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Monte Carlo modelling of a high resolution diffractometer using statistical time modulation to exploit the long pulse structure at the ICONE HiCANS.

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Abstract. Low energy accelerator-driven neutron sources are intrinsically limited by the peak flux they can provide. A way to increase the total brilliance of the source is to increase the neutron pulse length. However, the efficient use of time-of-flight techniques on long pulse sources is non trivial. ESS is building long instruments (up to 150 m) to be able to fully exploit the long pulse structure. Such a solution cannot be reasonably implemented on CANS or HiCANS, essentially for cost reasons. We are thus investigating the possibilities of implementing statistical time modulation on a diffraction instrument to be able to use very long pulse structures. We will present Monte-Carlo simulations using statistical time modulation and propose the design of a high-resolution powder diffractometer, which could be installed on the long pulse target station of the ICONE HiCANS source.

1 Introduction

CANS, Compact accelerator-based neutrons source, and HiCANS, High Current Accelerator-driven Neutron Sources are considered as new types of sources to perform neutron scattering with performances on par with medium power research reactors or spallation sources. The most efficient way to use neutrons for scattering techniques consists in using time-of-flight (ToF) techniques which allow using most of the neutrons produced by the source. However CANS and HiCANS sources are intrinsically limited by the peak brilliance they can achieve because of the low proton energies used to produce neutrons. This can be partially compensated by using longer neutron pulses so that the integrated flux can be of the same order of magnitude as the flux produced at spallation sources or at continuous sources after the monochromatization process. The price to pay for using long pulses, of the order of milliseconds, is that the time-of-flight resolution is reduced and is usually not adapted for higher resolution techniques such as powder diffraction for example.

In this communication, we are exploring the use of statistical choppers. They allow using a large fraction (~50%) of the produced neutrons while providing very high time resolution. In particular, we complement the considerations developed in [1] with Monte Carlo

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simulations. We propose a design for a short, very high resolution diffraction instrument which could be implemented on a very long pulse HiCANS such as ICONE.

2 Modelling and performances of a scattering instrument using a statistical chopper on a continuous source

The principle of statistical choppers is described in [1-2] and references therein. For the Monte-Carlo simulations, we will consider a modulation chopper with a sequence of length $N = 255$ rotating at a frequency of 200 Hz. The pulse lengths obtained with such a chopper are given by $1/f.N = 20 \mu\text{s}$. With such short pulses, it is possible to achieve good resolution ($\sim 1\%$) over a rather broad wavelength range with short instruments (6-20 m) (see Fig. 1).

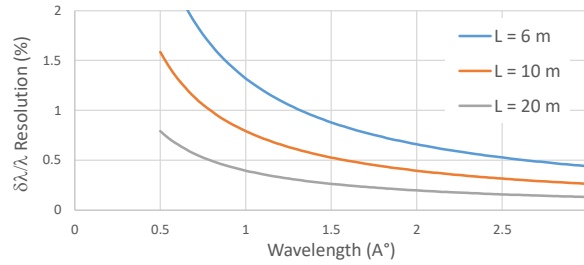


Fig. 1. Time of flight resolution with a statistical chopper providing $20 \mu\text{s}$ pulses. Even with short flight paths, resolutions below 1% can be achieved over a rather broad wavelength range.

We performed Monte Carlo simulations of a diffraction instrument using McStas. For these demonstration simulations, we defined a source with a flat wavelength distribution $\{ \lambda_0 - \delta\lambda ; \lambda_0 + \delta\lambda \}$. We used the components <StatisticalChopper>, <Powder_N> for the sample and <Monitor_nD> as the main detector. Various control monitors were also set along the flight path. The models used are made available at [3].

Monte-Carlo modelling allows to easily check the influence of various parameters of the instrument on the effective resolution. For testing the methodology, we considered a reference case where the source was reduced to a point source (1mm^2) and focussed on the sample ($D = 1 \text{ cm}$). Thus, in this setup, only the time-of-flight resolution as well as the modulation – deconvolution processes were probed. We used a “realistic” chopper with a diameter of 50 cm, so that the slit sizes are 6.2 mm.

The Monte-Carlo simulations provide a recording of the sample scattering measured on the PSD detector. The detector covers 2θ scattering angles spanning from 0 to 180° . We decided to use an angular resolution $\delta 2\theta$ of 0.5° which is a realistic setting. This corresponds to an angular resolution of $\delta 2\theta / 2\theta$ of 0.5% (at $2\theta = 90^\circ$) which is of the same order as the time resolution (see Fig. 1).

The demodulation matrix is mathematically defined from the modulation sequence as described in Figure 2 in [1]. We used the modulation sequence of length $N = 255$ implemented on the CORELLI instrument at SNS. For practical simulation purposes and data processing, the modulation sequence was “oversampled” over 1000 or 2000 time bins. Mathematically this has no influence on the deconvolution process. This was checked numerically. It was also checked that if the oversampling is not a multiple of N , this has no visible influence on the reconstruction.

Fig. 2a shows the raw signal measured on a Nickel powder sample in a $(2\theta, \text{ToF})$ representation. The measured signal is different for every 2θ scattering direction as it would in a usual ToF diffraction experiment. A typical signal as measured for $2\theta = 90^\circ$ (with $N=255$) is presented on Fig. 3a. Fig. 3b shows the reconstructed signal, while Fig. 3c shows

a reference scattering spectrum as measured in a classical ToF configuration. In the reconstructed signal pattern, the position of the peaks is perfectly reproduced (within a small error of 10-15 μ s). The width of the peaks is also preserved with values ranging from 25 to 35 μ s, to be compared to values ranging from 20 to 30 μ s in the ToF data. This suggests that time pulses of 20 μ s are good enough for most experiments as the time resolution is in practice limited by the angular detector resolution.

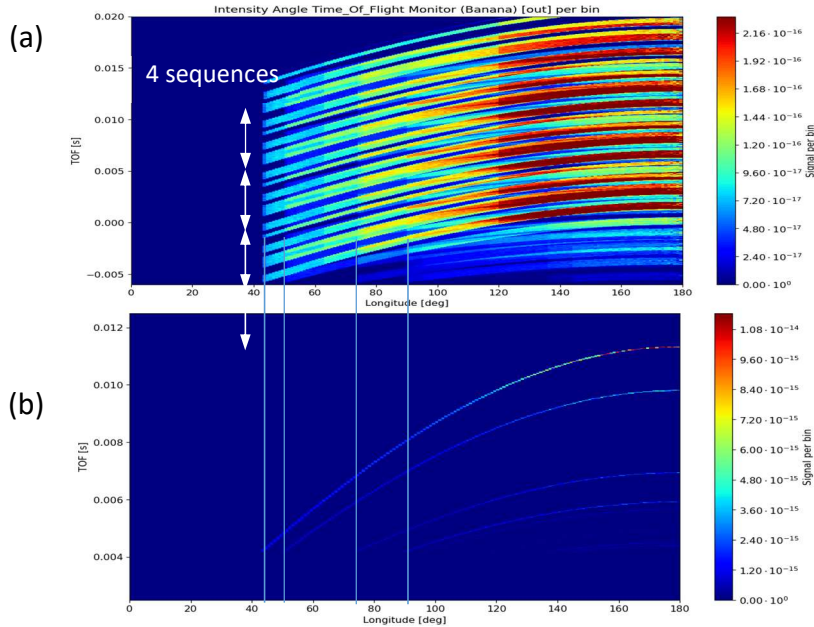


Fig. 2. Comparison of the signal obtained on a nickel powder sample from a regular Time-of-flight measurement (b) and the data as measured with a modulation chopper (a). In the modulation case, the sequence was reduced to a length $N = 14$ for the sake of illustration and the overlap of 4 sequences is presented. In a realistic setup ($N=255$) the vertical time structure would be much finer. The horizontal trajectories correspond to the usual diffraction lines. The vertical bands structure in the figure (a) corresponds to new diffraction lines which appear and start overlapping when the scattering angle is increased. For example, for $2\theta > 90^\circ$, 4 wavelengths contribute to the scattering pattern.

However, the diffraction peak intensities are not well reproduced. While the ratio of the third and fourth peak intensities is well reproduced, the intensities of the first and second peaks are poorly reproduced (with errors up to 20% in the peak intensities). This probably arises from the reconstruction noise. Fig. 4 shows simulations using low and higher statistics. When the statistics is increased, short range fluctuations disappear. However, from $N = 10^9$ to $N = 10^{10}$, the remaining longer range fluctuations are constant and follow the same pattern. These fluctuations are intrinsic to the reconstruction process and have an impact on the absolute values of the diffraction peaks. The smaller the diffractions peaks, the higher the bias. These effects may be smoothed out when averaging over a broader 2θ range and remapping from the $(ToF, 2\theta)$ space to the reciprocal space (Q, I) .

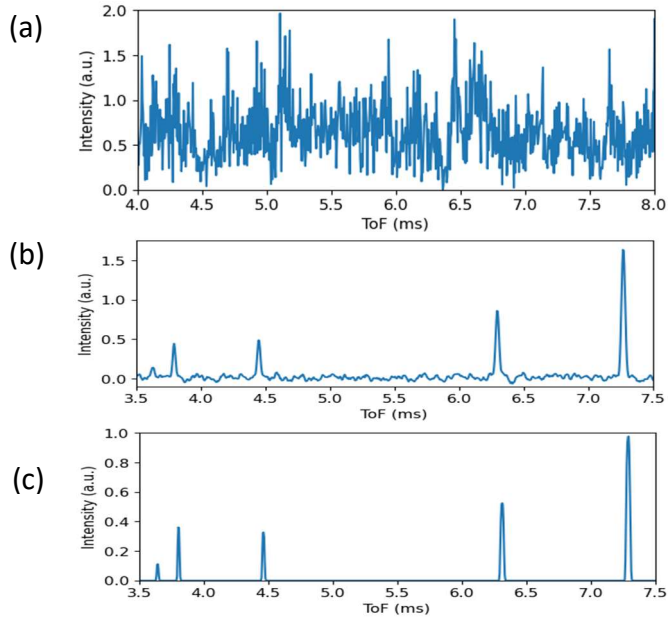


Fig. 3. (a) Signal as measured on the detector for $2\theta = 90^\circ$ (slice between 4 and 8 ms). (b) Signal after reconstruction. (c) Reference measurement in a classical ToF measurement. The diffraction peaks are found at the positions $\{3.805, 4.465, 6.315, 7.29\}$ ms. The broadening of the peaks arises from the finite angular resolution ($\delta 2\theta = 0.5^\circ$). The peak widths is of the order of $20\text{-}37\ \mu\text{s}$ (both in the reference ToF data and in the reconstructed data).

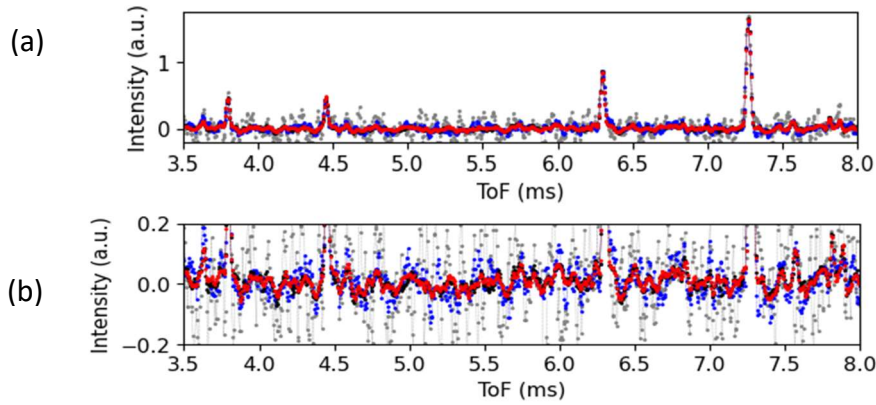


Fig. 4. (a) Simulation of the measured data at $2\theta = 90^\circ$ for different statistics in the Monte Carlo simulations ($N = 10^7$ (grey), 10^8 (blue), 10^9 (black), 10^{10} (red)). From $N = 10^7$ to $N = 10^9$, the statistical fluctuations decrease significantly. However, from $N = 10^9$ to $N = 10^{10}$, the remaining longer-range fluctuations are constant and follow the same pattern. These fluctuations are intrinsic to the reconstruction process.

We then probed the influence of the source size. The diffraction patterns were calculated using different source sizes $S = 1\text{mm}$, 6mm and 12mm (see Fig. 5b). Note that the beam modulation after the statistical chopper is very far from the ideal stepwise modulation (see Fig. 5a). After the reconstruction process, the peak positions are nevertheless accurately reproduced while the peak widths remain acceptable. The main peak width is increasing from

37 μs to 50 μs and 90 μs for $S=1, 6$ and 12 mm respectively. It was shown by F. Mezei in [4] that spatial convolution effects can be separated from time modulation resolution effects. This is qualitatively confirmed in this simulation, as the expected broadening of the diffraction peaks by the {source – slit} convolution is 20 μs for a point source and 40 to 60 μs for larger sources sizes. Beware that the shapes of the different spatial resolution function are not identical.

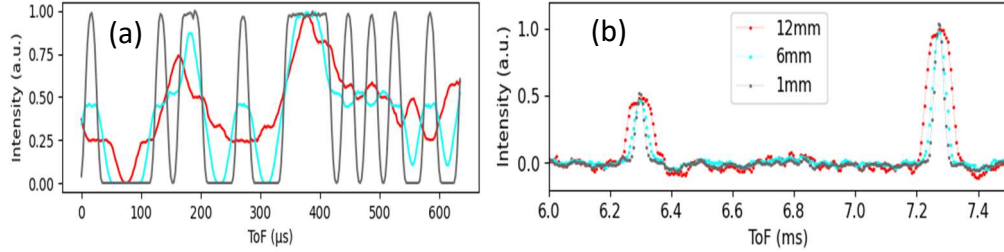


Fig. 5. (a) Evolution of the modulation pattern after the statistical chopper when the source slit is increased from 1 to 6 and 12mm. Evolution of the reconstructed scattering pattern when the source size is increased from 1mm to 6 and 12mm. The time width of the diffraction peaks increases from 37 μs for $s=1\text{mm}$, to 50 μs for $s=6\text{mm}$ and 90 μs for $s=12\text{mm}$.

3 Performances of a scattering instrument on a long pulse source

The use of statistical choppers was initially introduced in order to overcome background noise issues on experiments around reactors. While the background noise around reactors was fixed, the use of statistical choppers allowed using a much higher fraction of the neutron flux (from 1% on a monochromatic instrument up to 50% when using a statistical chopper), thus increasing the signal to noise ratio.

When operating on a pulsed source, the source background can be reduced by 4 to 5 orders of magnitude by performing measurements only after the prompt fast neutron and gamma pulses. On a short pulse source with a low duty cycle, modulation techniques are inefficient both at increasing the time resolution and at improving the signal to noise ratio. However, on long pulse sources, modulation techniques allow achieving high time resolution while using a large fraction of the neutrons and keeping a short instrument length.

We shall consider a long pulse source and try to define the maximum duty cycle that may be used. We consider a diffraction instrument which would use a bandwidth of $\Delta\lambda = 1 \text{ \AA}$, typ. $\lambda = \{1 - 2 \text{ \AA}\}$, similar to the POWGEN instrument at SNS. In an ideal situation, the Fig. 6 shows that a source operating with pulses up to 2.5 ms and a frequency as high as 133 Hz would allow avoiding any measurement during the prompt pulse for an instrument as short as 10 m. More realistic settings could be a pulse length of 2 ms to provide some decay time for the prompt pulse and a frequency of 80 Hz to provide more flexibility in the wavelength band range $\{1 - 4 \text{ \AA}\}$. Such setting would correspond to a duty cycle of 16%. Such parameters combined to a modulation chopper with 20 μs time resolution would allow building a very high resolution – short instrument ($L=10\text{m}$) using up to 8% of duty cycle of the accelerator.

On the other hand, let us consider an accelerator providing short pulses ($w \sim 200 \mu\text{s}$). We do not consider shorter neutrons pulses since this would require making compromises on the moderator performances by poisoning it for example. For $w \sim 200 \mu\text{s}$ pulses, achieving similar time resolution performances as the above design would require building an instrument with a length of $L = 100 \text{ m}$. Besides, if one aims at using a bandwidth such as $\{1 - 4 \text{ \AA}\}$, this requires operating at a repetition frequency of 10 Hz. Overall, the usable duty

cycle of the source is as low as 0.2 %. This is a factor 40 lower in terms of duty cycle compared to the “modulated long pulse” design.

A motivation for implementing statistical modulation is that the construction of high peak current accelerators (typ. $I_{\text{peak}} = 100 \text{ mA}$) is challenging. A machine using a high duty cycle accelerator but with a lower peak current ($\sim 10 \text{ mA}$), which is technically much easier to build and operate, may offer similar performances to a high-end high peak current machine together with much shorter and less expensive instruments.

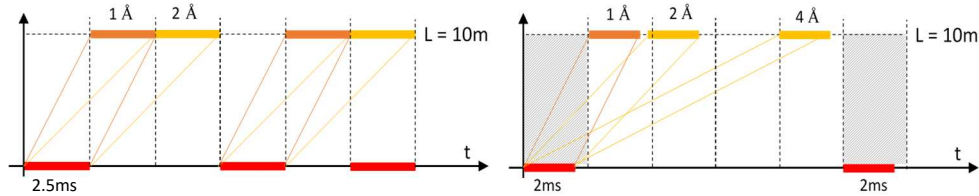


Fig. 6. (a) The upper limit for a very short bandwidth instrument $\{1 - 2 \text{ \AA}\}$, is an operation with pulse lengths of 2.5 ms and a frequency of 133 Hz. These settings correspond to a duty cycle of 33%. (b) More realistic settings: $w = 2 \text{ ms}$, $f = 80 \text{ Hz}$. The useful bandwidth is $\{1 - 4 \text{ \AA}\}$.

4 Conclusion

The peak brilliance of HiCANS is intrinsically limited by the low energy nuclear process used compared to spallation sources. The use of very long pulses on HiCANS (several ms) could help bridging the gap in total brilliance with spallation sources. Modulation choppers are a possible route to achieve such a goal. They allow building very high-resolution instruments that remain short. Some of the drawbacks are however a loss of flexibility in the resolution settings as well as issues related to reconstruction noise. These problems can however be minimized by the operation on a pulsed source which provides extra time information for the correlation analysis [2].

We are making McStas models available [3] for other contributors to explore the capabilities of statistical choppers on specific accelerators, either existing or in project. In the case of the operation in pulsed mode, the data processing in event mode, as proposed by Mezei et al [4] is better suited. We are planning to implement event mode simulations and data formatting so that they can be input into the SCIPP framework [5] for easy post-processing, in particular remapping from the $(ToF, 2\theta)$ space to the reciprocal space (Q, I) . This is made easier thanks to the new McStasScript interface which smooths the McStas data workflow.

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