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# Guiding Criteria for Instrument Design at Long-pulse Neutron Sources

J.P. de Vicente<sup>1,2</sup>, F. Sordo<sup>1,2</sup>, J.M. Perlado<sup>2</sup>, F.J. Bermejo<sup>3</sup>, and F. Fernandez-Alonso<sup>4,5</sup>

<sup>1</sup> Consorcio ESS-Bilbao, Polígono Ugaldeguren III, Pol. A, 7B. 48170 Zamudio, Spain

<sup>2</sup> Instituto de Fusión Nuclear, José Gutiérrez de Abascal, 2, 28006 Madrid, Spain

<sup>3</sup> Instituto de Estructura de la Materia, IEM-CSIC, Consejo Superior de Investigaciones Científicas, Serrano 123, 28006 Madrid, Spain

<sup>4</sup> ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom

<sup>5</sup> Department of Physics and Astronomy, University College London, Gower Street, London, WC1E 6BT, United Kingdom

E-mail: [jpvicente@essbilbao.org](mailto:jpvicente@essbilbao.org)

**Abstract.** We introduce and describe general criteria which characterize long-pulse neutron sources, with a view to guiding and facilitating subsequent instrument design and optimization for specific applications. The ensuing analysis shows that a long-pulse neutron source allows for the possibility of a wide range of flexible instrument concepts with variable resolution and dynamic range, tasks which invariably require the implementation of pulse-modulation techniques in the time domain, particularly for high-resolution applications. We also consider in some detail yet-to-be-tapped opportunities in the use of shorter proton pulses, characterised by a duration commensurate with typical moderation times at spallation sources.

## 1. Introduction

The *European Spallation Source* (ESS) project [22, 23] has undertaken the construction of the world's most intense neutron source for the study of condensed matter, including applications in physics, chemistry, geology, biology, materials discovery, and engineering [24]. The Spanish contribution to the ESS project is currently managed by the *ESS-Bilbao Consortium* (ESSB) and comprises both basic engineering tasks as well as the delivery of machine components [4]. Within the latter, ESSB is actively engaged in the design of the future ESS instrument suite. In this context, the aim of this contribution is to present basic criteria associated with the novel use of long neutron pulses, with a view to guiding and facilitating subsequent efforts in instrument design and optimization. To this end, we examine the merits (and limitations) of millisecond (ms) neutron pulses produced by third-generation spallation neutron sources such as ESS. The considerations described herein constitute a natural extension of previous studies, some of which were aimed at the construction of a medium-flux source in Spain to produce neutron pulses up to durations of 1.5 ms, a pulse length compliant with the ESS 2009 technical specification (see, e.g., Refs. [5, 6, 7]). These results can be easily extrapolated to the current (and longer) temporal width of 2.86 ms envisaged for ESS, or to other accelerator-driven systems aimed at maximising the production of pulsed neutron beams, particularly in the sub-thermal (cold) regime [8].



## 2. Useful neutrons within a pulse

In accelerator-driven neutron sources, the pulse length reaching a given instrument depends on both the length of the particle pulse impinging the neutron-production target (typically protons) as well as on the time taken by thermalization processes at the moderators to slow down spallation (MeV) neutrons to usable energies, typically below 1 eV. In this spirit, a pulsed source may be classified as long- or short-pulse depending upon which temporal width is longer. Long(short)-pulse sources are those where the temporal duration of the accelerator pulse becomes significantly longer(shorter) than the time required for neutron moderation down to thermal energies [9].

By their very nature, neutron scattering techniques with present-day technologies remain flux-limited [24, 10]. Although neutron-production reactions can yield total fluxes comparable to those characteristic of continuous reactor sources, the resulting *useful* flux at thermal energies is an extremely inefficient process, a disadvantage that can be partially mitigated via recourse to multiplexing schemes, i.e., the synchronous use of a broad band of incident neutron wavelengths within a pulse [11, 12]. In this context, instrument design is primarily driven by the underlying scientific requirements. As on steady-state sources, the use of monochromatic incident beams at pulsed sources by means of velocity-selection devices is typically restricted to spectroscopic applications requiring wide surveys of momentum and energy transfers – so-called direct-geometry spectrometers. In this particular case, beam monochromatization before use translates into an effective re-definition of the source. Aside from the above, the most efficient exploitation of pulsed neutron beams is predicated upon the use of a wide range of incident wavelengths and time-of-flight (TOF) techniques to isolate the scattering response of a given neutron wavelength. Such is the case of pulsed neutron diffraction and so-called inverted-geometry spectrometers. In the latter case, energy selection is performed after use and, again, TOF methods are used to determine the corresponding energy and momentum transfers associated with a given incident neutron wavelength. As neutron scattering cross sections at thermal energies are typically independent of incident energy, both direct- and indirect-geometry spectrometers provide access to the same observables associated with the structure and dynamics of the system under investigation [13, 14]. Judicious instrument design in the latter case also allows for the simultaneous implementation of high-resolution neutron diffraction in backscattering geometry, as currently implemented in the low-energy IRIS & OSIRIS spectrometers [15, 16], and the thermal and epithermal spectrometers TOSCA [17, 18, 19] and VESUVIO [20], respectively, all located at the ISIS Pulsed Neutron and Muon Source, Rutherford Appleton Laboratory, United Kingdom.

In any of the cases presented above, the ultimate useful flux associated with a given spectral resolution and dynamic range at a pulsed neutron source depend on a number of factors which are examined below.

## 3. Temporal response, spectral resolution, and dynamic range

In addition to the total neutron flux at the point of use, an analysis of the temporal pulse line shapes for a given neutron wavelength is an interesting exercise in its own right in order to examine how these may be related to optimal neutronic performance. During the time lapse of the proton pulse, neutrons of different energies will emerge from the moderator roughly at the same time. As they travel away from the source, this initial pulse will spread out in time and energy by virtue of the inverse relationship between neutron velocity and wavelength. As a result, the pulse leading edge at a given distance from the source will contain a larger fraction of faster neutrons. Traditionally, the analysis of temporal line shapes has been restricted to the definition of the time-integrated neutron flux at a given wavelength and its associated temporal width, typically defined as a full-width-at-half-maximum (FWHM) in the time domain. Such FWHM tends to increase monotonically with wavelength, a dependence which conforms to

physical intuition as the attainment of colder wavelengths requires on average a higher number of collisions with the moderating medium. For short-pulse neutron sources, wavelength-dependent FWHMs exhibit a (roughly) linear dependence on neutron wavelength in the thermal range, leading to a constant relative wavelength resolution [12]. This feature remains one of the primary virtues of both diffraction and indirect-geometry instrumentation at short-pulse sources where intrinsic FWHMs range from a few  $\mu\text{sec}$  at thermal wavelengths to 150-300  $\mu\text{sec}$  for the coldest wavelengths approaching 10 Å. For a long-pulse source, additional pulse-modulation techniques are invariably needed to attain a comparable energy at a given distance from the source. In either case, a sharp and symmetric temporal line shape represents the best-case scenario in order to optimise useful neutron flux and spectral resolution at a given wavelength.

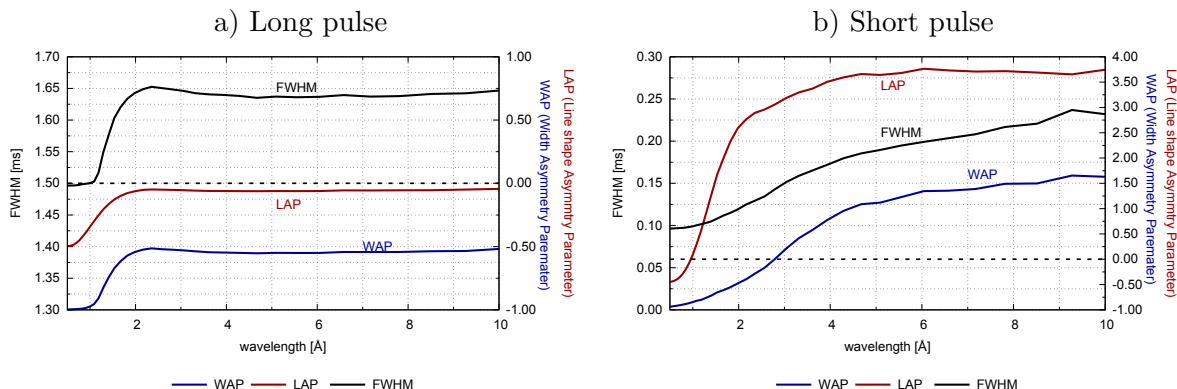
To examine deviations from the above scenario, we can extend previous treatments of neutron-pulse temporal line shapes in order to quantify deviations from a perfectly symmetric pulse around its most-probable (peak) value. In addition to the intrinsic FWHM, we can define Width and Line shape Asymmetry Parameters (WAP and LAP, respectively) as follows

$$WAP(\lambda) = \frac{HWHM_{right}(\lambda)}{HWHM_{left}(\lambda)} - 1 \quad (1)$$

and

$$LAP(\lambda) = \frac{\int_0^{\infty} \Phi(t, \lambda) dt}{2 \int_0^{t_{max}} \Phi(t, \lambda) dt} - 1 \quad (2)$$

where  $t_{max}$  stands for the most-probable time of the time- and wavelength-dependent neutron flux  $\Phi(t, \lambda)$  and HWHM denotes the half-width-at-half-maximum of  $\Phi(t, \lambda)$  on either side of  $t_{max}$ . With these definitions, the WAP is most sensitive to a temporal asymmetry of  $\Phi(t, \lambda)$  around  $t_{max}$  whereas the LAP provides an additional measure of long tails on either side of  $\Phi(t, \lambda)$ . Both WAP and LAP are positive(negative) depending on whether the time-dependent neutron flux is higher after(before)  $t_{max}$ . Positive WAP or LAP values are typical of short-pulse sources. Figures 1a and 1b show the FWHM, WAP, and LAP for two possible operational modes originally envisaged in the context of the ESSB project [6]. A few remarks on these results are in order. For the long pulse (1.5 ms), we observe a sharp transition for all three line shape parameters at around 1-2 Å. Following this step, all parameters remain roughly constant. The FWHM suffers a rather modest increase from 1.5 to 1.65 ms, whereas both WAP and LAP start at their minimal values at short wavelengths (undermoderated regime) and become markedly more symmetric beyond 2 Å. These considerations are in line with the notion that neutron pulses in this regime are largely dictated by the temporal structure of the proton pulse. Conversely, they also tell us that suitable schemes could be further developed to modify the temporal response of neutron pulses by changing the proton-pulse profile. For the shorter pulse (0.1 ms), the situation is markedly more complex as a consequence of the more similar timescales of the proton pulse and intrinsic moderation times. Both FWHM and WAP display a similar wavelength dependence, indicative of longer moderation times for colder neutrons. Both LAP and WAP become positive at 1 and 3 Å, respectively, indicative of the emergence of broad tails in the time-dependent flux. Interestingly, the LAP levels off to a constant value at much shorter wavelengths than the WAP indicating that temporal-pulse degradation is already important for energies sensibly above typical moderator temperatures. We also note that this proton-pulse width (0.1 ms) is intermediate between the short-pulse limit of second-generation spallation sources like ISIS at the Rutherford Appleton Laboratory, the SNS at Oak Ridge National Laboratory, or the MLF at J-PARC ( $\mu\text{sec}$ ) and the much-longer pulses at ESS (few ms). Given the similarities in timescales between proton-pulse widths and moderation times, it is worthwhile noting that this regime represents (at least in principle) a suitable starting point for the optimal delivery of *both* incident flux and spectral resolution. These considerations have been examined in more detail in



**Figure 1.** FWHM, WAP, and LAP for two possible operational modes originally envisaged in the context of the ESSB project: (a) long-pulse mode (1.5 ms proton pulse at a repetition frequency of 20 Hz); (b) short-pulse mode (0.1 ms proton pulse, 50 Hz). For further details, see the main text.

Refs. [23, 6], where it was concluded that a 0.1 ms/50 Hz proton pulse offers a wider spectrum of opportunities for neutron-scattering techniques than its long-pulse counterpart (1.5 ms/20 Hz).

On the basis of our discussion above, we can also use temporal pulse widths to define a characteristic wavelength-dependent resolution  $R(\lambda)$  which can be written as [6]

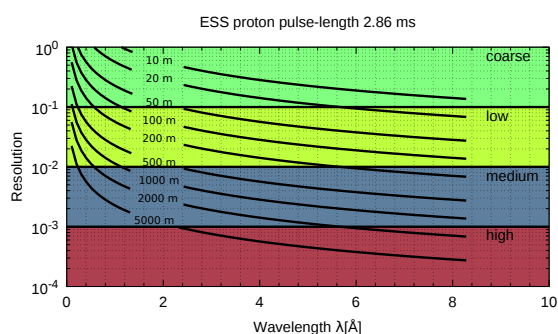
$$R(\lambda) = \frac{3.96}{\lambda[\text{\AA}]} \cdot \frac{\Delta t[\text{ms}]}{L[\text{m}]} \quad (3)$$

where  $\Delta t$  is the neutron pulse width and  $L$  is the length of the instrument. Figure 2 shows the minimum instrument length at ESS required to reach a certain value of  $R(\lambda)$ . From these data, we infer that medium-to-high resolution would only be within reach via the use of flight paths of hundreds of meters. This condition makes the use of pulse-modulation and pulse-shaping techniques a must in order to achieve high resolution at a reasonable cost.

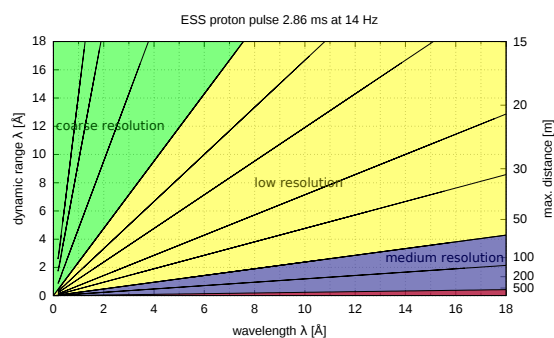
Unlike steady-state sources, pulsed neutron sources are unique in that it becomes possible to exploit a wide dynamic range within each neutron pulse using TOF techniques. This already-mentioned multiplexing advantage can lead to order-of-magnitude gains in count rate and also explains why the peak neutron flux is a more appropriate figure of merit to assess instrument performance, as opposed to analogous time-averaged quantities [11]. The dynamic range  $\Delta\lambda$  is both dependent on the distance to the source (as the spectral resolution) as well as on the repetition rate of the source ( $f$ ), as shown by the following equation [6]

$$\Delta\lambda[\text{\AA}] = \left( \frac{10^3}{f[\text{Hz}]} - \Delta t[\text{ms}] \right) \cdot \frac{3.96}{L[\text{m}]} \quad (4)$$

Figure 3 shows the requisite instrument lengths needed to attain a certain dynamic range for a given value of the spectral resolution. Also in this case, it reinforces the need to implement pulse-modulation and shaping techniques, otherwise the raw ESS pulse will never achieve high resolution while keeping a useful dynamic range. This requirement will necessarily reduce the number of useful neutrons per pulse to a fraction of the available total, although it also represents a timely opportunity for the further development of these technologies beyond the present state-of-the-art.



**Figure 2.** Spectral resolution for a number of instrument lengths at ESS. As a guide, qualitative resolution ranges are also shown.



**Figure 3.** Available dynamic range and spectral resolution for a given instrument length at ESS. For further details, see the text.

#### 4. Conclusions and outlook

In this work, we have presented a number of guiding criteria for instrument selection at state-of-the-art spallation neutron sources, where the proton-beam pulse can range from hundreds of  $\mu\text{sec}$  to a few ms. These considerations represent a natural continuation of our efforts to select optimal proton-pulse characteristics in the context of the ESSB project, yet at the same time are equally applicable to wider initiatives to develop third-generation neutron sources in the foreseeable future, ESS being an important and timely case in point. In addition to considering the maximisation and subsequent delivery of *sheer* incident flux, we have extended the traditional analysis of temporal neutron-pulse line shapes to quantify the overall width and underlying asymmetry close and away from the most-probable value. From this analysis, we conclude that medium-to-high-resolution applications with long (ms) pulses would require the extensive implementation of novel pulse-shaping and modulation techniques, leading to an unavoidable loss in useful flux. We also find that shorter proton pulses of the order of 0.1 ms are naturally matched to typical moderation times of sub-thermal neutrons at a spallation target and, therefore, they could offer a convenient starting point for the effective implementation of a wide range of neutron-scattering techniques at a reasonable cost.

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