

1      Design of a wavelength frame multiplication system  
2                      using acceptance diagrams

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6      **Abstract**

7          The concept of Wavelength Frame Multiplication (WFM) was developed to  
8          extend the usable wavelength range on long pulse neutron sources for instru-  
9          ments using pulse shaping choppers. For some instruments, it is combined with  
10         a pulse shaping double chopper, which defines a constant wavelength resolu-  
11         tion, and a set of frame overlap choppers that prevent spurious neutrons from  
12         reaching the detector thus avoiding systematic errors in the calculation of wave-  
13         length from time of flight. Due to its complexity, the design of such a system is  
14         challenging and there are several criteria that need to be accounted for. In this  
15         work, the design of the WFM chopper system for the potential future liquids re-  
16         flectometer at the European Spallation Source (ESS) is presented, which makes  
17         use of acceptance diagrams. They prove to be a powerful tool for understand-  
18         ing the work principle of the system and recognizing potential problems. The  
19         authors assume that the presented study can be useful for design or upgrade of  
20         further instruments, in particular the ones planned for the ESS.

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21      **1. Introduction**

22          There is currently an increasing demand for neutron instruments, at which  
23          the resolution can be adjusted, in particular towards high-resolution setups. The  
24          total instrument resolution in neutron scattering experiments always depends,  
25          amongst others, on the experimental  $\delta\lambda/\lambda$  resolution, where  $\lambda$  is the neutron  
26          wavelength. In time-of-flight (ToF) mode, the experimental resolution is deter-  
27          mined by pulse shaping choppers for all instruments at continuous sources and  
28          for high or medium resolution on long pulse sources. A particular system of  
29          rotating disc choppers provides the desired waveband and removes contaminant  
30          neutrons. For some experiments like small-angle neutron scattering or neutron  
31          reflectometry, it is often desirable to have a constant wavelength resolution over  
32          the entire usable waveband. For reactor sources, this can be achieved by intro-  
33          ducing a pulse shaping double chopper operating in optically blind mode [1]. In  
34          this case, the wavelength resolution is determined by the ratio of the distance  
35           $D$  between the pulse shaping choppers and the distance  $L_0$  between the center

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36 of the double chopper system and the detector:  $\delta\lambda/\lambda = D/L_0$ . This relation is  
37 valid for all wavelengths up to  $\lambda = \frac{3956}{D/\tau}[\text{\AA}]$ , where  $\tau$  is the single disc opening  
38 time.

39  
40 At pulsed sources, like the currently planned European Spallation Source  
41 (ESS) [2], the chopper design described above [1] is usually not applicable in  
42 its simple form. The reason is that due to the needed shielding volume, the  
43 first chopper can be placed only at a certain minimum distance away from the  
44 source, which is currently 6 m for the ESS. Depending on the desired wave-  
45 band, this implicates that not all neutrons will be at the first chopper at the  
46 same time, which limits the usable waveband at the detector. To extend this  
47 range, the WFM concept was developed [3]. It was then complemented with  
48 a blind double-chopper setup to create a wavelength dependent pulse length  
49 [4]. Here, the combination with a blind double-chopper setup is used to obtain  
50 a constant wavelength resolution. To achieve a sufficiently broadband pulse  
51 within the main frame (given by the pulse repetition rate), this concept utilizes  
52 multiple subframes. These subframes are constructed such that the wavelength  
53 resolution is the same for every subframe and they are separated in time at the  
54 detector, but at the same time the measurement time is efficiently used, i.e. the  
55 time gaps between individual subframes are minimised. The proof of principle  
56 of the WFM approach was achieved at the Budapest Neutron Center (BNC) [5].  
57

58 At the future ESS, several instruments will need to implement the WFM  
59 approach. The chopper layout must be carefully adapted to the long pulse  
60 structure of the ESS beam. Neutrons being detected in the wrong subframe  
61 can pose a significant source of systematic errors <sup>1</sup>, so in particular the choice  
62 of frame overlap chopper parameters must be done with great care. The need  
63 for a thorough analysis method was lastly shown by several technical challenges  
64 experienced during the conception of a WFM chopper layout using time-of-flight  
65 diagrams for the ESS test beamline in Berlin [8]. In this paper, the design of a  
66 WFM setup carried out in the context of a design study of a liquids reflectometer  
67 to be proposed for the ESS, is demonstrated by using acceptance diagrams based  
68 on the work presented in [6].

## 69 **2. Application of acceptance diagrams for WFM system of the ESS** 70 **liquids reflectometer**

### 71 *2.1. Designing the pulse shaping choppers*

72 In a WFM chopper setup, the parameters of the pulse shaping choppers  
73 (PSCs) have to be calculated first. These depend on the global parameters  
74 being the total length  $L_{\text{tot}}$  of the instrument and the width of the waveband  
75  $\Delta\lambda = \lambda_{\text{max}} - \lambda_{\text{min}}$ , where  $\lambda_{\text{min}}$  and  $\lambda_{\text{max}}$  are the minimal and maximal design

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<sup>1</sup>or spoil some fraction of the dataset and thereby lengthen the measurement time, if a contaminated part of a subframe has to be removed from the later data analysis.

76 wavelengths, respectively. The instrument length and the waveband width are  
 77 related through the source period  $T$ :

$$\Delta\lambda = h/m_n \times T/L_{\text{tot}}, \quad (1)$$

78 where  $h$  is Planck's constant and  $m_n$  is the neutron mass. In addition, it  
 79 is important to decide on the loosest wavelength resolution  $R_{\text{max}} = (\delta\lambda/\lambda)_{\text{max}}$   
 80 in the WFM regime. Once these parameters are given, then the distance  $D =$   
 81  $L_0 \times (\delta\lambda/\lambda)_{\text{max}}$  between the two choppers, the number of windows, their sizes  
 82 and offsets with respect to each other can be calculated (see Fig. 1). The  
 83 windows of the PSCs are designed such that they enable measurements with  
 84 the loosest design resolution  $R_{\text{max}}$ , with the distance between the two choppers  
 85 being

$$D = L_2 - L_1 = L_0 \times R_{\text{max}}, \quad (2)$$

86 where  $L_1$  ( $L_2$ ) is the position of the first (second) PSC chopper. Higher resolu-  
 87 tions are then achieved by reducing the distance between the two choppers [1].  
 88

89 The design of the chopper windows starts by calculating the time  $t_{1,1}^C$  when  
 90 the first window ( $W_{1,1}$ ) of the first chopper  $\text{Ch}_1$  closes. This time is set by  
 91 neutrons of wavelength  $\lambda_{\text{min}}$  starting at the end of the pulse, see Fig. 1:

$$t_{1,1}^C = L_1/v(\lambda_{\text{min}}) + t_0 \quad (3)$$

92 The PSCs operate in the optical blind mode, i.e. the second chopper opens  
 93 when the first one closes. Thus  $t_{2,1}^O = t_{1,1}^C$ . The opening time  $t_{1,1}^O$  of the window  
 94  $W_{1,1}$  is then given by the slowest neutrons that can reach the second chopper  
 95 when the window  $W_{2,1}$  opens, which start at the source at the beginning of the  
 96 pulse or after some offset  $\delta t_0$ :

$$t_{1,1}^O = \frac{L_1}{\tilde{v}_1} + \delta t_0, \quad (4)$$

97 where  $\tilde{v}_1 = L_2/(t_{2,1}^O - \delta t_0)$ . The closing time  $t_{2,1}^C$  of the window  $W_{2,1}$  is given  
 98 by the slowest neutrons with the wavelength  $\lambda_{\text{max},1}$  that reach the first chopper  
 99 when it closes:

$$t_{2,1}^C = \frac{L_2}{v_{\text{min},1}} + \delta t_0, \quad (5)$$

100 where  $v_{\text{min},1} = L_1/(t_{1,1}^C - \delta t_0)$ . Note that  $\lambda_{\text{min}}$  is not the shortest wavelength  
 101 that gets transmitted through the PSC (see Fig. 1), but is the shortest wave-  
 102 length for which the created pulse length  $\delta t$  corresponds to the resolution  $R_{\text{max}}$ .  
 103 At the same time, if  $\delta t_0 > 0$ , then  $\lambda_{\text{max},1} = \lambda(v_{\text{min},1})$  is also not the largest  
 104 wavelength that gets transmitted through the first window of the PSCs. For  
 105 the design of the second window, the shortest wavelength is set  $\lambda_{\text{min},2} = \lambda_{\text{max},1}$   
 106 to achieve a continuous spectrum and minimise time gaps at the detector, and

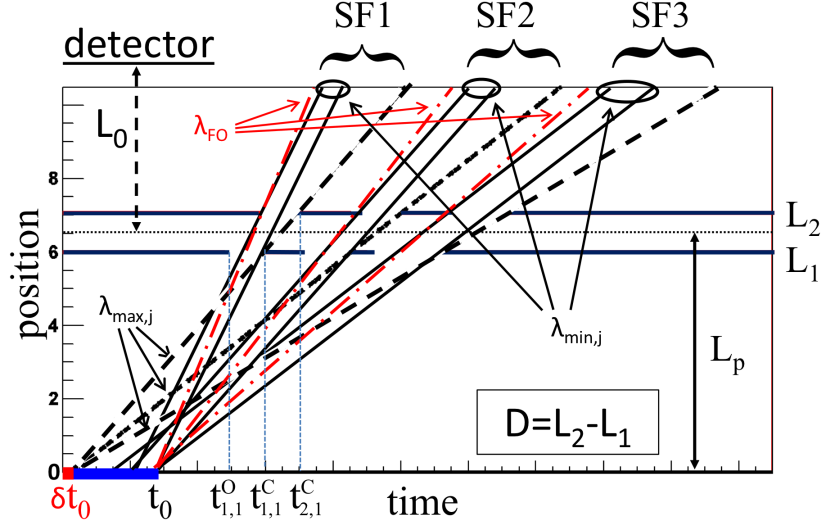


Figure 1: Illustration of the construction procedure of the PSC with a ToF diagram. The total pulse duration  $t_0$  is denoted by the blue bar, while the time offset  $\delta t_0$  is illustrated by the red square, thus the usable pulse length is  $t_0 - \delta t_0$ . The choppers are located at the positions  $L_1$  and  $L_2$ . For the  $j$ th subframe SF, neutrons having the wavelength  $\lambda_{\min,j}$  and  $\lambda_{\max,j}$  used in Eqs. 3 and 5 are shown by black lines. Neutrons with wavelengths  $\lambda_{FO} < \lambda_{\min,j}$  responsible for potential subframe overlap, are depicted by dashed-dotted red lines. In addition, the chopper system parameters  $D$  being the distance between both PSCs, the distance between the source and the centre of the PSC system  $L_p$  and  $L_0$ , which is the distance between the centre of the PSC system and the detector that is well outside the illustrated region, are also shown. See text for further details.

107 the construction procedure is repeated iteratively. Thus neutrons with wave-  
 108 lengths  $\lambda < \lambda_{\min,j}$  or  $\lambda > \lambda_{\max,j}$  that get transmitted through the  $j$ th window  
 109 of the PSCs can lead to overlap of the subframes in time at some distance be-  
 110 hind the PSCs and must be treated by frame overlap choppers. Their design is  
 111 discussed in the next subsection.

112

113

A PSC constructed in the way described above transmits a certain fraction  
 114 of the total available phase space. The latter is obtained by performing a fixed  
 115 grid scan through the  $[t, \lambda]$  parameter space assuming a constant spectrum as  
 116 a function of the wavelength  $\lambda$ , where  $t$  is the start time of a neutron at the  
 117 source. This can be visualised in an acceptance diagram (Fig. 2) displaying the  
 118 correlation between the neutron wavelength  $\lambda$  and the time  $t_{PS}$ , at which the  
 119 neutron is at the position  $L_p = L_1 + 1/2 \times D$  located in the center between  
 120 both PSCs. As an example, instrument parameters calculated for a potential  
 121 ESS liquids reflectometer (*instrument I*) (see Table 1) are used in the most of  
 122 the following discussion. The initially available phase space is split by the PSCs  
 123 into 3 subframes being disjoint in time but joint in wavelength ranging from  $2 \text{ \AA}$

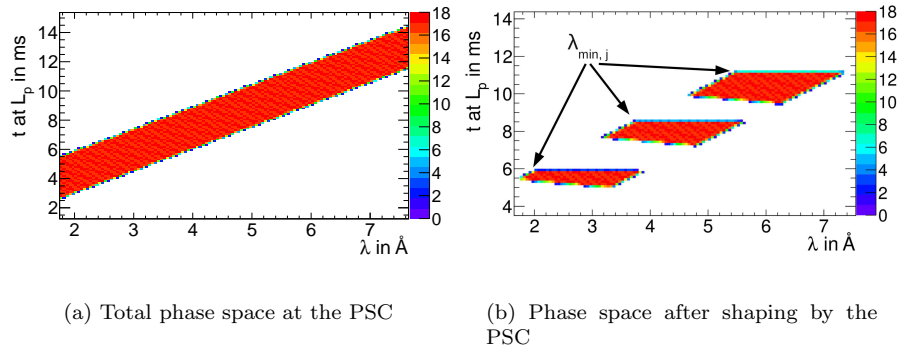


Figure 2: Neutron phase space available at the PSC for the *instrument I*, displayed as correlation between the neutron wavelength  $\lambda$  and the ToF at the position between the PSCs. This phase space has been determined by a fixed grid scan through the  $[\lambda, t]$  parameter space. The units on the z-axis are arbitrary and correspond to the phase space density. Without any pulse shaping, the phase space is linearly correlated and has the ESS pulse width of 2.86 ms for each wavelength. After pulse shaping, the phase space is divided into three subframes, with the width  $\delta t(\lambda)$  corresponding to the design resolution.

124 to 7.2 Å, based on a instrument length of  $L_{\text{tot}} = 55$  m. For each  $\lambda$ , the total  
 125 width  $\delta t(\lambda)$  of the modified pulse corresponds to the design resolution 2.2% of  
 126 the WFM system. If no further choppers would be included in the system, due  
 127 to wavelength overlap of individual subframes discussed above, the subframes  
 128 would inevitably overlap in time at some distance after the PSC. Thus frame  
 129 overlap choppers are needed to keep the subpulses separated until they reach  
 130 the detector. Their number and positions are optimised in the following using  
 131 acceptance diagrams.

### 133 2.2. Designing the frame overlap choppers

134 Frame overlap choppers (FOCs) can be visualised in the acceptance diagram  
 135 as linear functions indicating the opening and closing of the corresponding chop-  
 136 per window. Points in the phase space described by these functions correspond  
 137 to certain  $[t, \lambda]$  combinations such that these neutrons reach the corresponding  
 138 chopper at the time when it opens or closes. The analytical description of these  
 139 functions for the opening and closing time is:

$$\begin{aligned}
 t_{i,j}^{O/C} = f(\lambda) &= -((L_i - L_p)/v(\lambda)) + \Theta_{i,j}^{O/C}/\omega_i \\
 &= -((L_i - L_p) \times m/h) \times \lambda + \Theta_{i,j}^{O/C}/\omega_i,
 \end{aligned}
 \tag{6}$$

140 where  $L_i$  is the distance between the Chopper  $i$  and the source,  $v(\lambda) = \frac{h}{m\lambda}$   
 141 the neutron velocity,  $\Theta_{i,j}^{O/C}$  the angular offset of the window start (end)  $j$  with

142 respect to the guide position and  $\omega_i$  the chopper rotation frequency. At a  
 143 pulsed source, chopper frequencies have to be equal to the source frequency or  
 144 larger by an integer factor. Fractional distances between the PSCs<sup>2</sup> and the  
 145 detector act thereby as a limit for maximum possible multiple of the source  
 146 frequency, e.g. choppers only can rotate at twice (four times) the source fre-  
 147 quency, if their distance  $D_i$  to the PSCs fulfills  $D_i \leq 1/2L_0$  ( $1/4L_0$ ) and so on.  
 148 Thus as a first choice, three FOCs can be placed at  $1/8L_0 + L_1 = 12.125$  m,  
 149  $1/4L_0 + L_1 = 18.25$  m and  $1/2L_0 + L_1 = 30.5$  m. The windows of a FOC  $i$  are  
 150 then constructed such that they open when they are reached by the fastest neu-  
 151 tron starting at  $t_j^{\lambda_{\min,j}} = t_{2,j}^O - L_2/v(\lambda_{\min,j})$  and close upon arrival of the slowest  
 152 neutron of the corresponding subframe  $j$  starting at  $\delta t_0$ . Based on these fore-  
 153 going considerations, the window parameters  $j$  of the FOC  $i$  can be calculated  
 154 in a straightforward way:

$$\Theta_{i,j}^O = -\omega_i \times \left( \frac{L_i}{v(\lambda_{\min,j})} + t_j^{\lambda_{\min,j}} \right) \quad (7)$$

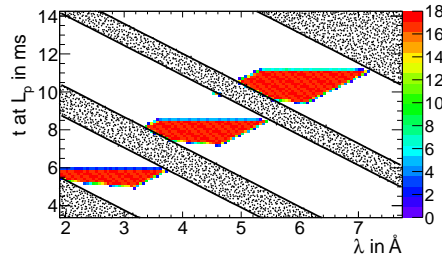
$$\Theta_{i,j}^C = -\omega_i \times \left( \frac{L_i}{v(\lambda_{\max,j})} + \delta t_0 \right) \quad (8)$$

155 The inclusion of FOCs restricts parts of the phase space transmitted through  
 156 the PSCs (Fig. 3). This leads to a reduced transmission for wavelengths be-  
 157 ing in the overlap region of the individual subframes. The level of such a flux  
 158 reduction also depends on other instrument parameters and is discussed in the  
 159 next section, while this discussion is more focused on whether the FOCs keep  
 160 all the unwanted phase space away from the subframes. While it appears that  
 161 for the loosest resolution of  $\delta\lambda/\lambda = 2.2\%$  the transmitted parameter space is in  
 162 accordance with expectations, at a higher resolution of 1%, when the discs of  
 163 the PSCs are closer together, there is a leakage of phase space into subframes  
 164 2 and 3, which spoils the desired resolution. Thus the previously chosen layout  
 165 of FOCs does not work properly for all adjustable WFM settings.

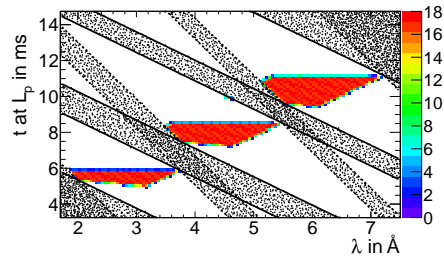
167 The position of the contaminant phase space in the diagram suggests that  
 168 an additional FOC located very close to the PSC, i.e. represented by lines with  
 169 a very small slope, would be able to remove the frame overlap while at the  
 170 same time not cut into the usable phase space. This is confirmed in Fig. 4,  
 171 showing the addition of a FOC at 7.5 m, while also the positions of other three  
 172 FOCs were slightly changed (see Tab. 1 and Fig. 6). Contaminant radiation is  
 173 now removed even for high resolutions while saving as much as possible of the  
 174 usable phase space. In Fig. 5, analytical calculations of neutron propagation  
 175 through this chopper setup show that all subframes are separated in time at the  
 176 detector position, while the adjusted resolution is achieved for a greater part  
 177 of the usable waveband. For wavelengths close to a neighbouring (sub)frame,  
 178 the resolution and thus the transmission is reduced due to prevention of frame

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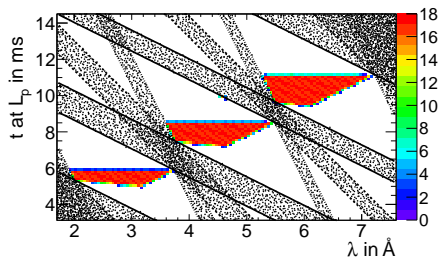
<sup>2</sup>or the source if the pulse is not shaped afterwards.



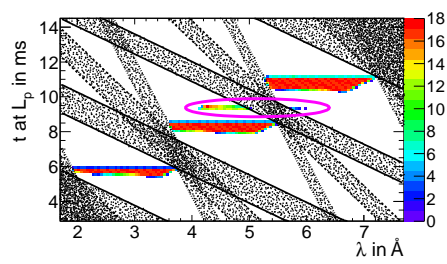
(a) Phase space after inclusion of FOC1 at 12.125 m



(b) Phase space after inclusion of FOC2 at 18.25 m

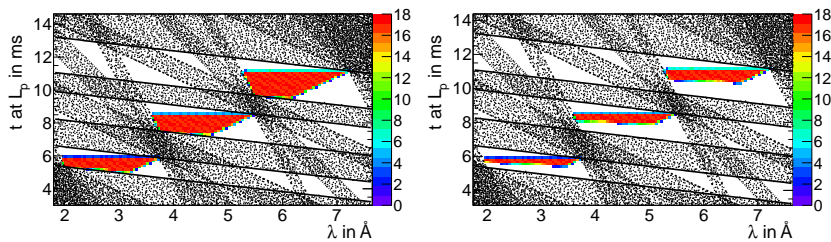


(c) Phase space after inclusion of FOC3 at 30.5 m



(d) Phase space for 1% resolution

Figure 3: Remaining phase space after subsequent inclusion of frame overlap choppers at 12.125 m, 18.25 m and 30.5 m. Areas that are excluded by the FOCs are shaded. While there is hardly any contaminant radiation left for the design resolution of 2.2%, there is a clear leakage of spurious neutrons highlighted by the magenta ellipse into the second and third subframe when reducing the distance between the two discs of the PSC to achieve a resolution of 1%.



(a) Phase space after all choppers for 2.2% resolution.

(b) Phase space after all choppers for 1% resolution.

Figure 4: The inclusion of a fourth FOC at 7.5 m removes the contaminant radiation present in the WFM setup shown in Fig. 3. Now even for resolutions of 1% (and higher) the transmitted phase space is free of spurious neutrons.

179 overlap. As the next step, the validity of this layout needs to be confirmed by  
 180 neutronic Monte-Carlo (MC) simulations, described in the following section.

181

### 182 3. Comparison with MC simulations

183 The analytical study described in the last section makes use of idealised  
 184 conditions. In a real instrument, the characteristics of the transmitted neutron  
 185 beam will be influenced by additional parameters like guide geometry, beam di-  
 186 vergence and pulse structure, and chopper rotation speed. Thus to confirm that  
 187 the WFM chopper layout derived from analytical considerations is suitable for  
 188 a real instrument, it needs to be tested by a neutron MC simulation, where all  
 189 of these criteria are included. In this work, the VITESS software [7, 9] package  
 190 was used. The chopper setup was included in the simulations of the *instrument*  
 191 *I*, which will be published elsewhere.

192

#### 193 3.1. Simulations of the reflectometer chopper layout

194 In order to include the choppers in the MC simulation, it is important to  
 195 decide on their parameters like radius and rotation speed. The radius and rota-  
 196 tion speed might be constrained by their position in the particular instrument  
 197 and engineering feasibility. It is also important to decide how to deal with the  
 198 finite time a chopper needs to fully open or close the beam. First, in order to  
 199 be conservative and prevent frame overlap as far as possible, the time  $t_{i,j}^O$  ( $t_{i,j}^C$ ),  
 200 at which the  $i$ th chopper opens (closes) the guide in the analytical calculation,  
 201 is defined as the time at which the chopper starts to open (fully closes) the  
 202 beam in the simulation, see Fig. 7. This requirement guarantees that for each  
 203 wavelength the neutron transmission starts and ends at the same time as in



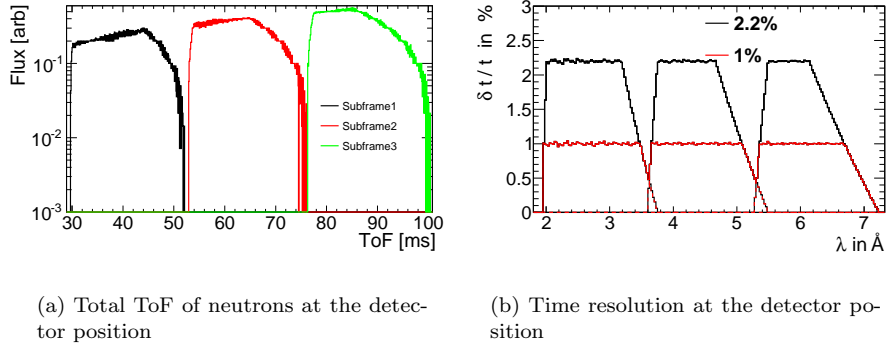


Figure 5: Left: ToF plot of 3 subframes coming from a single main pulse, which are well separated in time. Right: The wavelength resolution at the detector expressed as  $\delta t(\lambda)/t_{\text{tot}}(\lambda)$ , where  $t_{\text{tot}}$  is the ToF of neutrons between the centre of the PSC and the detector. The contributions of individual subframes are denoted by dashed lines, whereas the maximum resolution is depicted by the solid lines. Since the subframes are separated in time, it allows for an unambiguous reconstruction of the wavelength from ToF.

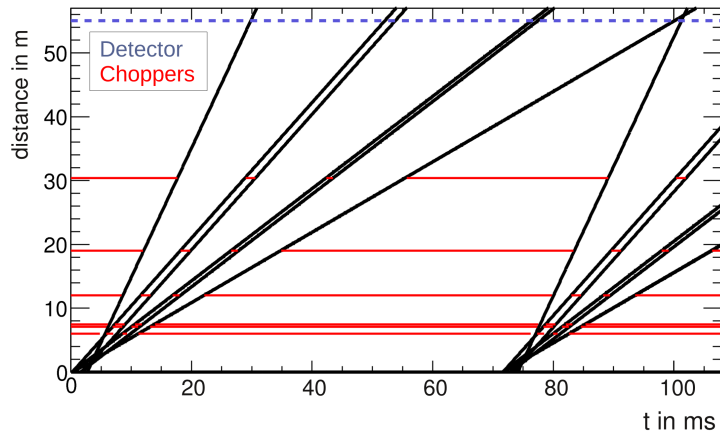


Figure 6: Time of flight diagram of the final chopper setup as worked out with the acceptance diagram method. The fastest and slowest of neutrons trajectories in the individual subframes are represented by black lines, while choppers and the detector are depicted by the red and blue lines, respectively. For completeness, the next main pulse is shown as well.

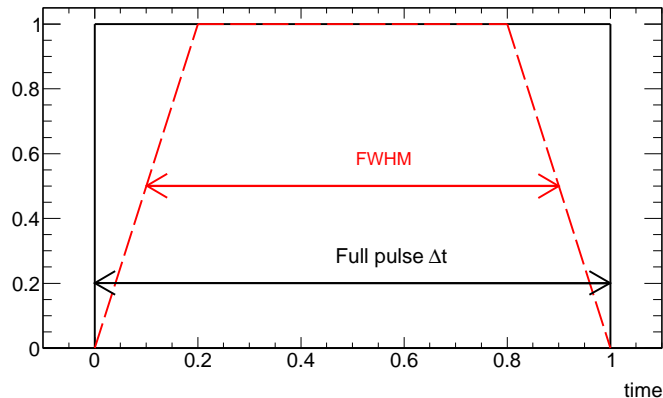


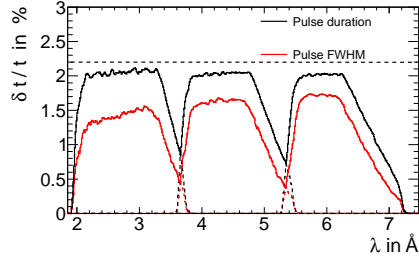
Figure 7: Illustration of the neutron pulse structure used in the analytical study and MC simulations. While in the analytical study the opening and closing time of choppers were assumed to be infinitely small and thus the pulse was a perfect rectangle with a width of  $\Delta t(\lambda)$ , the finite guide size and chopper rotation speed lead to a trapezoidal shape of the pulse. Its full width at half maximum (FWHM) is smaller than the pulse duration  $\Delta t$ , since in this work the points in time at which pulse starts and ends in the MC simulation were decided to exactly coincide with those from the phase space study.

204 the phase space study. Hence the size of the windows has to be reduced to  
 205 account for the time the choppers need to sweep through the guide. As a re-  
 206 sult, for a given nominal resolution simulations should yield a higher measured  
 207 resolution at the cost of a reduced transmission due to a smaller FWHM of the  
 208 pulse. A deviation from this strict requirement is considered in the next section.

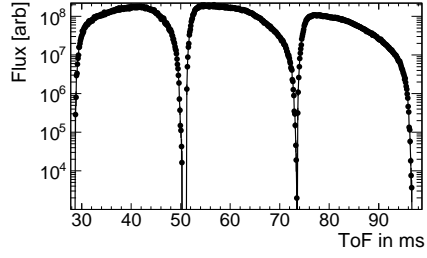
209  
 210 To prove that the WFM setup works in the MC simulation, it is important  
 211 to show that both the desired resolution is reached and the subframes are well  
 212 separated in time. Results of VITESS simulations shown in Fig. 8 confirm that  
 213 the subframes are well separated in time and the time gap between subframes  
 214 coincides with analytical results. As far as the achieved time resolution is con-  
 215 cerned, it can be observed that especially for short wavelengths it is higher than  
 216 the nominal resolution, thus the neutron transmission is slightly worse in MC  
 217 simulations compared with the transmission from analytical calculations. The  
 218 wavelength spectrum exhibits dips as a result of frame overlap prevention, see  
 219 Fig. 9 and Fig. 5 and 8 for comparison.

### 220 3.2. Impact of technical constraints

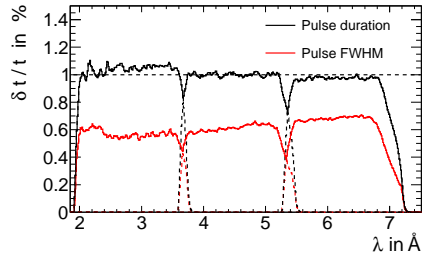
221 In the last section it was shown that the WFM setup as developed with  
 222 the help of acceptance diagrams proved to work in the MC simulation of the  
 223 *instrument I*. Compared to analytical calculations, geometrical constraints of  
 224 the instrument have an impact on the neutron transmission and lead to time  
 225 pulses, which deviate from the idealised rectangular shape (see Fig. 7). This



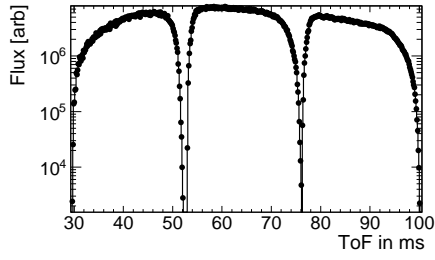
(a) Time resolution at the detector position for 2.2%



(b) Time distribution at the detector position for 2.2%



(c) Time resolution at the detector position for 1%



(d) Time distribution at the detector position for 1%

Figure 8: (a) and (c): Measured time resolution at the detector position as a function of wavelength, which was calculated using both the total pulse duration  $t_{\max} - t_{\min}(\lambda)$  and its FWHM (see also Fig. 7). As expected, the total pulse duration agrees well with analytical results while for the FWHM calculation the trapezoidal shape of the pulses due to finite guide geometry and chopper rotation speed comes into play. (b) and (d): ToF distribution at the detector position, all subframes are clearly separated in time by the WFM setup.

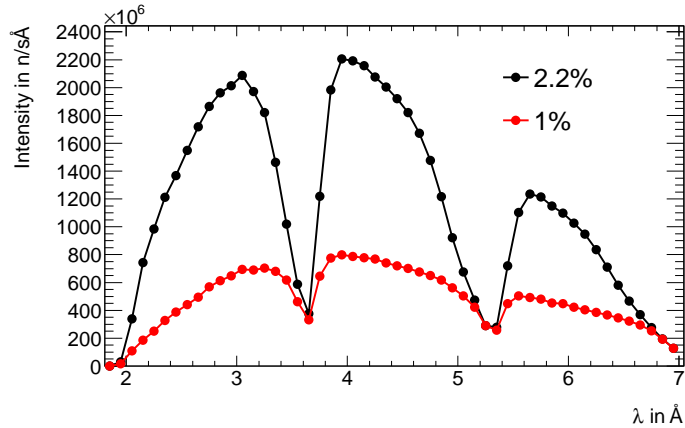
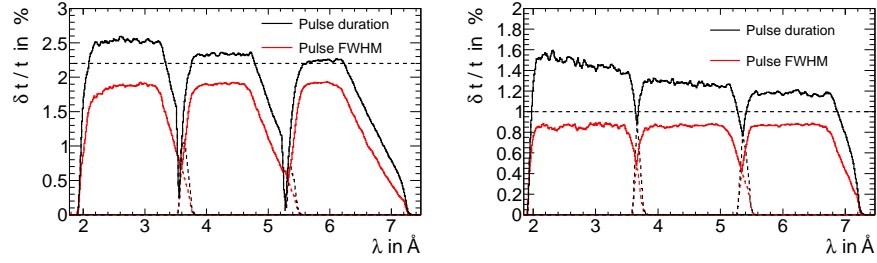


Figure 9: Neutron flux at the detector position for the *instrument I* comprising a WFM chopper layout for 2.2% and 1% wavelength resolution. For wavelengths close to the subframe edges a reduction of flux due to frame overlap prevention can be observed.

226 has an effect on the achieved wavelength resolution (Fig. 8) and overall neu-  
 227 tron flux (Fig. 9). As far as the resolution is concerned, in order to achieve  
 228 the desired value either the distance between the discs of the PSC needs to be  
 229 increased or the windows of the PSC should be modified. The latter can be  
 230 done by withdrawing the reduction of the window widths that accounted for  
 231 finite guide dimensions, i.e. dropping the strict requirement concerning chopper  
 232 opening and closing times by assuming that the beam is infinitely thin. This  
 233 leads to an increase of the total pulse width, but at the same time the FWHM  
 234 of the pulse, which is the factor determining the wavelength resolution at the  
 235 detector, better corresponds to the desired value, see Fig. 10. Such a choice of  
 236 window parameters for the PSC can be recommended as a solution to the pulse  
 237 shape problem coming from finite instrument dimensions. Flux losses in the  
 238 regions around subframe edges, which come from FOCs cutting into the beam  
 239 to avoid frame overlap, can be reduced by optimizing the sizes and offsets of  
 240 chopper windows such that the time gap between subframes is minimised and  
 241 the opening and closing time is reduced (see Fig. 11).

242  
 243 It should be mentioned that the *instrument I* does not have the most diffi-  
 244 cult conditions in terms of the complexity of the WFM system, both in terms  
 245 of the used wavelength band and instrument geometry, in particular taking into  
 246 account the small height of the neutron guide of 2 cm. To prove that the concept  
 247 still works in more challenging conditions as well, it was applied to a compara-  
 248 ble instrument (*instrument II*) requiring a constant resolution for wavelengths  
 249 between 1 Å and about 10 Å and having a guide cross section of  $9 \times 9 \text{ cm}^2$  for  
 250 the most of the length of the instrument. The chopper layout worked out with  
 251 acceptance diagrams was very similar to the one for *instrument I*, again com-



(a) Measured resolution at the detector position for nominal resolution of 2.2%

(b) Measured resolution at the detector position for nominal resolution of 1%

Figure 10: Wavelength resolution measured at the detector position using the total width and FWHM of time pulses as a function of wavelength. The effect of reduced and wavelength dependent FWHM due to finite instrument geometry and chopper speed (see Fig. 8) is corrected by modifying the windows of the PSC. See text for further details.

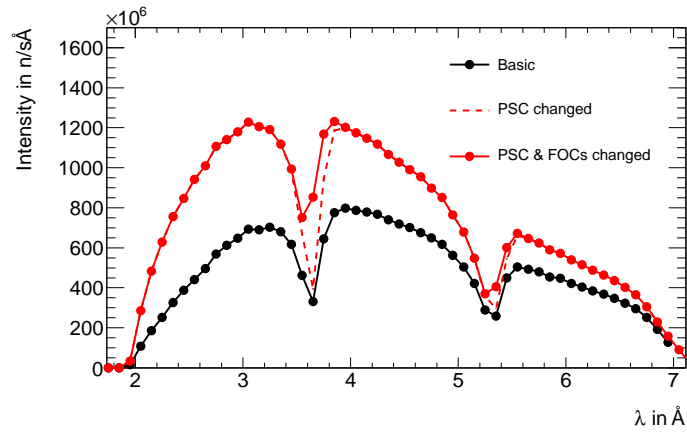
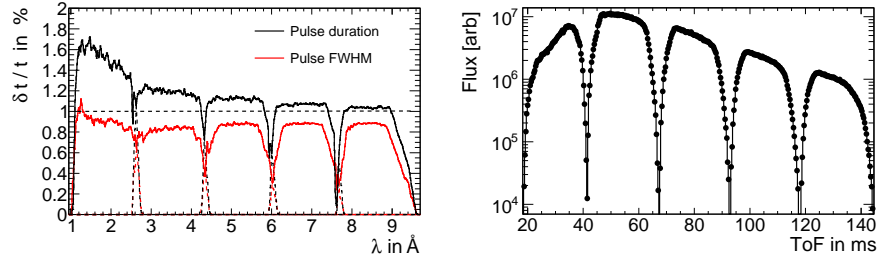


Figure 11: Neutron flux at the detector position for the *instrument I* comprising a WFM chopper layout for 1% wavelength resolution. The basic configuration of choppers, depicted by the black line, was modified to maximize the flux output in the regions where subframes overlap in wavelength. An improved performance was reached when modifying the windows of the PSC as well as those of FOCs.



(a) Measured resolution at the detector position for nominal resolution of 1%

(b) Measured ToF at the detector position for nominal resolution of 1%

Figure 12: Measured resolution and ToF distribution for the *instrument II* having a  $9 \times 9 \text{ cm}^2$  guide cross section for the most length and utilizing wavelengths between 1 and around  $10 \text{ \AA}$ . The chopper layout designed with acceptance diagrams allows to reach the adjusted resolution by splitting the waveband into five subframes that do not overlap in time.

252 prising six choppers and in particular with the first FOC being placed very close  
 253 to the PSC, which is again located at 6 m. While the PSC and the first FOC  
 254 deal with a focused beam of a  $2 \times 2 \text{ cm}^2$  cross section <sup>3</sup>, the full guide cross  
 255 section of  $9 \times 9 \text{ cm}^2$  is seen at the positions of the remaining three FOCs. MC  
 256 simulations show that also in this case the chopper system delivers the desired  
 257 resolution for the entire waveband, which is split into five subframes being all  
 258 separated in time as required (Fig. 12). The flux losses due to frame overlap  
 259 avoidance increase, since the larger guide dimensions and smaller chopper speed  
 260 due to the increased transmitted waveband require longer opening and closing  
 261 chopper times than for the *instrument I*. This situation can be improved by  
 262 minimising the time gap between subframes (see Fig. 13). For this, acceptance  
 263 diagrams once more prove to help by pointing out the right chopper parameters  
 264 for a modification. Compared to the *instrument I*, there is more flux lost in  
 265 the overlap regions, however the total flux reduction only amounts to about  
 266 20%, if compared to a layout in which FOCs would be excluded. In general, the  
 267 spectrum transmitted by a WFM system and its optimisation will be particular  
 268 to each instrument, whereas at the same time a chopper layout suggested by  
 269 the acceptance diagram approach can be expected to be already close to an  
 270 optimum solution.

<sup>3</sup>If high-resolution measurements are desired, the instrument concept should be such that at the position of the PSC the beam is narrow at least in one dimension. Since at the future ESS there are tight space constraints for choppers placed at around 6 m, a large beam cross section would render pulse shaping for high-resolution mode impossible.

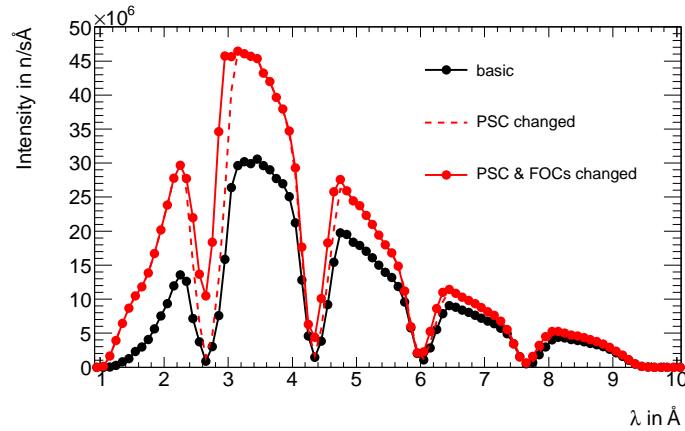


Figure 13: Neutron flux at the detector position for the *instrument II* comprising a WFM chopper layout for 1% wavelength resolution. The basic configuration of choppers, depicted by the black line, was modified to maximize the flux output in the regions where subframes overlap in wavelength. An improved performance was reached when modifying the windows of the PSC as well as those of FOCs. See text for further details.

#### 271 4. Conclusion

272 The WFM concept is a sophisticated chopper setup that enables to expand  
 273 the usable wavelength range, in particular in combination with a constant wave-  
 274 length resolution setup at long pulse neutron sources. Due to its complexity, the  
 275 design of such a system is challenging and there are several criteria that need  
 276 to be accounted for. As was shown in this work, acceptance diagrams can be a  
 277 powerful tool to design and optimise WFM systems, because they help getting  
 278 a thorough understanding of the interplay between individual choppers and are  
 279 at the same time much faster to process than neutron simulations, thus problems  
 280 like contaminant neutrons at higher resolutions would be more difficult  
 281 to recognise and solve in MC simulations. Acceptance diagrams allow one to  
 282 optimise the number and positions of the WFM choppers such that the beam  
 283 characteristics obtained in MC simulations match the instrument requirements  
 284 in terms of subframe separation and achieved resolution. The presented WFM  
 285 concept works for different instruments independent of their particular geomet-  
 286 rical constraints, thus the acceptance diagram method can be of significant help  
 287 when designing or upgrading instruments, in particular in view of the future  
 288 ESS facility.

289

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Parameter	Parameter value	
	<i>Instrument I</i>	<i>Instrument II</i>
ESS pulse length $t_0$	2.86 ms	
ESS source frequency	14 Hz	
Total instrument length $L_{\text{tot}}$	55 m	60 m
Wavelength band	2–7.2 Å	1–9.6 Å
Distance between the PSCs and detector $L_0$	49 m	54 m
Position of the first PSC	6 m	
Position of the second PSC at 2.2% (1%) resolution	7.08 m (6.49 m)	— (6.54 m)
Rotation frequency of the PSC	70 Hz	
Final position and rotation frequency of the 1st FOC	7.5 m, 70 Hz	7.4 m, 70 Hz
Final position and rotation frequency of the 2nd FOC	12 m, 56 Hz	11.7 m, 42 Hz
Final position and rotation frequency of the 3rd FOC	19 m, 28 Hz	18 m, 28 Hz
Final position and rotation frequency of the 4th FOC	30.4 m, 14 Hz	28 m, 14 Hz
Guide height	2 cm	2 – 9 cm
Guide width	10 – 26 cm	2 – 9 cm

Table 1: Basic preliminary instrument parameters used in the design of the potential future ESS liquids reflectometer (*instrument I*) and for the crosscheck instrument (*instrument II*).