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Image Analysis for Monitoring Crystal Growth

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There has been a vast increase in the efforts on the automation of crystal growth in the last few years. Crystallisation robots are capable of producing thousands of images per day and the number of functional crystallisation facilities worldwide is rapidly increasing. One main issue to be addressed at these facilities is to automatically determine as to whether the crystallisation drops contain crystals suitable for an X-ray diffraction experiment. Thus the optical properties of the crystallisation images are subject of active research [1,2]. Here we present a solution for this problem with a novel approach for classification and time series analysis of the images generated by a robot at a particular imaging event. The approach is based on a use of feature vectors generated with Gabor filter banks (harmonic functions modulated by a Gaussian distribution) within a window centred over the information points. For the latter we use the so-called two-dimensional features, which are well suited for a description of object's edges or corners. They have the advantage that no segmentation of the image content into well, drop, etc. is required. Gabor filters with different orientations are used in order to represent the neighbourhood information in the image. The feature vectors based on these filters are fed into a support vector machine for further texture classification. The preliminary results indicate overall 77% success of correct classification over 12 classes. The experimental reproducibility of the success rate requires thorough investigation. The method is being tested on the images obtained from different large-scale crystallisation facilities. The classification is complemented by a time series analysis of all images corresponding to a particular crystallisation well will be carried out.

- [1] Igor Jurisica, Patrick Rogers, Janice I. Glasgow, Robert J. Collins, Jennifer R. Wolfley, Joseph R. Luft and George T. DeTitta. Improving Objectivity and Scalability in Protein Crystallization, IEEE Intelligent systems, Nov/Dec 2001, 26-34.
 [2] Kuniaki Kawabata, Mutsunori, Takahashi, Kanako Saitoh, Hajime Asama, Taketoshi Mishima, Mitsuki Sugahara and Masashi Miyano. Evaluation of crystalline objects in crystallizing protein droplets based on line-segment information in greyscale images, Acta Cryst. (2006). D62, 239-245.

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Installation of mail-in system at SPring-8 protein crystallography beamlines

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Synchrotron radiation plays an essential role in high throughput protein crystallography because it enables both rapid and accurate data collection. However, use of synchrotron is not necessarily convenient because it is located far from users' laboratories in most cases, and unfamiliar operation at beamline is bothersome for many users. Mail-in data collection is one of the solutions to overcome such problems, and we have installed mail-in system at SPring-8 protein crystallography beamlines. The basic concept of our mail-in system is "a kind of remote data collection with a help of a beamline operator", meaning that users determine measurement conditions by themselves and the operator support users experiments by dealing with minimum routine tasks at beamlines. We have accomplished this by making use of data collection software BSS (Beamline Scheduling Software) [1], sample changer robot SPACE (SPring-8 Precise Automatic Cryo-sample Exchanger) [2] and beamline management database D-Cha (Diffraction Check Assistance utilities). Combination of BSS and SPACE enables a new measurement style called "two mode beamline operation" that consists of day time crystal screening and night time full automatic data collection. Web interface of D-Cha allows users to deposit measurement conditions and to observe recorded images at distant place. Following is the basic scheme of our mail-in system. At first, users send crystals mounted on a special tray for SPACE, and then upload crystal related information and crystal screening conditions on D-Cha. At beamline, the operator downloads the screening conditions and starts beamline operation in crystal screening mode. During crystal screening, crystals mounted on a goniometer are centered on X-ray beam path manually by the operator, and the centering coordinates of the goniometer are stored in D-Cha. These coordinates are used later to center crystals automatically when the crystals are remounted on the goniometer in data collection mode. After finishing crystal screening, users select crystals used for data collection and deposit data collection conditions on D-Cha. Then, the operator downloads the data collection conditions and starts automatic measurement. Diffraction images can be downloaded through the internet after finishing data collection. Our mail-in system is now routinely operated at RIKEN Structural Genomics Beamline (BL26B2). We are planning to start mail-in data collection for public users with this system.

- [1] Ueno, G. *et al. J. Synchrotron Rad.* (2005). 12, 380-384.
 [2] Ueno, G. *et al. J. Appl. Cryst.* (2004). 37, 867-873.