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Argonne NATIONAL LABORATORY

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

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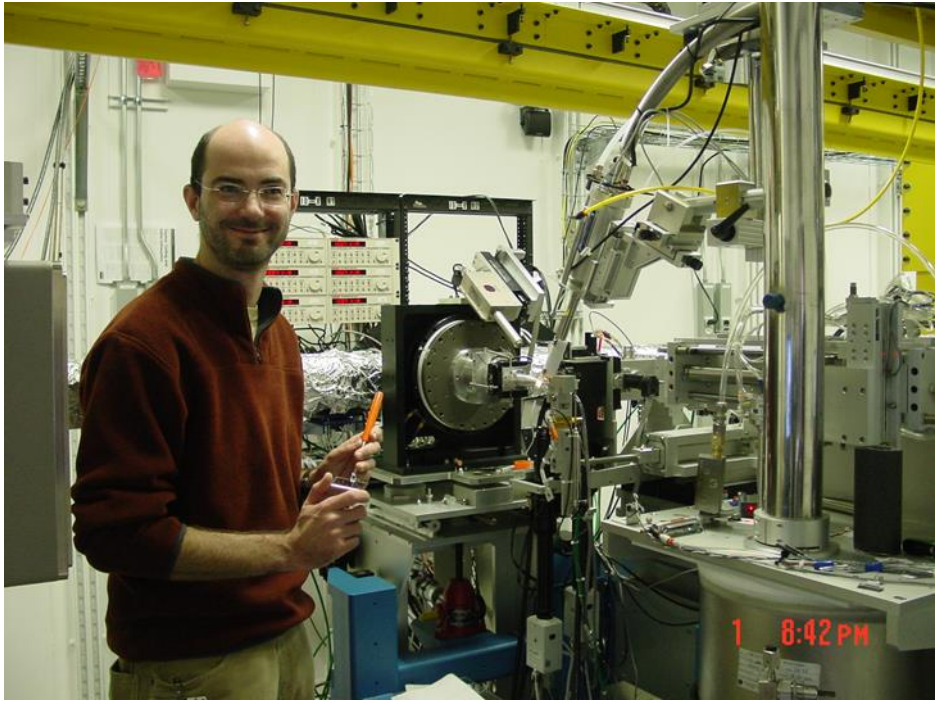
OUTLINE

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

INTRODUCTION

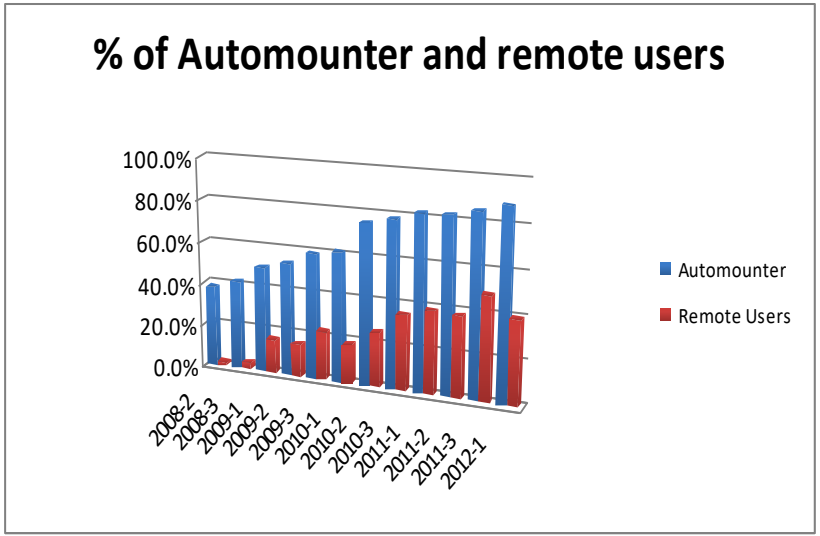
- High-throughput macromolecular crystallography implies:
  - Automated sample handling
  - Automated data collection
  - Automated data processing
- Sample changer is needed for:
  - Automated screening
  - Remote data collection



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

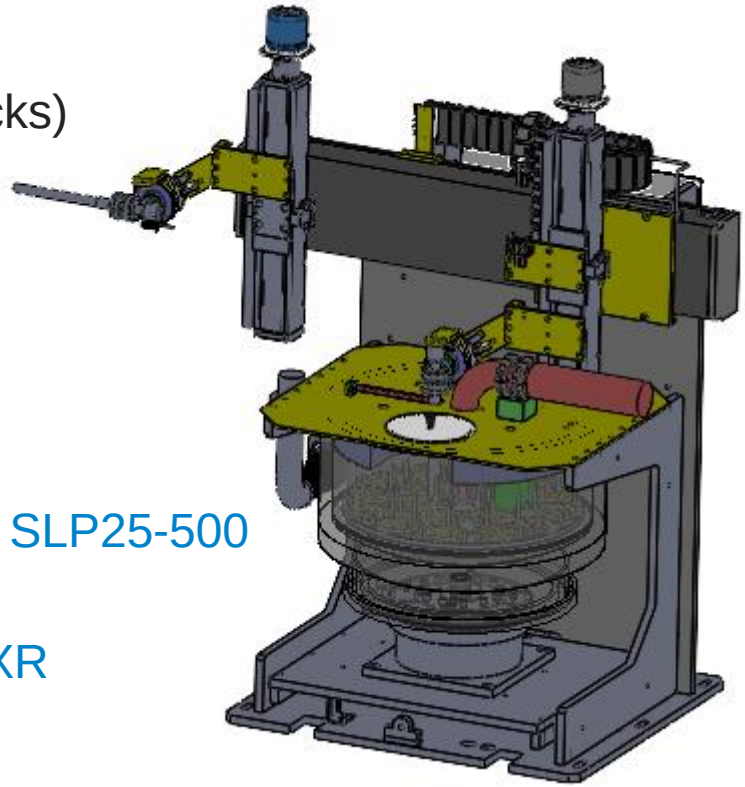
UPGRADE MOTIVATION

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



SELECTING COMPONENTS

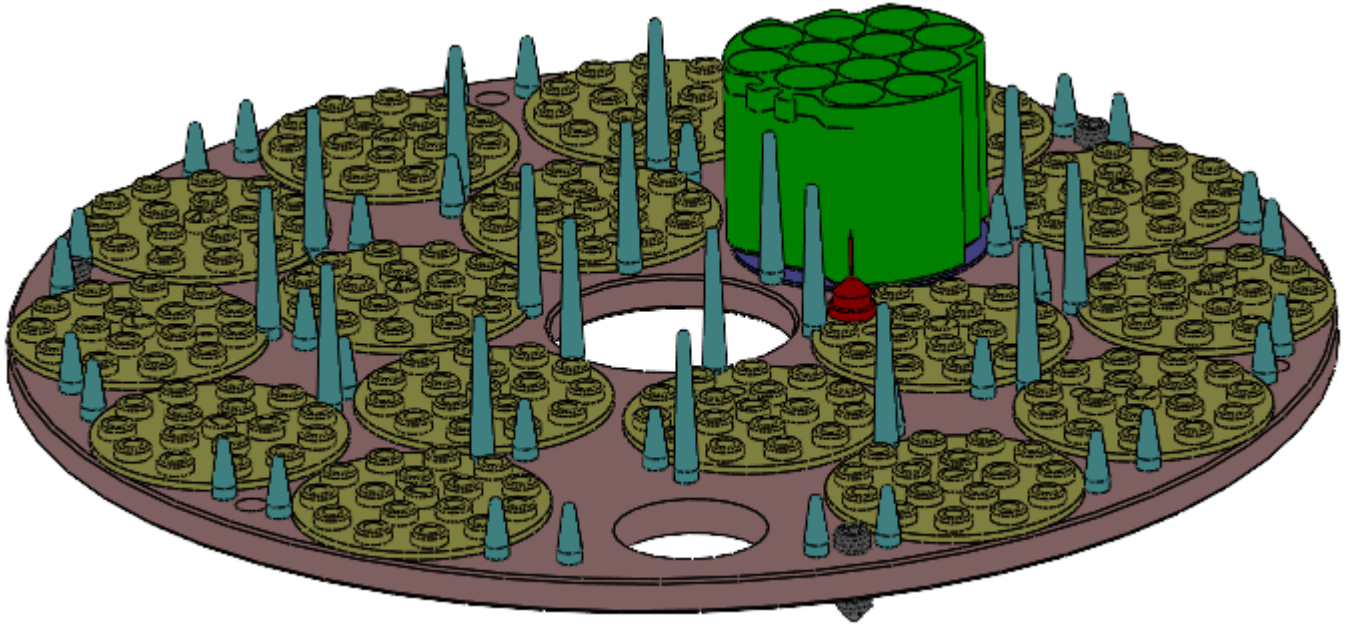
- Dewar capacity:
  - 18 pucks (ALS style, uni-pucks, Rigaku pucks)
  - 288 (216) samples



- 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

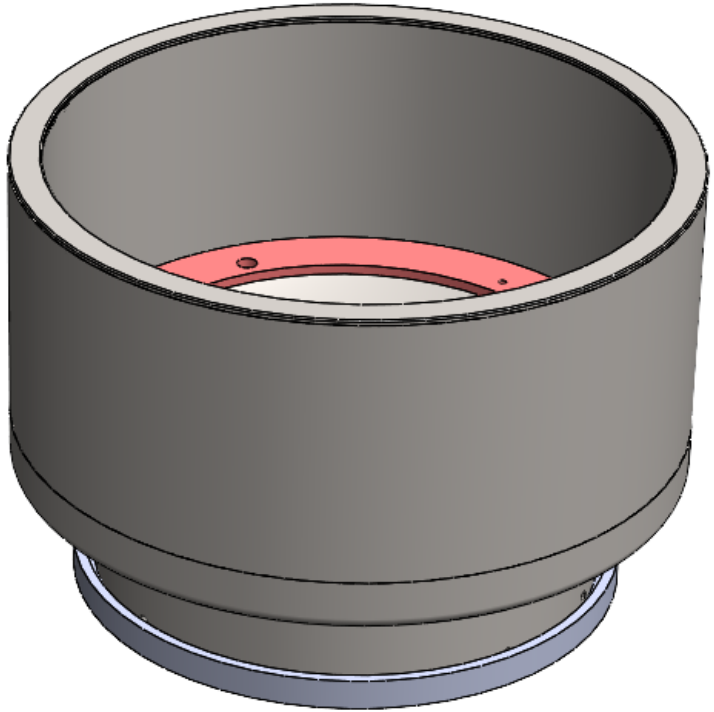
- Dewar base plate:
  - Adjusted with 3 set screws



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.

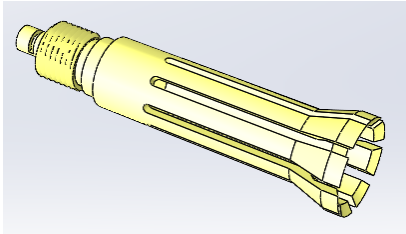


SAMPLE CHANGER UPGRADE

SAMPLE CHANGER UPGRADE

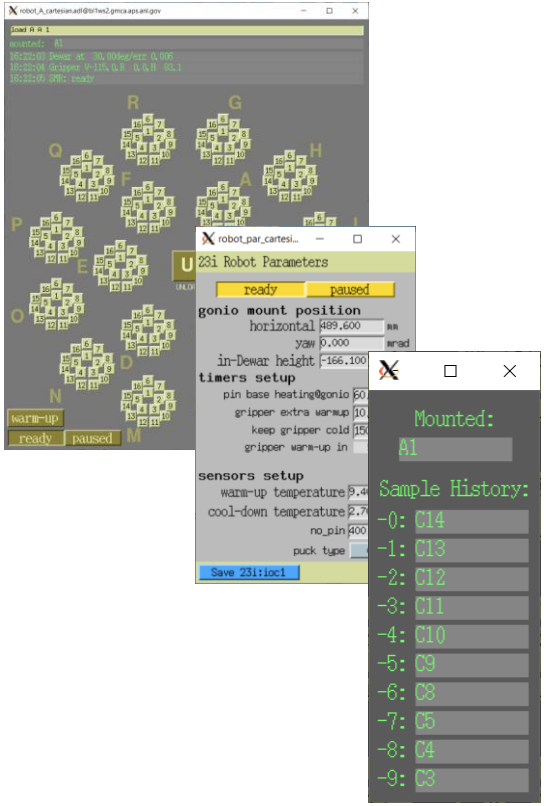
Design highlights

- 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

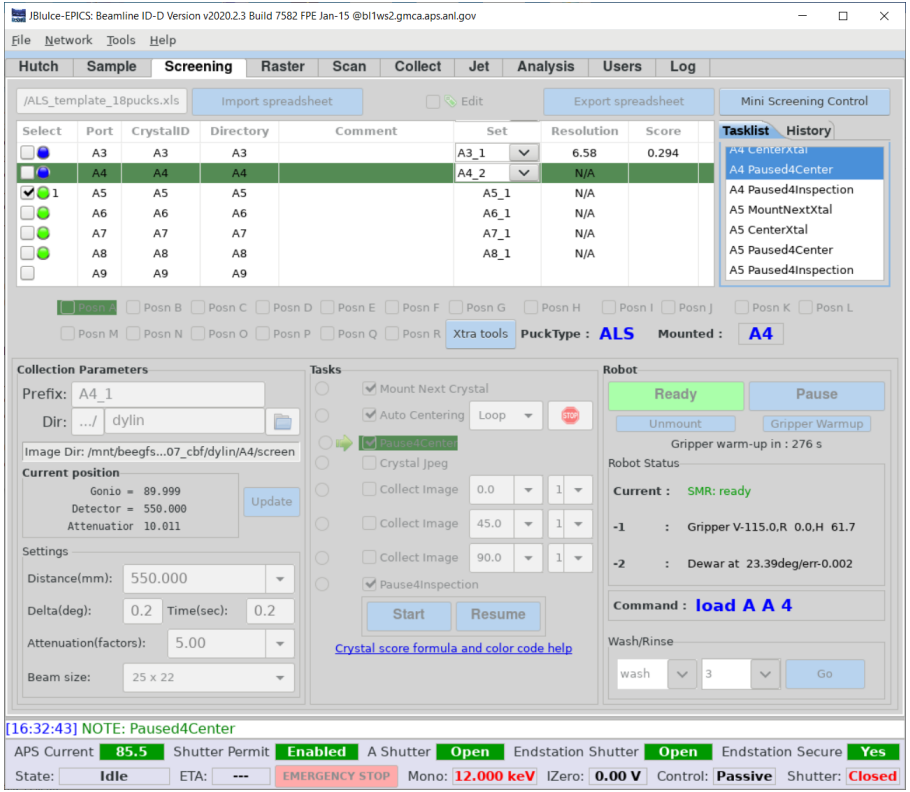
- Sample changer controlled by EPICS server
  - Uses SNL and Sequencer
  - Software runs in three threads:
    - Monitoring
    - State Sequence Set
    - Motion control
- EPICS interface PVs for clients:
  - Command string: <BL>:R:cmd
  - Status string: <BL>:R:sta
  - Sample Mounted string: <BL>:R:mounted



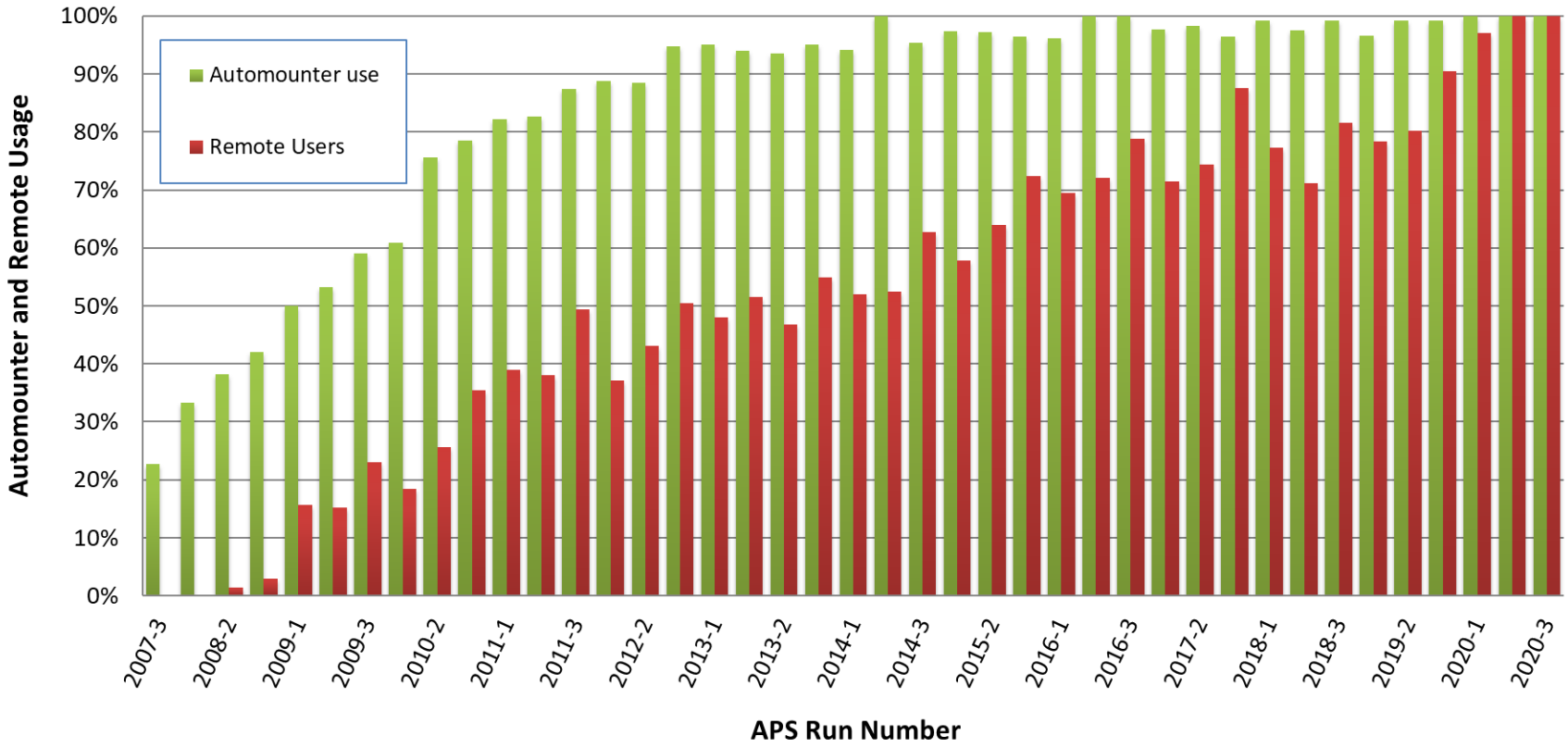
SAMPLE CHANGER EPICS SERVER

jBluIce 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



USAGE STATISTICS



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REFERENCES

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