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Computational techniques for efficient conversion of image files from area detectors

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ABSTRACT

Area detectors are used in many scientific and technological applications such as particle and radiation physics. Thanks to the recent technological developments, the radiation sources are becoming increasingly brighter and the detectors become faster and more efficient. The result is a sharp increase in the size of data collected in a typical experiment. This situation imposes a bottleneck on data processing capabilities, and could pose a real challenge to scientific research in certain areas. This article proposes a number of simple techniques to facilitate rapid and efficient extraction of data obtained from these detectors. These techniques are successfully implemented and tested in a computer program to deal with the extraction of X-ray diffraction patterns from EDF image files obtained from CCD detectors.

1. Introduction

In the recent years, the technology of detectors and data acquisition systems has witnessed a huge revolution. This, accompanied by the wide availability of intense radiation sources such as synchrotron radiation beams, contributed to the huge increase in the volume of data obtained in a typical experiment. It is not unusual these days to collect hundreds of thousands of experimental data files occupying several tera bytes of magnetic storage from a number of correlated measurements within just a few days. This situation necessitates the development of new computational algorithms and strategies to process and analyze such massive data sets. The current article presents a number of simple techniques that were developed and used recently by the author to deal with the processing of huge quantities of EDF (which stands for European Data Format) binary image files obtained from charge-coupled devices (CCDs) on synchrotron X-ray beamlines to extract numeric data in the form of 1D diffraction patterns. These techniques are simple and general and hence can be easily implemented and used by the interested scientists as a substitute for commercial and free software that rely on more sophisticated but slower algorithms. In the following we describe these techniques in the context of data extraction from binary image files of EDF format obtained from charge-coupled devices, although they can be equally applied to other data formats obtained by other types of detector.

2. EDF image processing

Charge-coupled devices consist of an array of light-sensitive solid-state cells that convert photons into quantified electric charges. These charges measure the intensity of the photon source in terms of energy and number of counts. The 2D spatial distribution of these cells produces a 2D image of the source object. Hence, an image of an object detected by a CCD consists of a 2D matrix of the same dimensions as the CCD array where each entry in the matrix indicates the intensity of radiation at the corresponding cell of the CCD array. Charge-coupled devices are used in many scientific and technological applications such as astronomy and X-ray imaging. Because CCDs are efficient area detectors, they can reduce the acquisition time substantially with improved resolution. A typical CCD used for X-ray imaging on a synchrotron beamline consists of an array of more than five million cells (2640 × 1920). Fig. 1 is a simple demonstration of the setting of a charge-coupled device in an X-ray diffraction experiment.

The purpose of EDF image processing is to convert binary image files obtained from CCD detectors to ASCII numeric format. While the binary image of an EDF file consists of a 2D rectangular matrix where the intensity of the diffracted radiation at each cell is given as a function of implicit *xy* coordinates of the pixel in the matrix, the extracted ASCII numeric data represent a 1D diffraction pattern of total intensity as a function of scattering angle. The radial dependence of the concentric rings in the 2D pattern is correlated to the scattering angle in the 1D pattern by a simple geometric relation. An image of the data contained in a typical EDF file is displayed in

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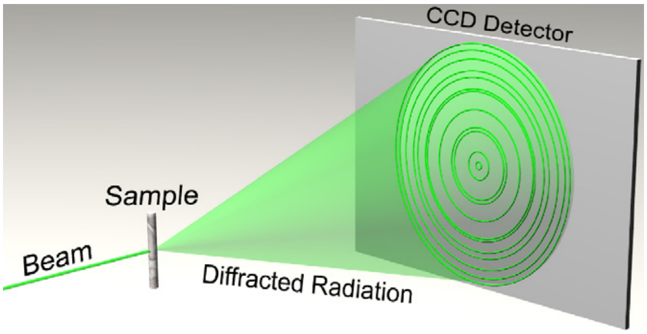

Fig. 1. The setting of a charge-coupled device in an X-ray diffraction experiment.

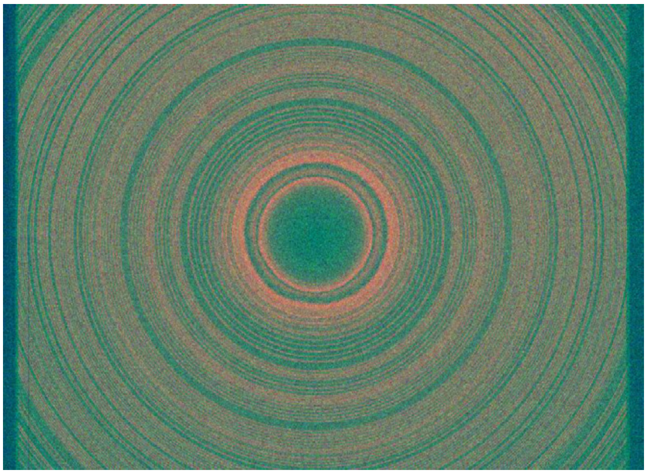

Fig. 2. Image of a 2D diffraction pattern contained in a typical EDF binary file. The 1D pattern of this image is shown in Fig. 3.

Fig. 2 while a sample of the extracted 1D pattern is shown in Fig. 3. Each EDF file contains, beside the binary data of the rectangular matrix, an ASCII header which normally consists of 24 lines of text. This header includes, among other things, the endian bit type (little or big), the data type (e.g. unsigned short or long integer), the horizontal and vertical dimensions of the image matrix in pixels, the size of the data file in bytes, and the date and time of data acquisition. In the following sections we outline the main steps of data extraction of these files.

2.1. Radial data vector

To convert the rings of pixel values in the rectangular data matrix to a 1D pattern, a radial 1D vector is used to store the cumulative intensity of each ring. Each cell in the rectangular data grid is assigned a certain radius according to its distance from the image center taking into account the tilt in the horizontal and vertical orientations as will be discussed in Appendix A. As the pixel values are read, they are assigned to the radial cells in the 1D vector immediately. This ensures rapid processing with minimal computing resources since no memory space is required to store the data in an intermediate processing stage. The radial dependence is computed from the pixel implicit coordinates in the rectangular matrix when the routine is run in single mode, while it is obtained in a more efficient way by using lookup table when the routine is executed in a multi batch mode as will be outlined later.

Because the pixel can be too coarse as a unit of length and as a unit of intensity storage due to its finite measurable size resulting in uneven distribution of intensity in the data points of the 1D pattern, the pixels of the CCD grid can be split to take into account these two factors. This splitting takes two forms:

1. By taking the radial unit length as a fraction of a pixel so that more than one ring can fit within one unit pixel of radial distance. The radial assignment of a pixel then depends on its radial distance from the image center as a float quantity rather than as an integer quantity.
2. By splitting the intensity of the pixel according to the area contained within the closest ring so each ring represents a strip with finite width in the radial direction. To do this, each pixel is divided into a grid of small squares (e.g. 10 × 10). The distance between the center of each small square in this grid and the center of the image is then computed and allocated to the nearest ring. The number of allocated points to a particular ring is then divided by the total number of points in the pixel (i.e. 100 for a

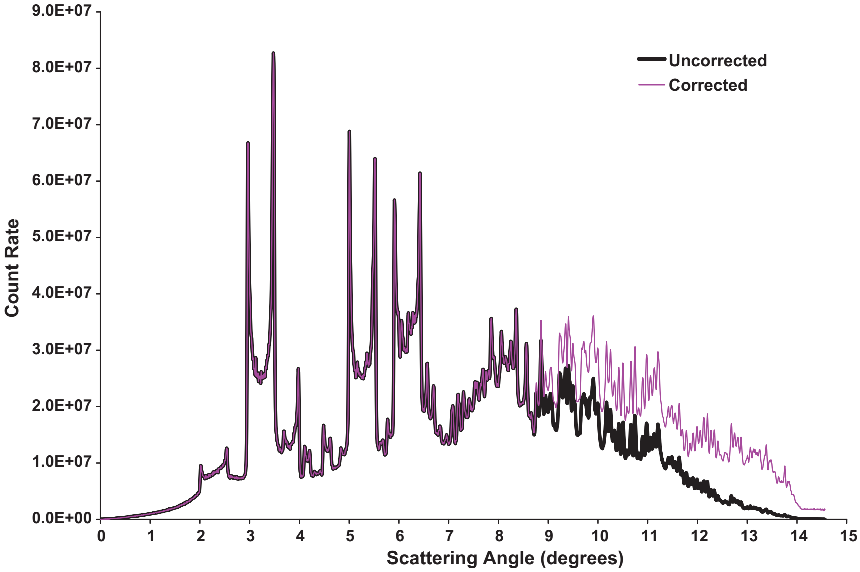

Fig. 3. Example of a 1D diffraction pattern extracted from a 2D EDF pattern. The pink curve is obtained with the application of missing-rings correction while the black is obtained without this correction. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)