four different instrument groups have to be considered.

- Instruments that can fully exploit the peak neutron flux of the pulsed source. Among these, powder diffractometers are the most notable, benefiting from pulses with peak intensities as high as two orders of magnitude above the average flux.

- Time-of-flight spectrometers that exploit short neutron pulses. These instruments also utilise the peak flux, but their duty cycle is low due to the insufficient repetition rates of pulsed sources compared to the optimum pulse rate which can be obtained by choppers at continuous sources.

- Broad-band instruments that, even at continuous sources, make use of a broad wavelength band that is a characteristic of pulsed source instruments. In this case, the benefit of pulsing is relatively small. The most prominent example of this class are the small angle neutron scattering (SANS) instruments exploiting a wavelength band $\Delta\lambda / \lambda \cong 10$ - 20%. This instrument class also includes neutron spin echo spectrometers, reflectometers, and, to some extent, instruments for diffuse scattering.

- Instruments which are only sensitive to the average flux of the pulsed source and which do not benefit at all from pulsing. The most important case is the triple axis spectrometer (and devices for irradiation work, which is not subject of this study).

The above considerations lead to a sophisticated weighting scheme that is explained in Appendix 1. Using Eq. (1) the calculated weights for the different instrument classes are included in Tables 6 and 7, and they are used for the source weighting and for the figures of merit presented in Section 3. We note that this assessment of instrument classes, and the comparison of performance at pulsed and continuous sources, is in general agreement with a recent evaluation by Mezei (contained in [1]).

As outlined in the introduction, neutron sources are most appropriately considered on a regional basis. Accordingly, we present regional outlooks for the three important instrument classes. Figs. 3, 4 and 5 display the projected development of the (unweighted) numbers of (a) powder diffractometers, (b) TOF spectrometers and (c) SANS machines in Europe, in North America, and in the Pacific region.

Based on this information we now take into account the different weights and introduce a time-dependent *performance index p(t)* for each instrument class

$$p(t) = \frac{\Sigma\, W_i\,(t)\, n_i(t)}{\Sigma\, n_i(t)} \qquad (3)$$

where $n_i(t)$ is the number of instruments of the particular class available at a source i at a given time t.

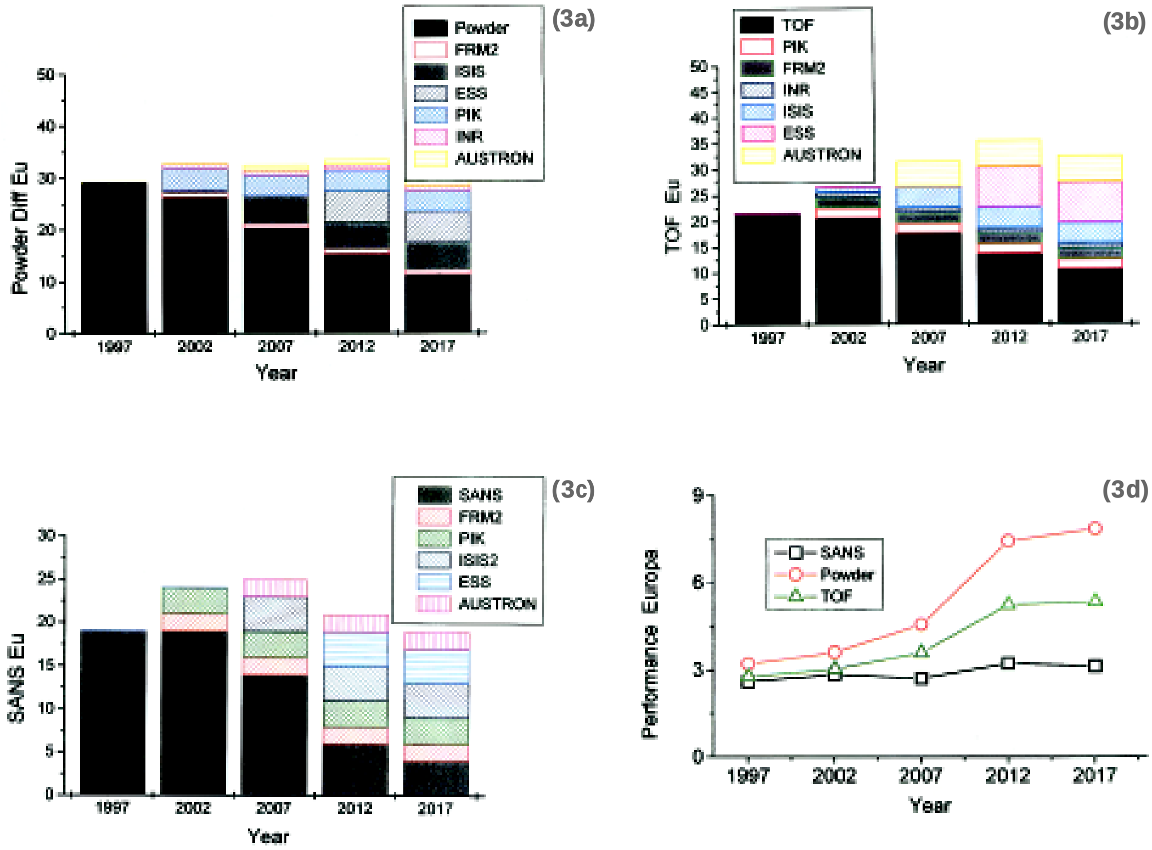


Fig. 3: Time-dependent availability of neutron scattering instruments of different classes, for the European region. The columns represent the number of available instruments in five-year steps, commencing with 1997. The black area indicates the time-dependent availability of presently existing instruments. The shaded areas display the growth in the number of instruments due to planned sources or upgrades. **(a)** powder diffractometers, **(b)** time-of-flight spectrometers, **(c)** SANS instruments, **(d)** average instrument performance, based on Eq. (3).

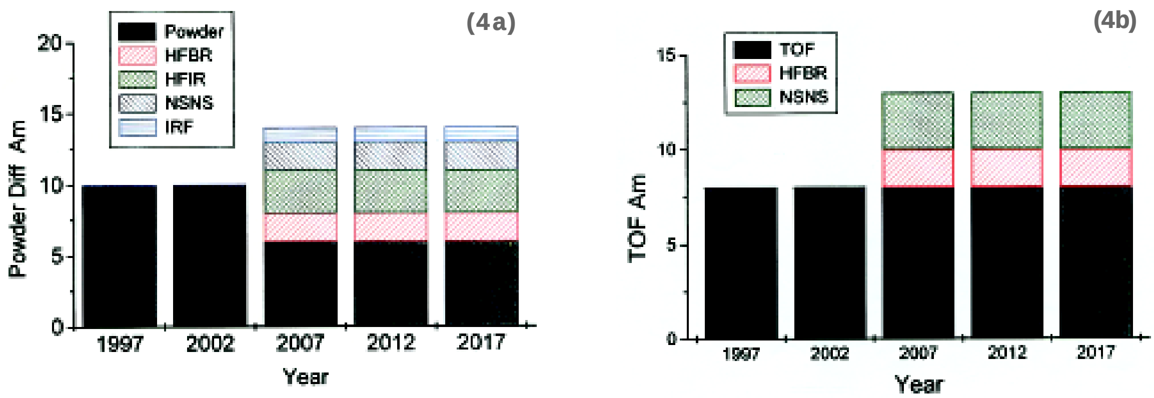


Fig. 4: Same as Figure 3 for the North American region. (See (c) and (d) following page)

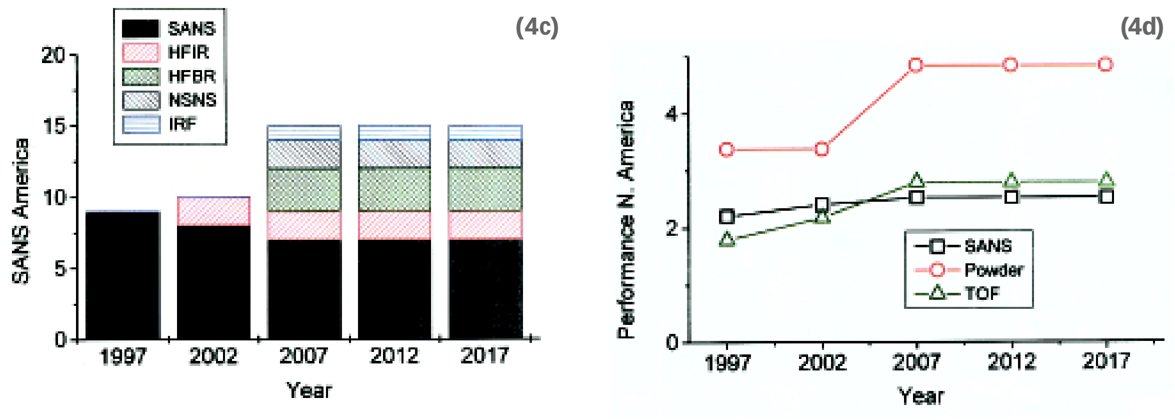


Fig. 4: Same as Figure 3 for the North American region.

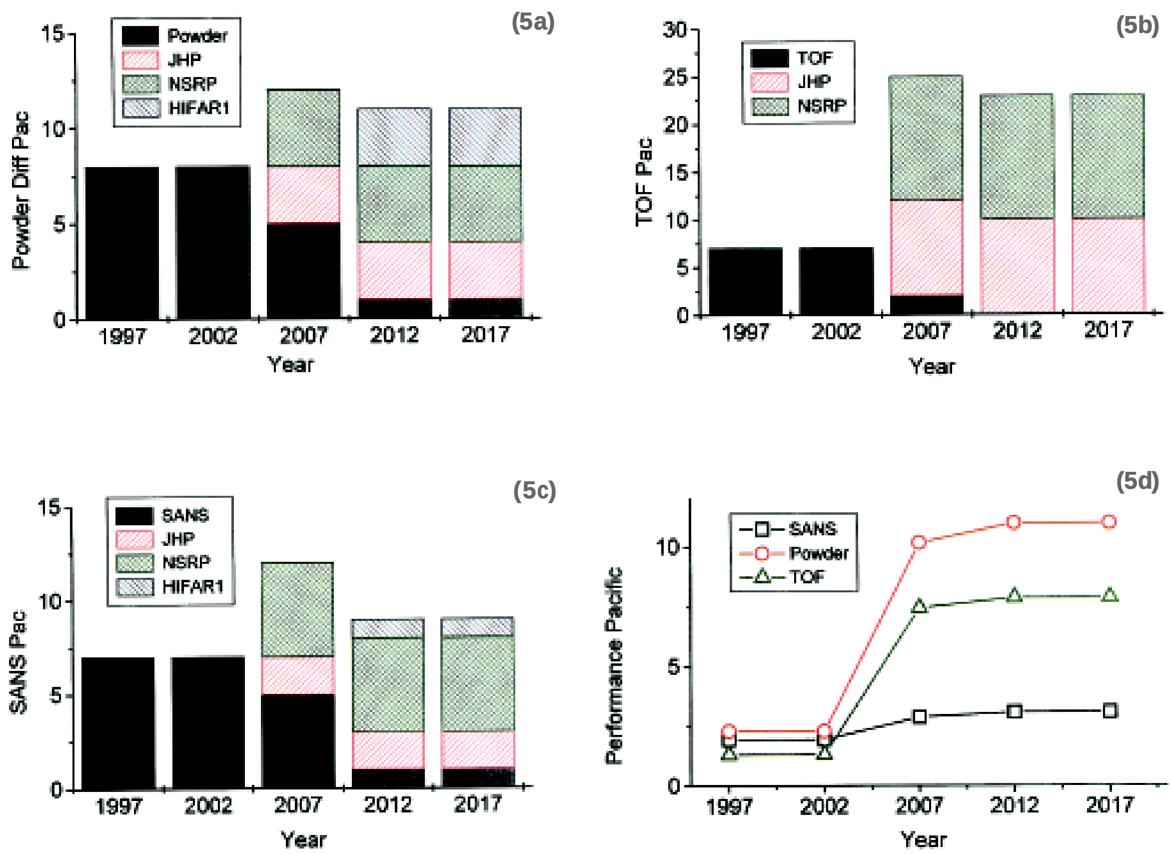


Fig. 5: Same as Figure 3 for the Pacific region.

The performance index thus quantifies the average weight of an instrument within its class in a certain region of the world. The performance indices are shown in Figures 3(d), 4(d) and 5(d).

We now discuss these results for the three world regions, considering first the time development of the instruments at *existing sources in Europe*. We note that, for all classes, there will be a major reduction over time in the number of instruments. The effect is most pronounced for the small angle scattering machines, which nearly vanish in 2017. Significant numbers of powder diffractometers and TOF instruments will remain, however, mainly due to the availability of the ISIS source. The figures show clearly that the five major plans for European sources have the capability to replace most of the older facilities, and to maintain or improve the present situation (especially for TOF instruments).

Regarding the performance indices of Fig. 3d, we observe that the change-over from continuous to pulsed sources will lead to major gains in performance for powder diffractometers and TOF spectrometers. Conversely, broad-band devices like the SANS instruments will not gain very much. We emphasise that an increase of the performance index by a factor of 2 implies an order of magnitude higher useful neutron intensity at a given instrument.

In *North America,* the evolution of available instrumentation at existing facilities is less dramatic than in Europe (Fig. 4). Because of the continuing important role of the existing reactors, the decline of instrument numbers will be less pronounced. Reactor upgrade programs, together with the planned large spallation source SNS, will significantly increase the number of all classes of instruments. The persisting importance of reactor-based neutron sources in North America also results in a smaller increase of the performance indices, compared with Europe. This holds true both for powder and TOF instruments.

The strongest predicted relative increase in instrument numbers, and in performance, will occur in the *Pacific region* - if all of the proposed sources are implemented (Fig. 5). The particularly high average performance of powder and TOF instruments in this region relates directly to the strong future weight of spallation sources.

In summary, while in Europe the totality of the presently planned sources will roughly compensate for the losses due to source shutdowns, in America and in particular in the Pacific region, important net gains can be anticipated, provided that the proposed projects are realised.

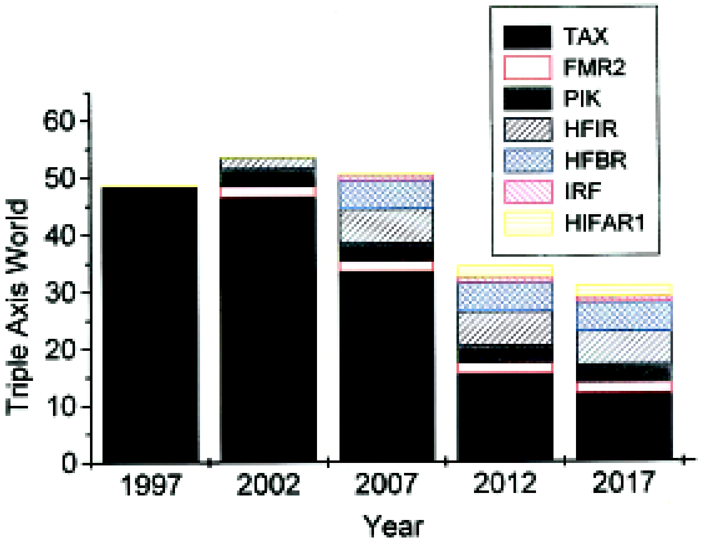


Fig. 6: World-wide availability of triple axis instruments as a function of time. The columns represent the availabilities in five-year steps, commencing with 1997. The black area displays the projected availability of instruments at existing sources. The shaded areas display the impact of instruments planned at new or upgraded sources.

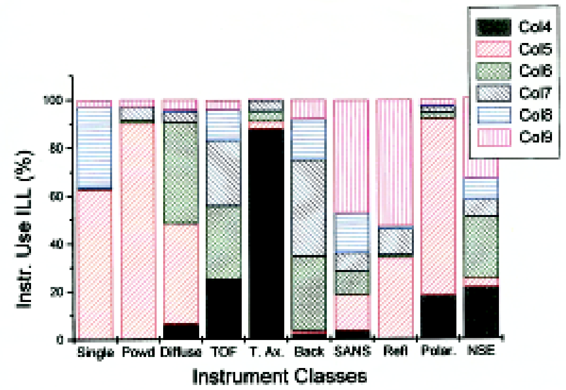
The projected world-wide increase in the number of TOF instruments has to be viewed in the context of the evolution of the other main class of spectrometers, the triple axis instruments. In Fig. 6 we display the world-wide availability of these instruments - they are, after all, the workhorses for inelastic scattering at continuous sources. As a consequence of the gradual shutdown of a large number of research reactors in the OECD countries, their total number will decrease with time, and this will not be compensated by the totality of all planned and proposed projects. Since triple axis machines are not well-suited to pulsed sources, their functions may have to be partly taken up by TOF instruments at spallation sources.

5. The correlation between instrumentation and fields of research

To predict future needs for different categories of instruments, the *correlation between scientific disciplines and instrument use* has to be known. We have analysed user statistics from three major neutron sources (Institut Laue-Langevin, ISIS, and the NIST Center for Neutron Research), and present these as representative of the field as a whole.

In addition, we have used data on European neutron users by disciplines (ENSA Survey of the European Neutron Scattering Community, 1996 [3]) which may be related to the use by scientific disciplines coming from the sources.

The data from the ILL (presented in detail in Appendix 2) describe the relative use of ten instrument categories by experimenters from six scientific colleges relating to different scientific disciplines (Fig. A1), and the oversubscription of these instrument categories (Fig. A2). Fig. 7 presents the percentage use of instruments at NIST, relative to various scientific disciplines. Comparison with the ILL shows that the correlation between scientific fields and instrument classes is similar, e.g.,



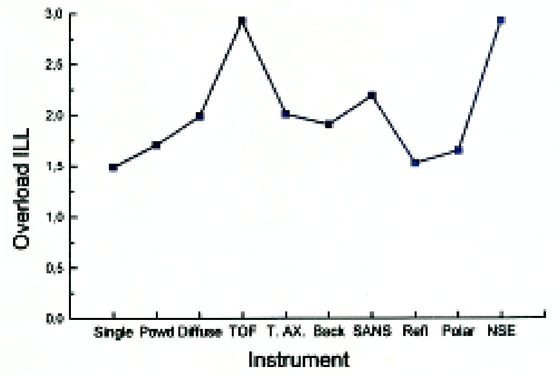


Fig. A1 (left): Percentage instrument use in different instrument classes in the various Colleges of the ILL: College 4: Excitations - Solid State Physics, College 5: Crystallography, College 6: Amorphous Materials and Liquids, College 7: Material Science, College 8: Biology, College 9: Soft Condensed Matter.
Fig. A2 (right): Overload factors for the different instruments at the ILL from 1995 until mid 1997.

in both cases the triple axis spectrometers are almost exclusively utilised by the solid state physicists. At both institutions, SANS instruments are used by researchers from several disciplines (soft condensed matter: ILL 47%, NIST 40%; biology: ILL 17%, NIST 22%; chemistry: ILL 15%, NIST 12% etc.). A similar multidisciplinary pattern of utilisation is found for neutron spin echo, backscattering, and TOF spectrometers. We note the particularly large oversubscription for TOF and neutron spin echo instruments (Fig. A2).

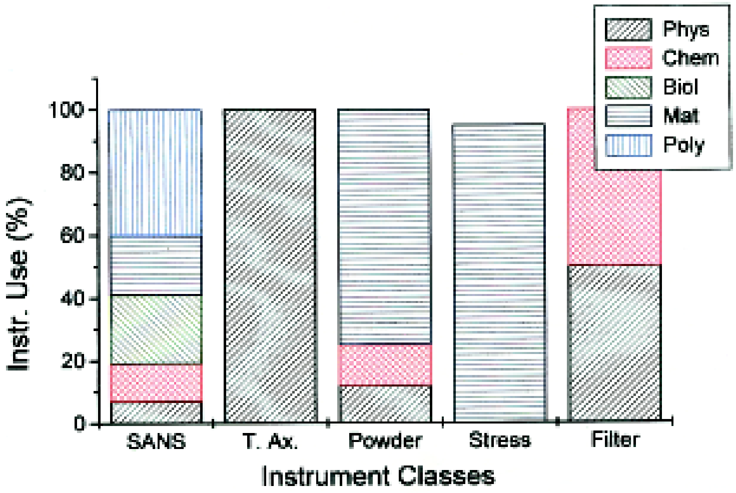


Fig. 7: Percentage instrument use of different instrument classes at the National Institute for Standards and Technology by different scientific disciplines.
(Stress: Engineering diffractometer; Filter: Triple Axis instrument with filter analyzer)

5. The correlation between instrumentation and fields of research

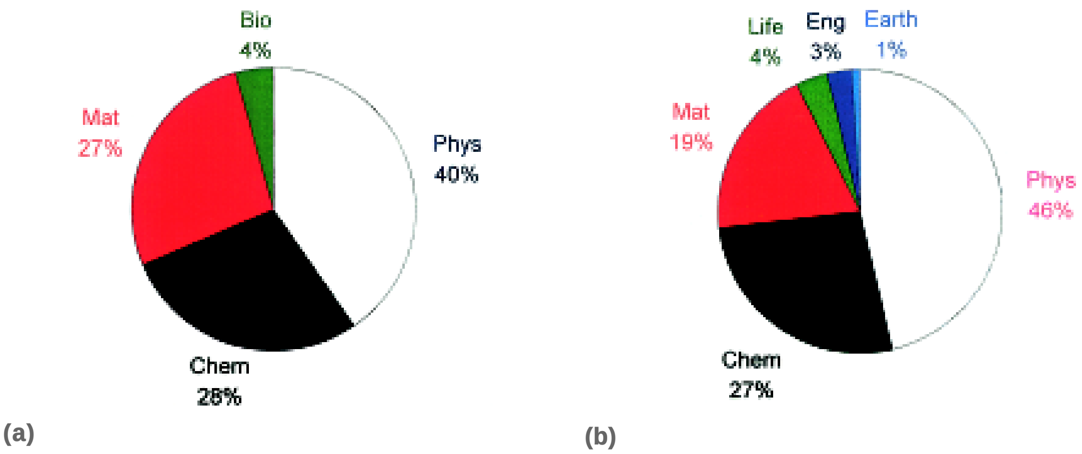


Fig. 8:
(a) Overall requests for ISIS by scientific disciplines, for the interval 1994 to 1996.
(b) European user statistics according to the ENSA Report (1996) for different scientific disciplines [3].

The ISIS statistics describe the requests for resources at this spallation source from researchers in different scientific disciplines. Data from the years 1994-1996 are displayed in Fig. 8a and compared with the European user statistics from the ENSA Report on European Neutron Users (Fig. 8b) [3]. Clearly, the two sets of data are consistent.

Given the consistency of the above data, we take them as representative of the global use of neutrons in condensed matter science. A number of conclusions on the *current status of* neutron research can then be drawn:

- The main application of powder diffractometry is the study of new materials, for example (Fig. A1) solid state chemistry and materials science.

- About one third of the users of single crystal diffractometers are biologists. Protein crystallography, which is pursued at synchrotron radiation sources, also benefits from neutron diffractometry studies, which provide insight into the structural role of hydrogen in these substances.

- Time-of-flight spectroscopy is widely used in most of the research fields. At the ILL, demand for this technique is nearly evenly distributed over solid state physics, liquids and glasses, materials science and, to a somewhat smaller extent, biology and soft matter. The instruments are heavily oversubscribed (Fig. A2).

- The applications of triple axis spectroscopy are essentially restricted to solid state physics, where elementary excitations, critical phenomena, magnetic susceptibilities, etc., are studied. These instruments have an inherent advantage for the study of selected points or paths in reciprocal space, through the investigation of single crystals.

- As in the case of the TOF spectroscopy, high-resolution backscattering, and spin echo spectrometry are used across a broad range of scientific disciplines. Slow dynamic processes, which require very high energy resolution, are, for example, associated with large-scale motions in soft matter, with the glass transition and with solid state diffusion.

- Small angle neutron scattering and reflectometry find their most popular applications in the study of soft materials. These methods, however, are also in strong demand for other disciplines such as biology, materials science, chemistry and, to a lesser extent, in physics.

- Finally, polarization analysis has, until now, mainly been used for static structure analysis in magnetic materials. The spectroscopy of magnetic excitations using polarized neutrons and spin analysis is a promising field, but its applications are still minor, pending progress in the development of improved spin filters.

6. Future needs for neutron sources and instruments in various scientific disciplines

In the previous section we have analysed the present global *status quo* in neutron sources and instrumentation, including the impact of proposed projects on the regional neutron supply. In this section, we attempt a forward look at the likely development of the demand for neutron scattering. We base our estimates on the Autrans report [2] which projects demand for neutron scattering in various disciplines in a way that we consider to be representative on a global scale. The study divided condensed matter science into 9 research fields: (1) magnetism and superconductivity; (2) amorphous materials and liquids; (3) polymers and soft matter; (4) biology; (5) atomic and molecular aspects of new materials; (6) chemical reactions, catalysis and electrochemistry; (7) materials science; (8) engineering and (9) earth science. These fields correlate to a certain extent with the scientific colleges of the ILL (Appendix 2). In Appendix 3, we present highlights of the Autrans report, by disciplines.

To predict the demand for neutron spectrometers based on the development of condensed matter

research as evaluated in the Autrans report, we have graded the importance of the different instrument types for each discipline as follows:
* = valuable, ** = very valuable, *** = essential . The results are shown in Table 8. (It is interesting to compare this table with Fig. A1, where the ILL colleges and instrument use are shown). We now use our grading scheme to make forward projections from the current situation which is depicted in Figs. 7 and A1.

Neutron *diffraction* will continue to be a basic technique for the exploration of the structure of materials. New users can to be expected from the fields of materials and earth sciences, as well as in engineering, where we anticipate a particularly strong demand for texture and strain analysis. With the advent of powerful Laue methods using image plate detectors, we expect an increased demand from biologists.

Inelastic neutron scattering will become increasingly important for disciplines which at present only rarely use neutrons. In particular, reaction chemistry and earth sciences will make use of spectroscopic methods. We also expect more demand in the life sciences, where the relation between biological function and molecular motion is receiving increased attention.

Table 8: Future instrument needs following the ESF evaluation "Scientific Prospects for Neutron Scattering"

	Solid State Magnetism	New Materials Chemical Aspects	Chemical Reactions Chemistry	Amorphous Materials	Material Science	Biology	Soft Matter	Earth Science	Engineering
Diffractometry									
single crystal	**					***		***	
powder	**	***	***		**				
diffuse				***					
engineering, texture								***	***
Inelastic scattering									
TOF	**	**	***	***	***	*	*	***	
3-axis	***							*	
NSE	*		**	***		*	***		
backscattering			***	**	**	*	**	**	
Large scale structures									
SANS	*	**		**	***	**	***		***
Reflectometer	*	**	**		**	***	***		**
Scattering with spin analysis	***			**		**	**		

* valuable, ** very valuable, *** essential

These growth areas primarily involve the study of disordered (or, at least, not single-crystalline) materials and therefore require the use of TOF techniques.

Small angle neutron scattering is already applied across a full range of disciplines. Increased demand is foreseen in materials science and engineering. *Reflectometry*, the other technique that probes large-scale structures, has only recently come to the attention of neutron scientists. With the increasing importance of surface science, and the study of thin layers, a strongly increased demand can be predicted in condensed matter research, in biology (research on membranes) and in materials science.

Finally, the use of *polarized neutrons* will be strongly enhanced, provided that more efficient techniques for polarization analysis become available. Currently, polarized neutrons are mainly used for structural research but, in the future, neutron spectroscopy with polarized neutrons will open up new avenues of research. Furthermore, the ability to distinguish coherent and incoherent scattering by spin analysis will make the use of polarized neutrons universal for condensed matter science, e.g., to separate single particle and collective motions (or coherent and incoherent scattering) in soft condensed matter.

The Autrans report convincingly demonstrates that research using neutrons is growing, with excellent prospects for expansion in the future. Growth is expected even in the *traditional fields* where most scientists are currently active (Fig. 8a,b), namely, solid state physics and selected topics in physical chemistry.

Furthermore, *new growth areas* are anticipated in the domains of biology, engineering, materials science and earth sciences. Engineering research has not yet made full use of the possibilities offered by the neutron. To stimulate such work, *certain characteristic requirements must be met:* ease of access, standardisation of the basic techniques, well-established procedures for data analysis and evaluation, and a specialised technical infrastructure. In addition, stronger links are needed between the engineers who define the industrial problems to be solved and, on the other side, the scientists who have an in-depth understanding of neutron diffraction and strain analysis. Such an interface could be developed, for instance, at a university engineering department close to a neutron source. Applied materials science also lacks adequate connections to neutron scattering, due to the inherent complexity of the substances being studied. For instance, an alloy with several constituents yields scattering patterns whose quantitative evaluation is extremely complicated; sophisticated numerical procedures are needed to arrive at reliable conclusions.

Independently of progress in neutron sources, entirely new and exciting results can be expected from the development of novel measurement techniques and data analysis methods. The history of neutron scattering reveals a clear pattern of advances of this kind. For example, when Bertram Brockhouse (Nobel prize-winner of 1994) developed his first spectrometers in the 1960s, the resolution of those instruments (on the order of 0.025 - 0.25 THz) was sufficient for studies of phonon dispersion and quasi-elastic scattering from liquids. At that time, the notion of resolutions at the MHz level - an advance of six orders of magnitude - seemed unrealistic, due to huge expected losses in intensity. Today, however, such resolutions have been achieved (although not yet for phonons), leading to major progress in the study of polymers and soft matter. This breakthrough was achieved, in GHz-backscattering spectrometers, through the decoupling of beam divergence from resolution, and, in the spin-echo method (which achieves MHz resolution), through the decoupling of resolution in energy *transfer* from the energy spread of the incident beam.

The use of polarized neutrons provides another example of progress via improved measurements techniques and instrumentation. The work that was pioneered by Clifford Shull (co-winner of the 1994 Nobel Prize) in the 1960s expanded rapidly with the advent of improved polarizers (for example, supermirrors at longer wavelengths). Even greater improvement is anticipated from the application of polarized *^{3}He filters*, which will decouple energy from polarization analysis, leading to new possibilities for spin analysis. For single crystal diffraction, particularly in biology, the step from two-dimensional scintillation or ^{3}He counters to image plate techniques with optical read-out will allow much higher data collection rates. Using high-quality *focusing mirrors* (originally designed for X-ray satellite telescopes), small angle neutron scattering (SANS) should be able to improve Q resolution by an order of magnitude, without appreciable intensity loss. The combination of a triple axis spectrometer with the new *spin echo-resonance* method will allow the investigation of phonon or magnon lifetimes with line widths in the GHz range.

In general, the Autrans report demonstrates that the novel fields for the application of the neutron, such as research on materials, in earth and in engineering sciences, require predominant use of the TOF methods (spectroscopy, powder diffraction, texture analysis etc.). For example, the study of disordered materials will benefit from the analysis of TOF spectra. For powder diffraction in general, the pulsed sources with MW-target power are highly superior even to a high flux reactor. Pulsed sources will be competitive with steady state sources for single crystal work, provided that new space-resolving detectors can be successfully developed, along with new algorithms for data analysis. The pulsed sources are definitely superior for time-resolved diffraction work.

There will be, however, a continuing *need for high average-flux sources.* For instance, the study of elementary excitations requires information from a selected region in reciprocal space, as provided by triple axis spectrometers; for small angle scattering and for the neutron spin echo method, (e.g. in polymer research) the benefit of pulsing is small and, in practice, the average flux determines the quality of the results. For relatively short small angle equipment, pulsing could be preferred (see Eq. A2); such short equipment can be implemented using focusing mirrors. Sufficiently high average fluxes can be achieved by modern research reactors, and by spallation sources as well, if their beam power is in the MW range, and provided they are equipped with high-quality moderators.

7. Summary

This study predicts a very significant decline of neutron scattering capabilities in the OECD countries within the next 15 - 20 years, if no major effort towards new sources and upgrades of existing sources is pursued (Figs.1 and 2). This presents a serious threat to the highly developed field of neutron scattering for the study of condensed matter, including new growth areas in engineering, materials science, earth sciences, and biology.

The *expected growth of the neutron demand* could be met by the implementation of the existing *plans* for new sources in the various regions of the world. Figs. 3a, b and c show that in *Europe* the anticipated shut-down of research reactors would be nearly compensated if several of the planned sources were built. For *North America*, where the current level is lower than in Europe, the planned upgrades (and new sources) would lead to a sizeable increase of scientific capability (Figs. 4a, b, c), thus restoring the leading position that North American countries once occupied, in the days of the first dedicated high-flux reactors at Brookhaven, Oak Ridge and Chalk River. A statement by the American Physical Society on neutron scattering, of November 5, 1997 addresses this situation:

"... For many decades, the United States was pre-eminent in neutron scattering science with state-of-the-art reactor and spallation neutron facilities. Today we have lost that pre-eminence and could well cease to be a major player in this field - in spite of its centrality to fundamental scientific studies as well as many areas of science important to national needs. The critical need for modern neutron scattering facilities has been well documented and recommendations have been made to upgrade US capabilities, but the needed developments have not come to fruition. If our neutron scattering facilities are not enhanced soon, this field will suffer damage to its research programs that will take decades to rebuild. As US leadership is lost, important technologies that depend upon the knowledge gained from neutron scattering studies - including the development of new polymers, superconductors and chemical catalysts and the use of neutron probes to study the stresses and impurities in materials that affect the performance and safety of structures such as bridges and aircraft -are increasingly at risk. ..."

In the *Pacific region*, given the relatively low starting profile, the capacity of the planned sources will approach or exceed the present level of other regions during the next decade, if all the plans are realised; (Fig. 5a, b, c).

Regarding the "performance" depicted in Figs. 3d, 4d and 5d, for diffraction and TOF methods, an impressive upward step is expected, mainly due to new pulsed sources. The increase of performance will increase the quantity of scientific output, but, more importantly, it will enhance the *data quality*, e.g. statistics or resolution. Generally, this analysis emphasises that the *growth fields are mainly related to TOF methods*. This underlines the tendency to build spallation sources. On the other hand, *dual-purpose reactors* still play an important role for materials irradiation (for example, isotope production), activation analysis, medical applications, and materials testing, and for traditional triple axis spectroscopy as well.

An urgent need for new sources in the future is obvious. Funding authorities must make the appropriate decisions between now and 2005, given the period of 10 to 15 years between a funding decision and full operation of a new source. These new sources should be regional, as explained in the report, and should provide high neutron fluxes (10^{15} n/cm^{2}s for reactors, and above 1 MW beam power for pulsed sources). A high flux ensures the quality of data, but, as has been seen in the past, also stimulates international cooperation, promotes progress in instrumentation design, and in research with neutrons in general.

Appendix 1: Weight factors for instruments at pulsed sources

To compare the scientific and technological impact of pulsed and continuous sources, the performance of different instrument types has to be examined quantitatively. While for a continuous source the average flux is the relevant figure, for a pulsed source the *peak flux* ⊠, the pulse *repetition rate* ν and the *average flux* ⊠, all have to be considered. These quantities depend on the design of the target station, the reflector, the moderators, the degree of moderator coupling, etc.

Since we are only interested in order-of-magnitude estimates, we adopt the following strategy:

- To create a uniform basis for comparison, the design values of the ESS are used as a point of reference [4]. With an optimized reflector the ESS can produce an average thermal neutron flux of ⊠= 6 ∞ 10^{14} n/cm^2s at a proton beam power of 5 MW. With a 50 Hz repetition rate, a thermal peak flux ⊠ = 2000 ∞ 10^{14} n/cm^2s is achieved.

- Based on these figures, hypothetical peak and average fluxes for each spallation source are calculated by scaling with the proton beam power, and taking into account the ratio of the repetition rates. These calculated fluxes are, in general, similar to those quoted by the various facilities, and can be used to evaluate weight factors for the different instrument classes, as well as to establish weight factors for the facilities themselves.

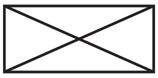
As outlined in Section 4, different neutron techniques utilize the peak flux of a pulsed source with varying degrees of efficiency. Following the classification outlined in Section 4, we have derived characteristic weights for each of the four instrument classes: powder diffractometers, TOF spectrometers, SANS instruments, and instruments that essentially use the average flux.

These steps lead us to the following weighting procedure:

1. Powder diffractometers utilize the thermal peak flux ⊠ of the source in a resolution regime where the full repetition rate may be used. Thus, powder diffractometers may be viewed as typical examples of instruments that make full use of the peak flux. The gain over the average source flux is then given by the ratio of the peak flux ⊠ to the average flux ⊠. When weighting using Equation (1), ⊠ is used, provided the repetition rate of the source is not too low. For standard powder diffraction, an optimal minimum repetition rate of 20 Hz is assumed.

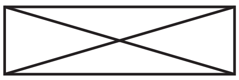
2. Thermal time-of-flight (TOF) spectrometers also utilize the peak

flux of the source. Its value, however, has to be reduced to an effective flux, taking into account the ratio of the source repetition rate ν and the optimized rate which can be obtained at a continuous source $\nu_{opt} \cong 400$ Hz. Consequently, the effective useful flux F_{TOF} becomes

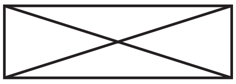
 (A1)

For a typical pulsed source with a repetition rate of ν = 50 Hz, Φ_{TOF} is reduced by $^1/_8$ compared to the peak flux . Similar reductions apply to cold neutron TOF instruments, where the inherently lower optimum repetition rate is largely counterbalanced by the weaker peak flux from the cold neutron moderators in a pulsed source.

3. For a broad band instrument, such as a small angle scattering (SANS) device, the intensity gain over the average flux of the pulsed source can be evaluated by comparing the usable wavelength band at a spallation source with the optimal band width utilized at a continuous source. For a pulsed source, the usable band width depends on the time interval between pulses, and the length of the neutron flight path, *L*:

 (A2)

For a comparison with a continuous source, the average flux is the point of reference. The effective optimal flux F_{SANS} then becomes

 (A3)

The gain factor with respect to the average flux then becomes the ratio of the possible bandwidth Δλ at the pulsed source, and the optimal band width $\Delta\lambda_{opt}$ at a continuous source.

As an example, we consider a typical *SANS* instrument with *L* = 40 m, at a pulsed source with a repetition rate of ν = 50 Hz. For a reactor instrument, the optimum bandwidth is Δλ / λ ≅ 10%. Thus, at a nominal wavelength, λ= 6 Å, $\Delta\lambda_{opt}$ = 0.6 Å holds, yielding a gain factor of 3.3 over the average flux . The specific parameters *L* = 40 m and λ = 6 Å were used in our weighting procedure.

4. Certain instruments derive essentially no benefit at all from pulsing, and for them the average flux  is applicable. Triple axis spectrometers are examples of this class. Other neutron applications, e.g. neutron capture and irradiation, are in this category.

Based on this classification of instruments, we introduce four different weight factors (flux in units of 10^{13} n/cm^{2}s).

Powder instruments are weighted with

$$W_{DIFF} = 2^{\log \boxtimes} \qquad \text{(A4)}$$

TOF instruments with

$$W_{TOF} = 2^{\log \boxtimes_{TOF}} \qquad \text{(A5)}$$

Broadband instruments with

$$W_{SANS} = 2^{\log \boxtimes_{SANS}} \qquad \text{(A6)}$$

and, finally, we define a weight factor associated with the average flux

$$W_{AV} = \boxtimes 2^{\log \boxtimes} \qquad \text{(A7)}$$

These weight factors for each pulsed source are listed in Table 6.

For the weighting of a pulsed source overall, we define the average weight factor to be

$$W = \frac{1}{4} \sum_{1}^{4} W_i \qquad \text{(A8)}$$

where the sum goes over the four categories explained above.

These values are included in Tables 2 and 4.

Finally, it should be noted that the impact of cold sources installed in many of the medium and high flux reactors was not *explicitly* considered in this evaluation. However, a cold source in general increases the number of instruments at a source by allowing the use of neutron guides. The larger number of instruments leads to a higher figure of merit, thus reflecting the impact of the cold source in an *implicit* way.

Appendix 2: ILL user statistics

The most detailed user statistics that illustrate the correlation between research fields and instruments come from the ILL. For each scientific college, a detailed breakdown of the requested instrument days is available. Unfortunately, only about half of the colleges are directly related to scientific disciplines, others relate to specific physical phenomena. College IV ("excitations") covers mainly solid state physics, e.g., topics such as lattice dynamics and dynamic magnetic susceptibilities. College V focuses on crystallography, involving chemistry, solid state physics, engineering and geophysics. College VI covers liquids and glasses and involves mainly physics and chemistry. The remaining colleges are discipline-specific and cover: VII: materials science; VIII: biology; and IX: soft condensed matter.

Table A1 displays the requested instrument days in the various colleges, from 1995 until the first half of 1997. Fig. A1 (see p. 31) presents the data per college broken down into different instrument classes. Fig. A2 (see p. 31) displays the overload factors, i.e., the ratio of requested to allocated time.

Table A1: Requested beam days during the period 1995 - first half 1997 according to instruments and scientific colleges at the ILL

Instrument class	College 4	College 5	College 6	College 7	College 8	College 9	total requested	total available	overload
single crystal diff	0	2091	18	21	1117	93	3340	2235	1.49
powder diff.	0	1897	29	114	0	61	2101	1227	1.71
diffuse sc.	76	491	491	51	10	51	1170	587	1.99
TOF	591	0	725	643	308	92	2359	804	2.93
TAX	2356	83	113	123	4	0	2679	1335	2.01
backsc.	32	16	423	546	229	109	1355	708	1.91
SANS	48	201	131	106	223	632	1341	611	2.19
reflect.	0	256	8	81	11	393	749	481	1.53
pol.analys.	327	1332	43	47	10	46	1805	1096	1.65
NSE	252	45	302	87	101	393	1171	399	2.93

College 4: Excitations
College 5: Crystallography
College 6: Liquids and glasses
College 7: Material science
College 8: Biology
College 9: Soft condensed matter

Appendix 3: Prospects of neutron research in condensed matter science

This chapter highlights the key elements of the ESF-Autrans report on "Scientific Prospects for Neutron Scattering with Present and Future Sources" [2], illuminating briefly the different fields of research.

Magnetism and superconductivity. Neutron spectroscopy and structure analysis in crystalline substances have had numerous important applications, beginning with Cliff Shull's pioneering work on magnetism and, more recently, with the advent of high-T_c superconductors and highly correlated electronic systems. The main goal of neutron scattering is the determination of the susceptibility $\chi''(Q,\omega)$ for a wide range of scattering vectors Q and frequencies ω. Thereby, magnetic systems often serve as model systems for statistical physics. Furthermore, topics like the fractional quantum Hall-effect, Fermi glasses, lifetimes of electronic states or the dynamic structure factor at the energy gap of superconductors are on the agenda. Many other topics in condensed matter physics are highlighted, such as quantum liquids and solids, magnetic layers, nuclear magnetic ordering, and the kinetics of phase transitions. Industrial aspects, like the optimization of hard magnets or magnetic storage devices, are discussed in the ESF report as well.

Further experimental progress is expected from more efficient means of spin analysis using ^{3}He spin filters. Also, the combination of triple axis spectrometry with the neutron spin echo or resonance spin echo method will extend the range of resolution to GHz frequencies for the study of the lifetime of elementary magnetic or non-magnetic excitations. It is worth noting here that the field of phonon spectroscopy, flourishing in the previous decades, seems to have nearly disappeared, except for selected applications like overdamped modes and diffusive motions.

Regarding instruments, triple axis spectrometry and magnetic diffraction play the most important role for 3d spin analysis. Other methods are coming into play, such as reflectometry and SANS, for studying magnetic layers, flux lines, domains and ferrofluids. Also, micro focusing of neutrons may make them a probe for local magnetic imaging.

Amorphous materials and liquids. Research on amorphous disordered materials is concerned with melts, liquids, solutions, glasses, quasi crystals, ionic conductors, nanocrystalline materials, porous media, and also quantum systems like liquid ^{3}He and ^{4}He. This research aims at an understanding of the microscopic and mesoscopic structure of such materials, their dynamics, and the forces acting between their constituents.

Of special interest are topics like the connection between hydrodynamics and microscopic dynamics, universal features of the glass transition, ion distribution in ionic solutions, and also hydrogen-containing materials for batteries, or the use of hydrogen as a tool for amorphisation. Important insights into the atomic-level structure of these materials can be achieved via an interplay of neutron scattering and computer simulation.

For many of these investigations, neutrons are irreplaceable, e.g., neutron scattering yields absolutely calibrated results for the structure factors S(Q,ω) or S(Q), and neutrons allow the observation of diffusion and local motion in disordered solids at GHz and MHz resolution; they facilitate the separation of dynamic from static disorder. In the future, ^{3}He filters may lead to an efficient separation of the self and the pair correlation functions by spin flip analysis, which would be a major step forward for the understanding of liquids and glasses.

The most important methods for the study of these topics are specialized diffractometers to investigate the diffuse scattering intensities, TOF analysis, Brillouin spectroscopy, SANS, backscattering, spin echo spectroscopy, and spin analysis with filters.

Polymers and soft matter are a major growth area with strong links to industrial applications. During the last twenty years, the understanding of soft materials has been significantly advanced by SANS, combined with labeling through the H-D replacement method, and by neutron spin echo (NSE) spectroscopy, thus facilitating the determination of the properties of the substances on mesoscopic length and time scales. Today, SANS is the pre-eminent technique for determining polymer conformations, with important implications for, among others, chain deformation and rubber elasticity, polymer brushes stabilizing colloids, or for chains at interfaces relevant for gluing, etc. Multicomponent systems may be studied by contrast-matching techniques, and tasks like the exploration of micro heterogeneities in multiblock copolymers or interfacial reactions may come into focus. Dynamic experiments with NSE provide insight into molecular rheology. Another challenging research field is the self-organization of multi-component systems, like amphiphilics in oil or water, where structural, kinetic and dynamic aspects can be investigated by time-resolved SANS and by NSE-spectroscopy. The response of soft materials to external fields like shear, temperature or pressure, is another area of interest, with clear technological implications, such as an understanding of processing methods such as drawing, spinning, etc. of various materials, including rubbers. Complex fluids in confined geometries may be accessed, allowing, e.g., an exploration of techniques for tertiary oil recovery. Neutron reflectometry is the technique of choice for studying the morphology of artificial membranes, interfaces, films, or for studying, among others, lubrication, interdiffusion phenomena and adhesion.

The main tools are SANS, which now penetrates into the region of 1000 nm, i.e., resolutions of 10^{-4} $Å^{-1}$ by focusing instruments, reflectometry and microsecond time resolution using spin echo spectroscopy. GHz spectroscopy and diffuse scattering also play a role.

Biology. Compared to the wealth of protein structures analyzed with synchrotron radiation, the quantitative contribution of neutron diffraction is small. Neutrons work well for the determination of hydrogen positions, such as the hydrogen bonds involving functional amino-acid residues, or water molecules at active sites, both of which are harder to observe using X-rays. Among the difficulties in using neutron diffraction are the small data rates and/or the relatively large single crystals needed for the experiments. The introduction of the image plate technique in Laue neutron diffraction, combined with higher source fluxes, may lead to major progress, making this method more attractive to biologists.

SANS combined with the H-D contrast variation is a tool for low resolution studies on the morphology of biological objects, such as the protein-DNA distribution in a nucleosome. Neutron reflectometry gives the depth profile of the lateral average for the scattering amplitude. This yields morphological information on biological membranes. Also, neutron spectroscopy has been applied, e.g., for investigating the dynamics of proteins. Though difficult to interpret, such studies on biomaterials are a stimulus to perform molecular dynamics calculations which, in turn, may directly be tested by inelastic neutron scattering.

Major instrumental requirements relate to single crystal diffraction (Laue method), reflectometry, SANS and, to a smaller extent, TOF, and the neutron spin echo method.

Atomic and molecular aspects of new materials; materials science. The main objective of scattering experiments in this field is the atomic-level understanding of applied materials, and the correlation of the macroscopic properties (like mechanical strength or ductility) with atomic and mesoscopic properties. In contrast to solid state physics where, in general, the study of physical phenomena in simple crystalline materials is the main research object, materials research deals with very complex materials. As examples we cite alloys with many constituents and complicated precipitate structures, fracture toughened ceramics materials with intergranular stresses, glasses, artificial fibers, composite materials, and complex magnetic compounds. Because of the complexity of such materials, one often combines the scattering experiment with other techniques, for instance stress/strain data, and surface imaging techniques like transmission electron microscopy. Neutrons have a considerable advantage for texture and microstructure studies because they give an accurate bulk average, whereas techniques with small sampling volumes may only sample a few grains.

The production process for certain materials (for example, densification in powder metallurgy, precipitate growth, drawing of fibers, grain kinetics during annealing) may be studied in real time and *in situ* by scattering methods, in order to understand and control materials processing. The behavior of materials under operational conditions are another important issue, where problems like the discharge of batteries, ion conduction in fuel cells, the action of catalysts, or aging processes may be investigated. Finally, interfacial properties are gaining increasingly more attention, with broad implications for protective coatings and corrosion, lubrication and adhesion, functional layers, biocompatibility, and other topics.

The most common techniques are powder diffraction, SANS for mesoscopic structures, also diffuse scattering, reflectometry and TOF spectroscopy.

Chemical reactions, catalysis and electrochemistry. Physical methods like X-ray diffraction, optical spectroscopy and various kinds of relaxation spectroscopy are the traditional tools in chemical research. Neutron scattering is a complementary technique with a great future potential. Chemical reactions can be observed in real time by time-resolved neutron diffraction and spectroscopy, particularly for proton transfer reactions, including pathways and dynamics. In addition to its analytical application, neutron spectroscopy of molecular solids and liquids identifies vibrations and librations whose frequencies and spectral intensities permits investigators to study model potentials, if combined with appropriate computer simulations. In this way, one may finally approach a deeper and more systematic understanding of the inter- and intramolecular forces in chemical compounds. The investigation of proton motion along hydrogen bonds, in tunneling states of hydrogenous groups or in protonic conductors is of fundamental interest. Open questions are related to the sites and dynamics of hydrogenous molecules in zeolites. Neutron spectroscopy allows for the identification of catalytic sites with hydrogenous molecules and the evaluation, in real time, of their relative occupancies. Depth profiles of oxidation, corrosion, and hydrogen ingress at surfaces or interfaces in operating electrochemical cells can be studied by neutron reflectometry. Very recently, pioneering work has been reported on the *in situ* observation of polymerization reactions by SANS.

The methods in this field are neutron spectroscopy (backscattering and TOF), from GHz up to 100 THz energies, powder diffraction, and reflectometry.

Earth sciences. In this field, some well-known advantages of neutrons (as compared to X-rays) come fully into play, namely: their ability to localize light atoms (H, Li, Be, ...) in the presence of heavy atoms, the ease of penetration of thick specimens, and the potential of investigating samples under ultra high pressures and/or temperatures, thanks to the transparency of sample containers. For instance, studies can be carried out of phase transitions of minerals, changes in chemical composition, and dehydration processes. Neutron spectroscopy is essential for investigating soft modes in phase transitions under extreme conditions, measuring the vibrational spectra to predict thermodynamic properties and, especially, observing the dynamics of hydrogenous components in minerals. Important work is being done in the study of crystalline texture in minerals, for example, those recovered in deep drilling projects. The corresponding texture patterns image the history of geological materials related to crystallization, recrystallization and the influence of shear deformation. In this area, the study of microstrains is also significant. Studies on laboratory-deformed specimens help to simulate these processes under controlled conditions. The investigations are obviously relevant to highly practical problems, namely minerals prospecting, earth mantle rheology, volcanism and seismology.

The relevant methods are powder diffraction, texture and internal strain analysis, and diffraction and TOF spectroscopy under extreme pressures and temperatures.

Engineering. From space-resolved diffraction measurements one obtains the stress in the interior of a sample. The knowledge of the stress in machine components (for example, in the vicinity of welds) is important in determining how far the material is from yielding. Another application is the *in situ* investigation of the redistribution of atoms by thermal diffusion, e.g., in a turbine blade. This method can help determine the lifetime of critical mechanical components. The corresponding diagnostic methods are diffraction or SANS. An exciting potential new application would be to use diffraction to follow heat treatment, to optimize the thermal treatment process. Stress, as well as the grain orientation, would have to be measured as a function of time in different regions of a machine component. The process of forging could be investigated in a similar way.

The main methods are diffraction, specialized for texture and strain analysis, and small angle scattering. A recent and very attractive development is neutron tomography, for example, for imaging hydrogenous fluids in the interior of machine components, and structural reinforcement of concrete.

Appendix 4: Questionnaire used for the inquiry
(example for projects)

1. History of your source

- Date of first operation:
- Years of major upgrades:
- Years of significant minor upgrades:

- Annual operating time (days):
- Anticipated shutdown date (if known):

2. Parameters of your source

Reactor

- Thermal power (MW):
- Maximum thermal flux at beam hole noses (10^{14} n/cm^{2}s^{-1}):
- Number of moderators:
  Hot source: ☐
  Cold source: ☐

Pulsed Source

- Proton beam power (kW):
- Pulse length (µs):
- Repetition rate (Hz):
- Peak flux (thermal) (10^{14} n/cm^{2}s^{-1}):
- Number of moderators:
  hot ☐
  thermal ☐
  cold ☐

3. Classes and Numbers of Instruments on your source

(please specify how many)

	cold	therm.	hot	epith.
a) Diffraction (non magn.) • single crystal • powder • diffuse (liquid, glass, disordered alloys etc.) • dedicated engineering diffractometers				
b) SANS				
c) Reflectometers				
d) Spectrometers • tof • triple axis • backscattering • spin echo				
e) Diffractometers/Spectrometers for polarized neutrons				
f) Others • Tomography • Test position				

Number of unused beam positions:

4. Neutron Beam Users at your source

- Number of internal users:
- Number of external users:

(*users* are persons who perform at least one experiment per year)

- Please describe availability of:

-"local contacts": yes ☐ no ☐
- travel expenses: yes ☐ no ☐

5. Terms of Access

- Formal proposal system with peer review: yes ☐ no ☐

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