Event-Based Processing of Neutron Scattering Data

Peter F. Peterson, Stuart I. Campbell, Michael A. Reuter, Russell J. Taylor, Janik Zikovsky

*Neutron Data Analysis and Visualization, Oak Ridge National Laboratory,
Oak Ridge, TN, USA*

Abstract

Many of the world's time-of-flight spallation neutrons sources are migrating to recording individual neutron events. This provides for new opportunities in data processing, the least of which is to filter the events based on correlating them with logs of sample environment and other ancillary equipment. This paper will describe techniques for processing neutron scattering data acquired in event mode which preserve event information all the way to a final spectrum, including any necessary corrections or normalizations. This results in smaller final uncertainties compared to traditional methods, while significantly reducing processing time and memory requirements in typical experiments. Results with traditional histogramming techniques will be shown for comparison.

Keywords: neutron, software

1. Introduction

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory [1, 2] measured first neutrons April 28, 2006. Besides the promised neutron flux increase over existing sources and novel instrument design, the biggest

Preprint submitted to Nuclear Instruments and Methods

August 31, 2015

5 feature advertised was event mode data acquisition. Event mode provides
6 three pieces of information for each detected neutron: detector pixel identi-
7 fier, total time-of-flight from source to detector, and wall clock time of the
8 proton pulse the neutron is associated with. The full list of events can be
9 stored for later processing. The time-of-flight is the time from the neutron
10 to be emitted from the moderator until it is measured by the detector. The
11 detector pixel identifier, or pixel id, is a unique index to the detector pixel
12 in the instrument. This differs from the traditional data acquisition mode of
13 measuring histograms where each detected neutron is given a pixel identifier
14 and time-of-flight then collected into histograms, without information about
15 the pulse the neutron is associated with.

16 Limited memory and bandwidth of computers when time-of-flight neu-
17 tron scattering was being developed is the reason for histogram mode [3, 4, 5].
18 Generally the experimenter made a choice of either having more detector pix-
19 els or time-of-flight bins, balancing them as anticipated for the experiment.
20 With event mode, the neutrons are recorded at full resolution of the data
21 acquisition electronics. At SNS this is 100ns for time-of-flight and each in-
22 dividual pixel. While this new acquisition mode was available since the first
23 neutrons were measured, techniques for processing the events had not been
24 developed. For the first few years of operation data was reduced by first his-
25 togramming the events, then processing them using traditional techniques.
26 Note that this is still an available option, but much of the data reduction at
27 SNS has been converted to use the techniques described below.

Figure 1: Schematic diagram of histogramming. Dashes below are individual events. Boxes are the histogram representation. Curved line is the normal distribution for reference.

28 2. Histogramming

29 Before the SNS, most experiments on time of flight neutron sources, data
30 was collected in what is known as Histogram Mode. What do we mean by
31 this? Histograms divide the total range of time-of-flights ($t_{min} \rightarrow t_{max}$) into
32 a number of channels or bins. When a neutron is detected, its time-of-flight
33 (TOF) is determined and the scaler counter for the corresponding histogram
34 channel is incremented.

35 The time-of-flight (TOF) of a neutron recorded into the time channel N
36 can be defined as

$$t_{min} \leq t_{min} + t_N \leq TOF < t_{min} + t_{N+1} \leq t_{max} \quad (1)$$

37 where t_N is the starting time boundary for the N^{th} histogram channel.
38 Figure 1 illustrates this. For the N^{th} histogram channel, the most likely
39 time-of-flight for the neutron is given by

$$TOF = t_{min} + \frac{1}{2}(t_{N+1} - t_N) \quad (2)$$

40 From this we can see that the time-of-flight accuracy of a given feature in
41 the collected spectrum will depend on the width of the time channels that we
42 use in the data acquisition. Furthermore, an increase in the channel width
43 would also move the position of any feature by half the increase in channel
44 width. For a more detailed discussion of choosing histogram bin widths can
45 be found in [3].

Figure 2: A comparison of the relative differences observed in diffractograms arising from the rebinning of histogram or event data. Each lower figure is a rebinned version of the one above it. All four are done with constant $\Delta T/T$ binning with the left column being the with event data and the right being histogram, for comparison. The data presented is from a Diamond sample measured on the instrument POWGEN.[6]

46 3. Dynamic Histogramming

47 One great advantage of event-based processing is that histogramming can
48 be performed dynamically, using the raw event data. In histogrammed data,
49 the distribution of neutrons' times of flight within a single bin is unknown,
50 that information has been discarded, requiring that assumptions be made
51 when rebinning. Generally the assumption is that the events are evenly
52 distributed within a histogram bin. As a result, rebinning always smooths
53 the data. By retaining the distribution of events, one can continue using the
54 notation of rebinning, when all that is really being done is histogramming.
55 Figure 2 shows the ability to rebin event-based data (left) as compared to
56 histogram data (right). As can be seen, the diffraction pattern is revealed
57 as the bins are made smaller. With traditional histogram data, there is an
58 effective smoothing of the data as seen in the figure. As mentioned in Section
59 1, at any point data processing can continue with the histogram version of the
60 data. In practice this can be done making a copy of the dynamic histogram.

61 In order to efficiently histogram the data, it is best to sort the events
62 for the histogram by time-of-flight. Then the algorithm iterates through the
63 sorted event list, adding events to a bin, then moving on to the next bin
64 when the next event's time-of-flight goes to a new bin. While the initial sort
65 of n events has a computational complexity of order $O(n) = n \log n$, any
66 subsequent re-binning is performed in approximately linear time $O(n) = n$.
67 Histogram errors are calculated to be simply equal to the square root of the
68 number of counts in each bin as according to Poisson statistics [7, 8].

69 4. Propagation of Uncertainties

70 4.1. Existing histogram mode data processing

71 To provide a framework for understand event data processing, we will
 72 first describe processing histograms. A histogram can be made from event
 73 data by ignoring the wall clock time and summing together all events within
 74 histogram bin boundaries together. The term "wall clock time" refers to the
 75 absolute time of the proton pulse on target. If we sum the wall clock time and
 76 the time-of-flight, we will get the absolute time the neutron was detected.
 77 The uncertainties are just the square root of the measured intensities, $\sigma^2 = I$,
 78 as traditionally assumed. The four types of arithmetic that one can generally
 79 do are add, subtract, multiply and divide. When doing these operations for
 80 individual histogram bins uncertainties are propagated according to tradi-
 81 tional equations assuming there is no cross-correlation between parameters
 82 [7, 8].

$$C = A + B \quad \text{then} \quad \sigma_C^2 = \sigma_A^2 + \sigma_B^2 \quad (3)$$

$$C = A - B \quad \text{then} \quad \sigma_C^2 = \sigma_A^2 + \sigma_B^2 \quad (4)$$

$$C = A \times B \quad \text{then} \quad \left(\frac{\sigma_C}{C}\right)^2 = \left(\frac{\sigma_A}{A}\right)^2 + \left(\frac{\sigma_B}{B}\right)^2 \quad (5)$$

$$\text{or} \quad \sigma_C^2 = (B \cdot \sigma_A)^2 + (A \cdot \sigma_B)^2 \quad (6)$$

$$C = A/B \quad \text{then} \quad \left(\frac{\sigma_C}{C}\right)^2 = \left(\frac{\sigma_A}{A}\right)^2 + \left(\frac{\sigma_B}{B}\right)^2 \quad (7)$$

$$\text{or} \quad \sigma_C^2 = \left(\frac{\sigma_A}{B}\right)^2 + \left(\frac{A \cdot \sigma_B}{B^2}\right)^2 \quad (8)$$

83 4.2. Weighted Events

84 Typical data reduction steps performed on histogrammed scattering data
 85 include background subtraction, absorption corrections, normalization, and

86 dividing by a reference spectrum. The discussion so far has assumed that
 87 each neutron event counted as exactly one; handling these reduction steps
 88 requires the introduction of *weighted events*.

89 A weighted event consists of a neutron event with the addition of a weight
 90 and an error (discussed in the next section). One can handle weighted events
 91 by converting un-weighted events to weighted events dynamically, only as
 92 required. Say, for instance, that an event is multiplied by a scalar, 2.0: a
 93 new *weighted* event will be created with a weight of 2.0, and this will replace
 94 the original, un-weighted event. When histogramming weighted events dy-
 95 namically, this event will count as two, and the resulting histogram will be
 96 the same as if the multiplication had been performed on a histogram.

97 The following arithmetic operations can be performed on the event data
 98 A and B :

99 $A + B$: List of events are simply appended.

100 $A - B$: List of events are appended, with B 's weights set to negative.

101 $A \times B$ **and** A/B : Here, the dynamic histogram of B is used. The weight
 102 of each event in A is multiplied/divided by the value (and error) of the
 103 histogram at the corresponding bin in the B histogram. This is one
 104 occasion when the bin sizes matter.

105 In all four cases, the results are still lists of events, and further arithmetic
 106 can be performed with no loss of information.

107 4.3. Event Data Specifics

108 When using weighted events, it is necessary to propagate uncertainties
 109 in a way that is consistent with histogram methods. In essence, a list of

110 events should be treated as a *sparse* histogram with bins of negligible width.
 111 Each of these sparse bins contains a single event ($N = 1$) and therefore its
 112 uncertainty is $\sigma = \sqrt{N} = \sqrt{1}$. There is debate as to whether or not this is an
 113 appropriate value for the uncertainties of a "small" number of counts. That
 114 is not germane to how the uncertainties are propagated [9, 10, 11].

115 The methods for uncertainty propagation of histogram data, described in
 116 section 4.1, can then be applied in the usual way. With w_i and w_f as the
 117 initial and final weights of an event; σ_i and σ_f as the initial and final errors
 118 on an event:

119 **Multiply by scalar A :** $w_f = A \cdot w_i$; $\sigma_f^2 = A^2 \cdot \sigma_i^2$

120 **Multiply by scalar with error $A \pm \sigma_A$:** $w_f = A \cdot w_i$

121
$$\sigma_f^2 = (A \cdot \sigma_i)^2 + (w_i \cdot \sigma_A)^2$$

122 **Adding N events into a bin :** Weights are simply summed: $w_{tot} = \sum w_i$.

123 Errors are summed in quadrature: $\sigma_{tot}^2 = \sum \sigma_i^2$

124 With these values, the uncertainty in a bin during on-the-fly histogram-
 125 ming can be performed by simply summing the square of the uncertainties
 126 of each event. For N un-weighted events, $\sigma = 1$, this is simply $\sqrt{N}$.

127 5. Applications

128 5.1. Saving Memory

129 When dealing with large numbers of events, processing speed and memory
 130 use become concerns. A way to handle this is to compress the events. This
 131 technique can be used to reduce both the number of events and their memory

Figure 3: The data presented is from a water (in a Al holder) sample measured on the instrument VISION [12] separated into inelastic (a) and diffraction (b) detectors as a function of time since the measurement started. The vertical axis is in number of raw events (solid), weighted events (dot-dashed), or histogram bins (dashed).

132 footprint. The algorithm iterates through the events and combines into a
133 single weighted event any separate neutron event objects that have times-of-
134 flight within a given tolerance. As an example in time-of-flight, if 10 events
135 have the same time-of-flight of exactly 1.000 ms and a weight of 1.0, they are
136 combined into one event with a weight of 10.0: a 90% reduction in memory
137 use. At the SNS, events' time-stamp are measured with a resolution of 100
138 ns; therefore, compressing events can be safely done using a tolerance of 50
139 ns (for example) without removing any information. In large data sets, the
140 memory savings and speed improvements can be very significant.

141 There is an obvious drawback if the chosen compression tolerance is too
142 large, then time-of-flight resolution is lost. This will leave artifacts in the
143 data analogous to coarse binning of histogram data. A related, but separate,
144 artifact comes from the machine precision of storing the time-of-flight, which
145 is originally an integer number of 100ns steps, as a floating precision number.
146 This will have a undesirable effect as the storage format will move the time-
147 of-flight as the difference between floating point numbers and integers vary.

148 An additional benefit of on-the-fly histogramming is reduced memory re-
149 quirements for visualization. Since histograms are generated on-the-fly, they
150 do not need to all be stored in memory at once. In many cases there is
151 less memory needed to store the events than to store fine histograms at full
152 instrument pixel resolution. Therefore, fine histograms that would overflow
153 a computer's available memory can still be generated. Some experimental
154 techniques, like single crystal diffraction, require many pixels and fine time-
155 of-flight resolution in order to have accurate measurement of peak position
156 and intensity. With histograms, this traditionally means a large number of

bins. On TOPAZ [13, 14], a single crystal diffractometer at SNS, this would
 be $256 \times 256 \times 3000 \approx 2 \times 10^8$ for a single detector panel. Storing the
 events will automatically only record where there were counts which will be
 overwhelmingly where the Bragg peaks are. As a second example, a NeXus
 [15, 16] file from the SEQUOIA spectrometer at SNS [17, 18] is 265MB in
 size. The file contains approximately 5.0 million events which compresses to
 4.8 million weighted events. However, with $10\mu s$ bins, this data requires 193
 million histogram bins for the time-of-flight range. Independent of storage
 format, this is a tremendous difference. Figure 3 shows a comparison of mem-
 ory usage as a function of measurement time using the VISION instrument.
 While it is significantly less memory to store events than histograms for the
 inelastic detectors (3a), the diffraction detectors (3b) are more efficiently
 stored as histograms.

5.2. Flat Background Subtraction

We have shown above that subtracting a measured background from a
 given data set is straightforward. In some cases we want to subtract a con-
 stant background from the whole data set, and the value of this constant
 is often estimated by taking the average value over a given "flat" region of
 measured data. If we consider the background as a histogram, then this
 poses a problem if we want to subtract it from a list of events. Namely, it
 is impossible for us to know the distribution of events within the histogram
 correctly.

As a practical method to overcome this problem, our approach is to ex-
 tract the list of events from the original dataset. This is then treated as
 a characteristic representation of the distribution of events. This region is

Figure 4: Schematic diagram of how we generate a flat event data set from a region of (simulated) experimental data.

182 replicated and shifted until it fills up the entire data range. We now have two
183 event lists covering the same range of data and we can simply subtract them
184 as shown previously. Another approach would be to generate a sequence of
185 fictitious events with a flat distribution over the entire data range.

186 5.3. *Filtering Events*

187 Since the pulse time of every event is recorded, it is possible to perform
188 filtering on data after acquisition is complete; such filtering is impossible on
189 histogrammed data. Filtering can reduce background noise or allow selecting
190 parameter space more finely. Figure 5 shows a schematic of such a filtering.
191 For filtering based on logged information there is a requirement that the
192 clocks are all synchronized to an accuracy that is no larger than the time res-
193 olution scale of the phenomenon being observed. In practice, the resolution
194 of commonly used time synchronization techniques [19] is adequate (e.g. 1ms
195 upto 100ms) for "slow control" values (e.g. temperature). Filtering based on
196 a "slow control" value is done by converting the log values to absolute times,
197 then selecting the events based on those times[20, 21]. This can be general-
198 ized to "slicing" data where ranges of log values are used to create a list of
199 time ranges that belong in multiple workspaces. Continuing the temperature
200 example, slicing a measurement of temperature ramping from 100K to 200K
201 in 5K chunks would result in 20 event data sets from a single measurement.
202 The experimenter can then decide whether there are sufficient statistics in
203 each slice and increase or decrease the temperature range for the slice.

204 For "fast" logs which are measured at a frequency similar to the wall-clock
205 time for the events a different technique can be used for filtering and splitting.
206 An example of this is a magnet whose power and cooling requirements dictate

Figure 5: Schematic diagram showing event filtering capabilities. Each of the lower plots shows a wall clock integrated diffractogram of the data within the dashed lines from the upper plot. The data shown is from a simulated measurement.

207 that it can only produce its field for a few microseconds then cool for several
208 minutes. In this case, the synchronization of the times is done by the observed
209 phenomenon. The time resolution of the log allows for frame correcting the
210 data before filtering. The events should be filtered based on the state of
211 the sample when the neutrons were interacting with the sample, rather than
212 when they were at the detector. Therefore, we need to estimate how far back
213 in time the neutron was at the sample and remove it from the events absolute
214 time[22, 23]. The absolute time is simply the wall-clock time of the pulse
215 added to the time-of-flight of the neutron. It is this (corrected) absolute time
216 that should be compared to the time of the log.

217 **6. Summary**

218 We have introduced how event data can be used to process data at time-
219 of-flight spallation neutron sources. The propagation of uncertainties for
220 events has been shown along with some practical considerations of using this
221 technique.

222 **7. Acknowledgments**

223 Work was sponsored by the Division of Scientific User Facilities, Office
224 of Basic Energy Sciences, US Department of Energy, under Contract No.
225 DE-AC05-00OR22725 with UT-Battelle, LLC. A portion of this research
226 used data from the POWGEN and VISION instruments at Spallation Neu-
227 tron Source. The authors would also like to thank Nick Draper and Timmy
228 Ramirez-Cuesta for useful discussions.

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