

# EPICS controlled sample mounting robots at the GM/CA CAT

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## Abstract

GM/CA CAT at Sector 23 of the advanced photon source (APS) is an NIH funded facility for crystallographic structure determination of biological macromolecules by X-ray diffraction [R.F. Fischetti, et al., GM/CA canted undulator beamlines for protein crystallography, *Acta Crystallogr. A* 61 (2005) C139]. The facility consists of three beamlines; two based on canted undulators and one on a bending magnet. The scientific and technical goals of the CAT emphasize streamlined, efficient throughput for a variety of sample types, sizes and qualities, representing the cutting edge of structural biology research.

For this purpose all three beamlines are equipped with the ALS-style robots [C.W. Cork, et al. Status of the BCSB automated sample mounting and alignment system for macromolecular crystallography at the Advanced Light Source, SRI-2003, San-Francisco, CA, USA, August 25–29, 2003] for an automated mounting of cryo-protected macromolecular crystals. This report summarizes software and technical solutions implemented with the first of the three operational robots at beamline 23-ID-B. The automounter's Dewar can hold up to 72 or 96 samples residing in six Rigaku ACTOR magazines or ALS-style pucks, respectively. Mounting of a crystal takes approximately 2 s, during which time the temperature of the crystal is maintained near that of liquid nitrogen.

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## 1. Robot control program

The automounters [1,2] are controlled by an EPICS server written in State Notation Language [3] that interfaces all the motions [4] (servo drives and pneumatics), as well as a gripper temperature and a laser-based pin presence sensors.

The program interface is implemented via EPICS string process variables, so the server can be accessed from any software talking EPICS channel access. In particular at GMCA CAT beamlines the automounter controls were made available as a part of BluIce GUI [5] for data acquisition.

The program receives a request via EPICS PV string “{beamline}:R:cmd” and returns automounter status via EPICS PV string “{beamline}:R:sta”.

The format of the request string for loading sample is:  
**load** <puck\_position> <puck\_style> <sample #>,  
puck\_position: {A|B|C|D|E|F}, puck\_style: {R|A}, sample #: 1..12 for RigakuMSC ACTOR magazine, 1..16 for ALS puck. The request string for unloading sample is:

### unload

When a sample is loaded and another request for loading is made, the control program will unload the sample first, and only then perform the next load request.

The automounter server program consists of three state sets. A block diagram of the program is shown in Fig. 1. State set “robot” contains all control logic for automounter, state set “monitorer” monitors all limit switches, and state set “warm\_up” monitors elapsed time for mounted samples.

State “init” waits until all EPICS PVs are connected, state “pause” waits for the operator's permit, state “recover” safely sets automounter into idling configuration and then transits to the state “ready”. Should a collision or

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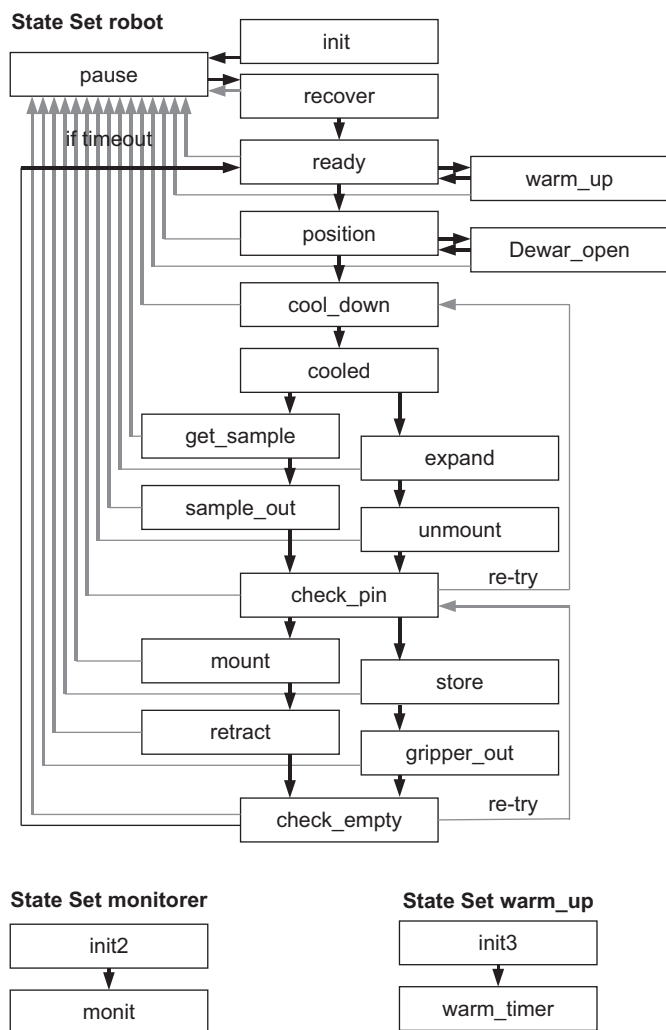


Fig. 1. Block diagram of the SNL program.

malfunction happen in the course of automounter operation so that a timeout occurs or an operation is paused, the control program transits to the state “pause” and awaits for operator’s permit to resume. State “position” controls all motions done by servo motors at the automounter, goniometer support and goniometer to which sample is being mounted/dismounted. In the state “cool\_down” the sample gripper is cooled before loading or unloading the sample. Through the state sequence “position”—“cool\_down”—“cooled”—“get\_sample”—“sample\_out”—“check\_pin”—“mount”—“retract”—“check\_empty” the automounter loads the sample. It unloads the sample with “position”—“cool\_down”—“cooled”—“expand”—“unmount”—“check\_pin”—“store”—“gripper\_out”—“check\_empty” sequence.

If a load request is pending, the gripper warm-up procedure is postponed, so the automounter loads the next sample right after unloading is complete, and only then does the gripper go to warm up and dry cycle.

To load samples into the Dewar the operator sends a request to the control program by pressing the Dewar switch to the “open Dewar” position, and to close the

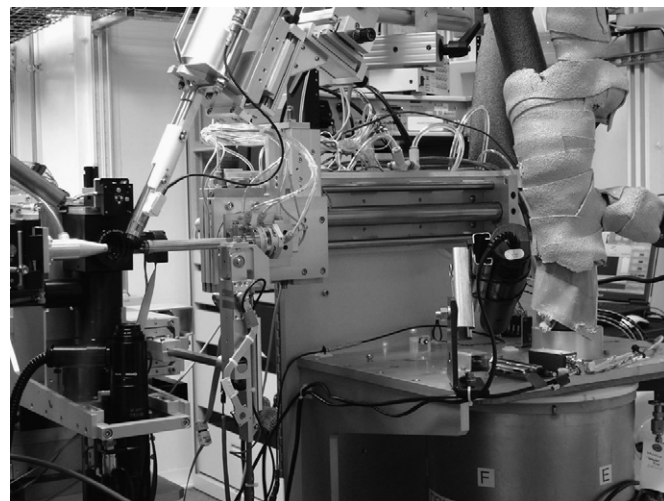


Fig. 2. ALS-style sample mounting robot at the 23-ID-B APS beamline.

Dewar the operator sets the switch to the “close Dewar” position. Setting the switch to the middle position stops Dewar motion.

## 2. Further development

- (1) Automate sample screening. This includes automated crystal centering, taking a few diffraction images, and making an evaluation regarding the crystal quality.
- (2) Install a longer gripper and longer small motion stage. This change will allow the gripper to be kept cold while the Dewar is being positioned for the selected sample. The warm-up cycle for gripper de-icing could be performed once per hour or even longer period. This change will boost automated screening throughput.

## 3. Conclusion

The project is in a testing stage since 12/2006, but it has served close to 1000 successful mounts of crystals for outside users. Implementation of sample mounting robots is an important milestone for the goal of high-throughput data collection and automated sample screening. Fig. 2 shows the robot at the 23-ID-B APS beamline.

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