

MARCH 16, 2021



**GM/CA@APS
MACROMOLECULAR CRYSTALLOGRAPHY
SAMPLE-CHANGER UPGRADE
FOR HIGHER CAPACITY AND
THROUGHPUT**



OLEG MAKAROV



Argonne National Laboratory is a
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Current and Future Trends in

Macromolecular Crystallography Experiments:

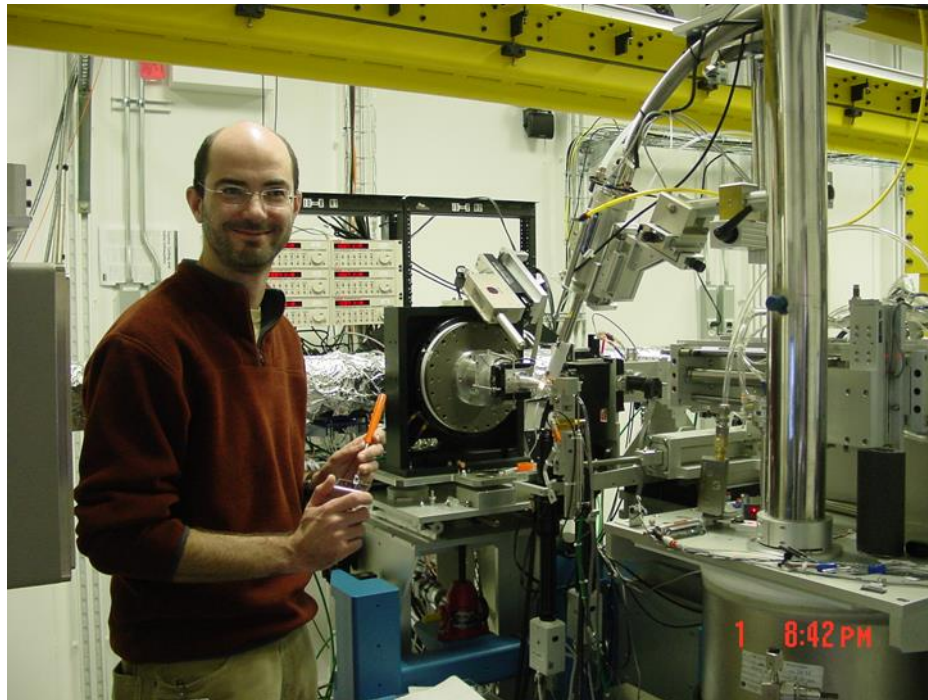
Focus on Automation, High Data Rate Analysis and User Interfaces

OUTLINE

- Introduction
- Upgrade motivation
- Selecting components
- Sample changer upgrade
- Sample changer EPICS server
- Usage statistics
- Acknowledgments

INTRODUCTION

- High-throughput macromolecular crystallography implies:
 - Automated sample handling
 - Automated data collection
 - Automated data processing
- Sample changer is needed for:
 - Automated screening
 - Remote data collection



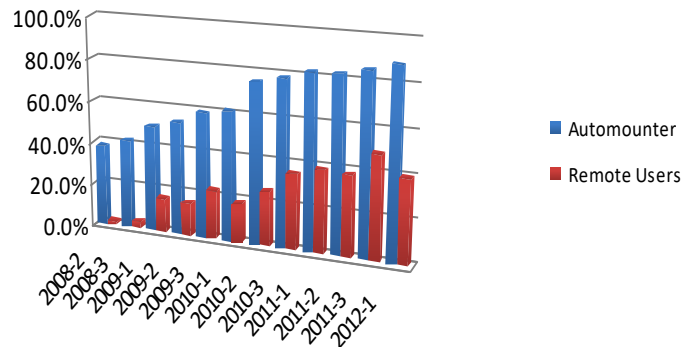
The first sample changer user:
Gyorgy Snell, Takeda Inc. December 1, 2006

UPGRADE MOTIVATION

- Growing beamline automation
- Pixel array detectors with higher throughput
- Steady increase in remote data collection

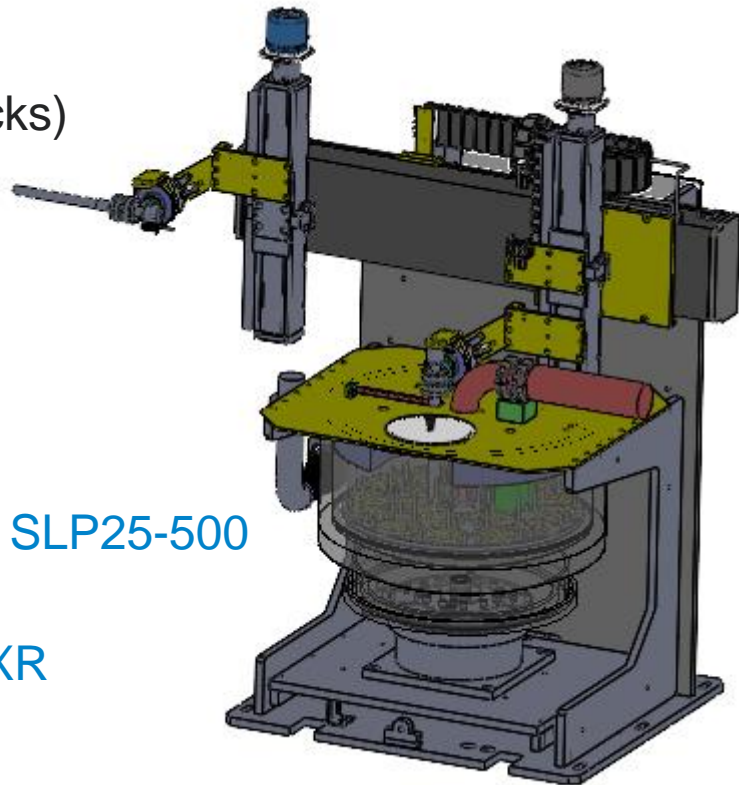


% of Automounter and remote users



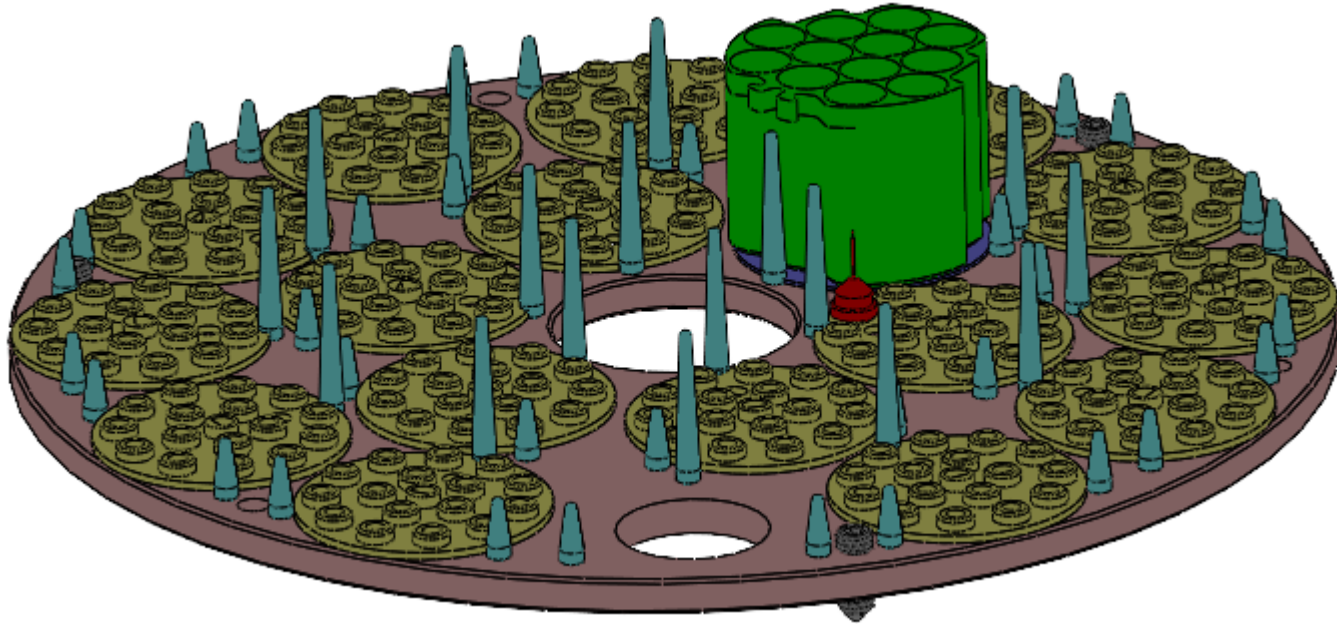
SELECTING COMPONENTS

- Dewar capacity:
 - 18 pucks (ALS style, uni-pucks, Rigaku pucks)
 - 288 (216) samples
- Direct drive components:
 - Dewar rotation: [IntelLiDrives PSR-200](#)
 - Gripper rotation: [ThinGap TG-2310](#)
 - Gripper horizontal translation: [NipponPulse SLP25-500](#)
- Ball screw driven components:
 - Gripper vertical translation: [Parker 402200XR](#)



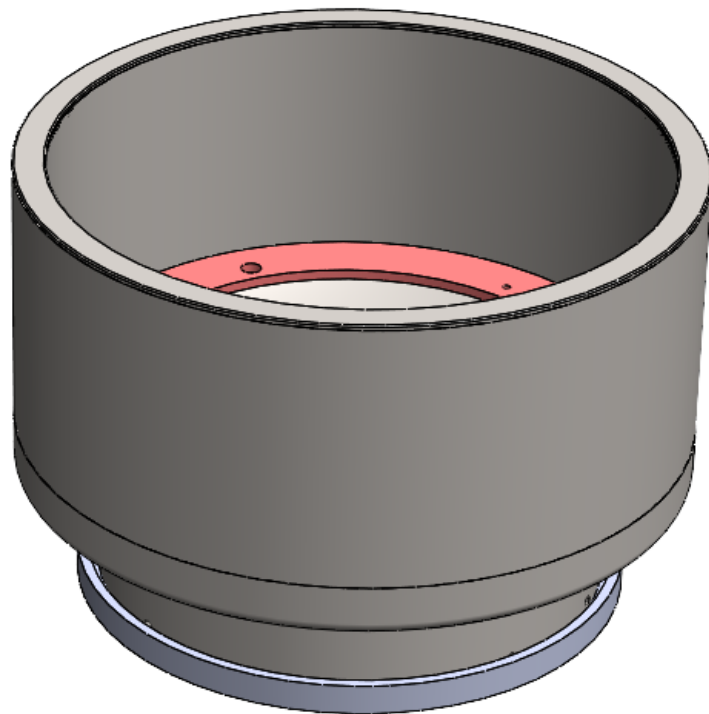
SELECTING COMPONENTS

- Dewar base plate:
 - Adjusted with 3 set screws



SELECTING COMPONENTS

- Dewar:
 - Diameter: 16 inches
 - Hight: 11 inches
- Dewar base plate has set screws
 - To tweak rotation axis to be perpendicular with the top surface.
 - To tweak Dewar base plate axis to be on rotation axis.



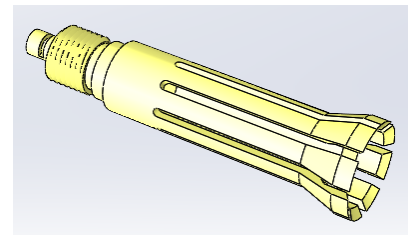
SAMPLE CHANGER UPGRADE



SAMPLE CHANGER UPGRADE

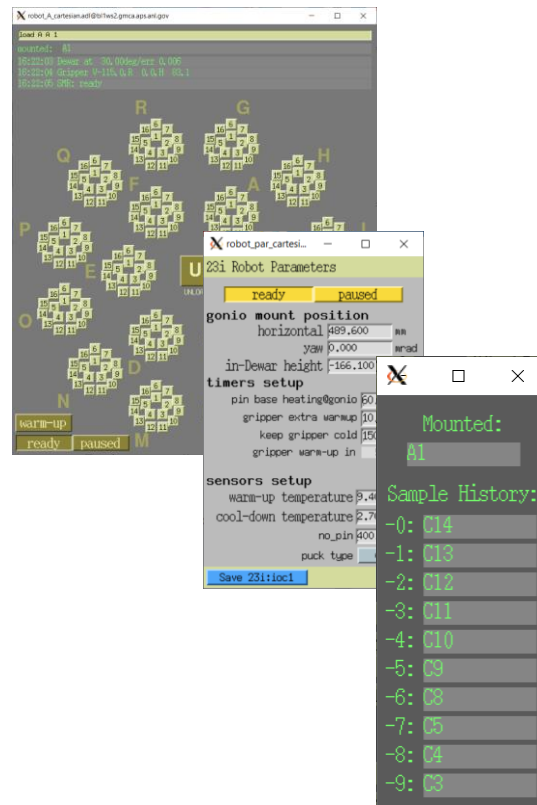
Design highlights

- The use of servo motor positioners results in reduced vibrations and faster operation.
- Same simple operation moves as it was designed for the original Berkeley Lab sample changer
- Heated cover prevents icing at the Dewar top surface.
- Sensors:
 - Hall Effect – for detecting pin base at the goniometer.
 - Fiber optic – for detecting pin base in the gripper.
- More robust eight finger gripper:
 - Less frequent gripper warm-ups.
- Fast sample retrieval with direct drive rotation stage.



SAMPLE CHANGER EPICS SERVER

- Sample changer controlled by EPICS server
 - Uses SNL and Sequencer
 - Software runs in three threads:
 - Monitoring
 - State Sequence Set
 - Motion control
- EPICS interface PVs for clients:
 - Command string: <BL>:R:cmd
 - Status string: <BL>:R:sta
 - Sample Mounted string: <BL>:R:mounted



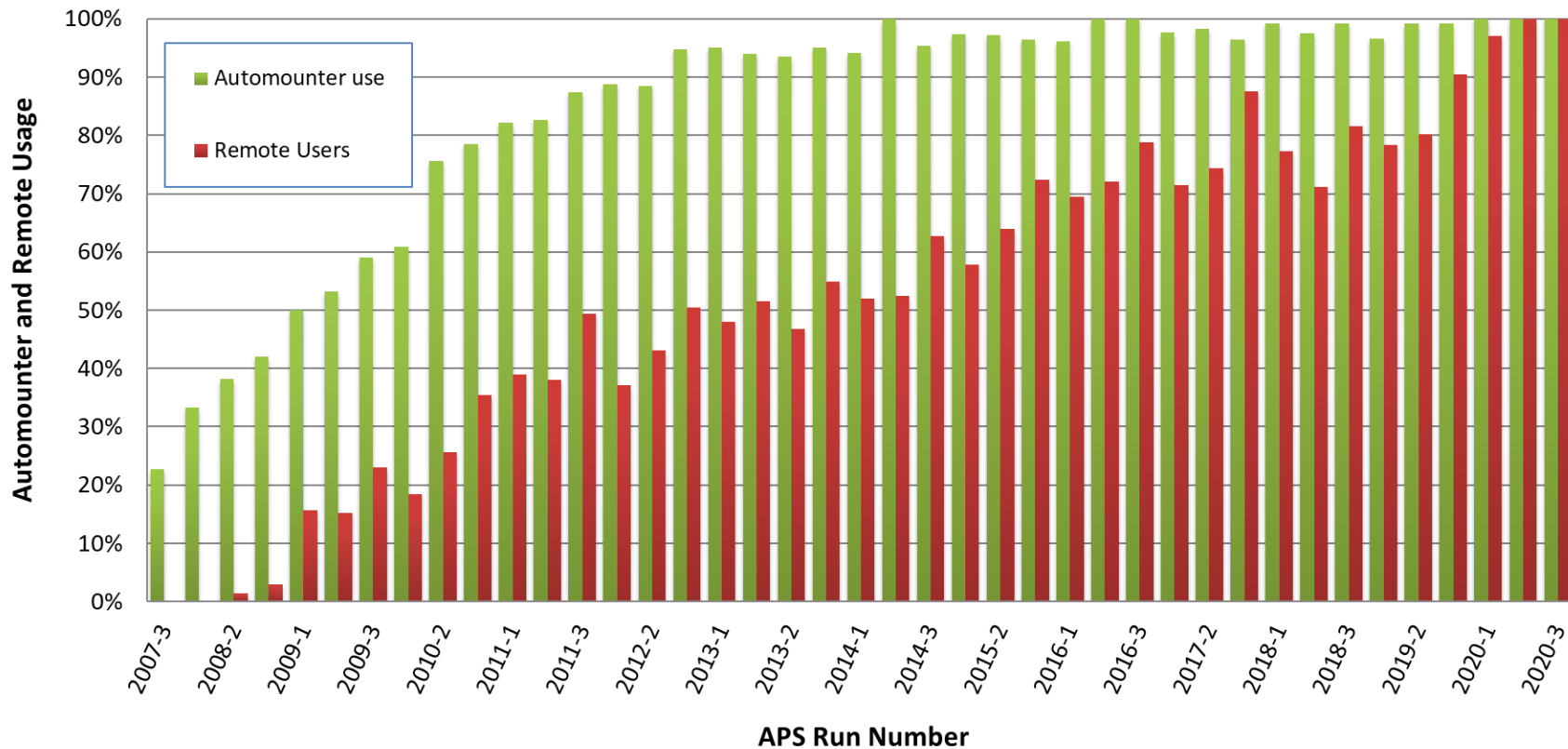
SAMPLE CHANGER EPICS SERVER

jBlulce graphical user interface

- Screening tab – interface for automated sample screening:
 - Uses sample list from Excel spreadsheet.
 - Allows user to select samples for screening
 - Allows user to choose screening options from the task list.
 - Allows user load/unload sample to/from goniometer.
 - Shows screening progress

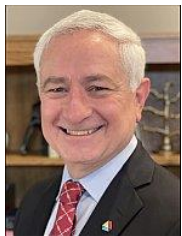
The screenshot displays the jBlulce-EPICS Beamline ID-D Version v2020.2.3 Build 7582 FPE Jan-15 @bl1ws2.gmca.aps.anl.gov window. The 'Screening' tab is active, showing a table of sample data with columns: Select, Port, CrystalID, Directory, Comment, Set, Resolution, and Score. The table lists samples A3 through A9. Sample A4 is selected, and its details are shown in the 'Mini Screening Control' panel on the right. The 'Tasklist' panel shows a list of tasks including 'A4 CenterXtal', 'A4 Paused4Center', 'A4 Paused4Inspection', 'A5 MountNextXtal', 'A5 CenterXtal', 'A5 Paused4Center', and 'A5 Paused4Inspection'. The 'Collection Parameters' panel shows settings for Prefix (A4_1), Dir (dylin), Image Dir (mnt/beegfs...07_cbf/dylin/A4/screen), Current position (Gonio = 89.999, Detector = 550.000, Attenuator = 10.011), Settings (Distance(mm) = 550.000, Delta(deg) = 0.2, Time(sec) = 0.2, Attenuation(factors) = 5.00, Beam size: 25 x 22), and Tasks (Mount Next Crystal, Auto Centering, Crystal jpeg, Collect image, Collect image, Collect image, Collect image, Paused4Inspection). The 'Robot' panel shows the robot status (Ready), current (SMR: ready), and command (load A A 4). The 'Status' bar at the bottom shows the system state: APS Current: 85.5, Shutter Permit: Enabled, A Shutter: Open, Endstation Shutter: Open, Endstation Secure: Yes, State: Idle, ETA: ---, EMERGENCY STOP, Mono: 12.000 keV, IZero: 0.00 V, Control: Passive, Shutter: Closed.

USAGE STATISTICS



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- GMCA@APS
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 - Craig Ogata
 - Shenglan Xu
 - Steve Corcoran
 - Dale Ferguson



REFERENCES

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Acta Cryst. D (2006). **62**, 852-858
2. *EPICS controlled sample mounting robots at the GM/CA CAT*,
Makarov O.A., Benn R., Corcoran S., Devarapalli S., Fischetti R., Hilgart M., Smith W.W., Stepanov S., and Xu S.,
Nucl. Instrum. & Methods Phys. Res. A (2007) **582**, 156-158.

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