Continuous Mode Data Collection in Protein Crystallography

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ABSTRACT

In the traditional start/stop rotation method of data collection, the overhead for proper implementation of the rotation is high and this overhead increases as exposure time or oscillation width decrease. A more efficient alternative approach is a continuous rotation mode. In this mode the spindle axis is rotated at constant speed with the shutter opening and closing at specific motor positions to select which rotation ranges are recorded. The objective is to minimize overall system overhead as exposure time per image becomes small (less than one second); this overhead should be closely related to the detector readout speed and diminishes with a fast readout detector. An example would be collecting every second or third image possible while performing two or three passes to complete a data set. Methodology and characterizations necessary for implementing continuous mode data collection in general are described.

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Introduction

The traditional rotation method for protein crystallography data collection consists of a simple linear sequence of images from a starting phi angle to an ending phi angle. For each image the detector is enabled for data accumulation, the required rotation is performed, and the detector is read out. The proper implementation of this rotation motion together with the operation of the X ray shutter during the rotation directly affects the quality of the data. Errors in the rotation, whether timing or mechanical, are a direct cause of systematic errors (the worst sort) in data sets. A proper implementation of the rotation can add two to three seconds of overhead in addition to the actual exposure time. As the exposure time per degree decreases or the rotation width decreases, the percentage of the total image cycle time consumed by overhead in executing an accurate rotation motion increases substantially. Since the trend at synchrotron beam lines is for higher flux and faster detectors, this overhead poses a significant challenge to efficient use of synchrotron sources.

We propose a method in which the spindle axis rotates continuously and thus data collection overhead is related primarily to the exposure time and detector readout time. We will show that the continuous rotation method can take advantage of faster detector readout times and that the percentage of overhead for this method is lower than for the traditional start/stop method.

We will describe the continuous rotation method in detail, and then discuss the minimum information and functions required to implement this algorithm in a general setting. Some timing examples will be shown comparing the standard rotation method with the continuous rotation method.

We choose to describe this method independently of any specific hardware implementation of the spindle axis and shutter or its control software (Galil or Compumotor controllers, EPICS or SPEC control programs). Similarly, it is too simplistic to view the issue in terms of system interconnections such as: “You take this cable, plug it into the motion controller’s digital IO channel, and run it over to the detector where…” This is a general approach, and we approach it generally in this discussion; the details of specific implementations will vary.

The Continuous Rotation Method

In the continuous rotation method, the data are taken as a series of passes with the spindle axis phi rotating at constant velocity. Each pass consists of moving the phi angle several degrees prior to the first image to be recorded in the pass, ramping phi to a constant velocity, then recording every *nth* image in the pass until the end of the data collection range has been reached, followed by ramping down the phi angle to rest. Passes are repeated until all images have been collected. Since the actual exposure timing consists only of opening and closing the shutter at appropriate phi values, it is hoped that this method can be implemented easily at most beam lines. Many motion controllers used to drive the spindle axis at synchrotron beam lines, such as Galil or Compumotor controllers, can be programmed easily to perform this exposure.

Figure 1 illustrates the basic timing elements of the continuous rotation method. In this example the detector readout time is a bit longer than the rotation exposure time; every third image will be collected on each pass with three passes required to collect all the data.

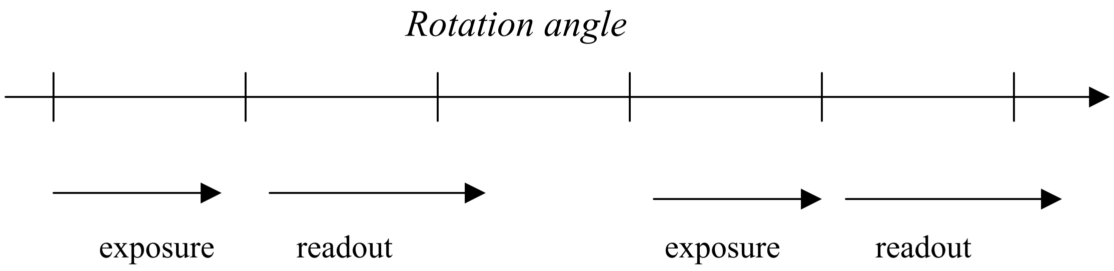

Figure 1

An actual implementation of the algorithm will require the following goniometer commands in addition to those in general use: ramp phi to constant velocity (which will be the rotation time divided by the rotation angle range), take an exposure beginning at a specified phi angle whose duration is the rotation angle width, ramp phi to rest (used at the end of each pass), and read current phi position. The detector readout time, which is the time from the start of detector readout until a new start or detector enable command can be issued, must be determined. The exposure time and the detector readout time determine the number of passes. There will be a small overhead in issuing commands to the goniometer and detector; this should be taken into account when calculating the number of passes.

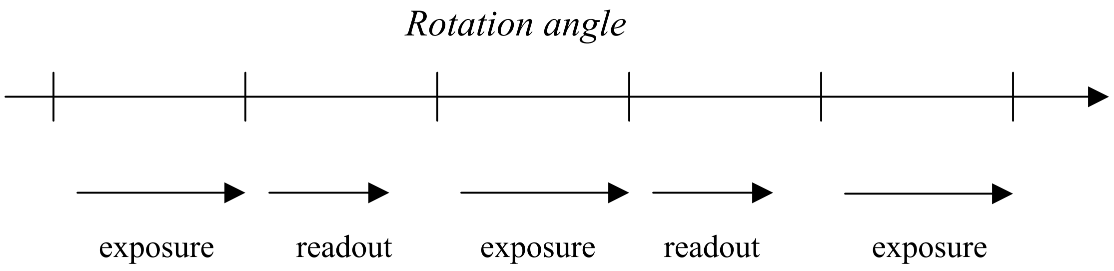

Figure 2

Figure 2 shows an example where the readout time is smaller than the exposure time so only two passes will be required to collect the data. It is apparent that small changes in the readout time or the exposure time can change the number of passes required to collect the data.

We can calculate the total time taken for the standard rotation method as:

$$t\_total = (t\_exposure + t\_overhead) * n\_images$$

For the continuous rotation method the total time is given by:

$$t\_total = t\_exposure * n\_images * n\_passes + (n\_passes - 1) * rewind\_time$$

where *t_exposure* is the exposure time for each image, *n_images* is the number of images in the data set, *t_overhead* is the larger of the detector readout time and the motor repositioning overhead per image, *n_passes* is the number of passes for the continuous rotation method, and *rewind_time* is the time to move the rotation spindle from the end of the data collection run to the beginning of the run.

Timing Examples

We can construct some timing examples for a sample 100 degrees data collection. In this example we assume *t_overhead* of three seconds, and *rewind_time* of 13 seconds. These are typical values for the SBC-CAT beam line 19ID at the APS. All runs use a velocity of 1.0 degree per second for the spindle axis, so a 1.0 second run is for 1 degree of rotation, and an 0.5 second run is for 0.5 degrees of rotation. The readout times are typical times, including control and system overhead, for ADSC Q210 and Q315 CCD detectors. The results are summarized in Table 1.

Exposure Time (sec)	Readout Time (sec)	Total Data Collection Time (sec)	
		Standard Method	Continuous Rotation Method
1.00	1.35	400	326
1.00	0.70	400	213
0.50	1.35	700	439
0.50	0.70	700	326

Table 1. Comparison of times for 100 degrees of data.

Some interesting observations can be made. Since the goniometer overhead is larger than the readout time, improving the readout speed of the detector system does not result in lower data collection times when using the standard data collection method. However, in the continuous rotation method, the reduction in detector readout speed results in a reduction in overall data collection time.

Sometimes it is desirable to collect data with the same total flux but with finer slices (the final two entries in Table 1). This can reduce saturation effects and result in lower background (and better statistics) for a significant percentage of the data. Using the standard method this results in a 75% increase in data collection time for either readout speed, but using the continuous rotation method the increase is only 35% or 48% for the slower or faster readout speed.

With the continuous rotation method we can devise minimum overhead data collection strategies. An exposure time can be chosen so that during data collection the system is either exposing or reading out the detector. In Table 2 we show for comparison times for 100 degrees of data. The first two entries are for 1.0 degree rotations, the last two entries are for 0.5 degree rotations and half the exposure time. The exposure times were chosen to allow for a bit more system overhead than just the readout time (1.5 sec. vs. 1.35 sec., and 0.80 sec. vs. 0.70 sec.).

Exposure Time (sec)	Readout Time (sec)	Total Data Collection Time (sec)	
		Standard Method	Continuous Rotation Method
1.50	1.35	450	313
0.80	0.70	380	173
0.75	1.35	750	476
0.40	0.70	680	266

Table 2. Comparison of times for minimum data collection overhead.

Table 2 shows the exposure time with minimum overhead as a function of detector readout time, and the data collection times associated with collecting each image with half the angle range and half the exposure time.

Exposure Time (sec)	Readout Time (sec)	Total Data Collection Time (sec)	
		Standard Method	Continuous Rotation Method
0.50	0.42	350	113
0.20	0.17	320	53
0.25	0.42	650	176
0.10	0.17	620	86

Table 3. Minimum overhead times using faster detector.

Table 3 shows how fast data sets could be collected if the detector readout were about a factor of three faster. Looking at the differences in the standard method as shown in Tables 2 and 3, there is only a modest improvement when the detector readout times and exposure times are decreased by a factor of three, but for the continuous rotation method almost all of the increase in speed is reflected in the decrease in total data collection times.

Conclusion

The trend at synchrotron beam lines is for higher flux, shorter exposure times and oscillation ranges (fine slicing), and as shown above this will cause data collection times to rise substantially, and no advantage can be taken for faster detector readout. We proposed a continuous data collection method for which it is possible to take advantage of faster detector readout and for which the data collection times increase modestly for faster exposure times and smaller oscillation ranges. We also showed that if the detector readout speed can be made much smaller that almost all of this benefit is reflected in much faster overall data collection times.