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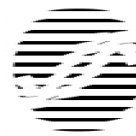
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Integration of sample automounters at GMCA CAT protein crystallography beamlines

Oleg Makarov

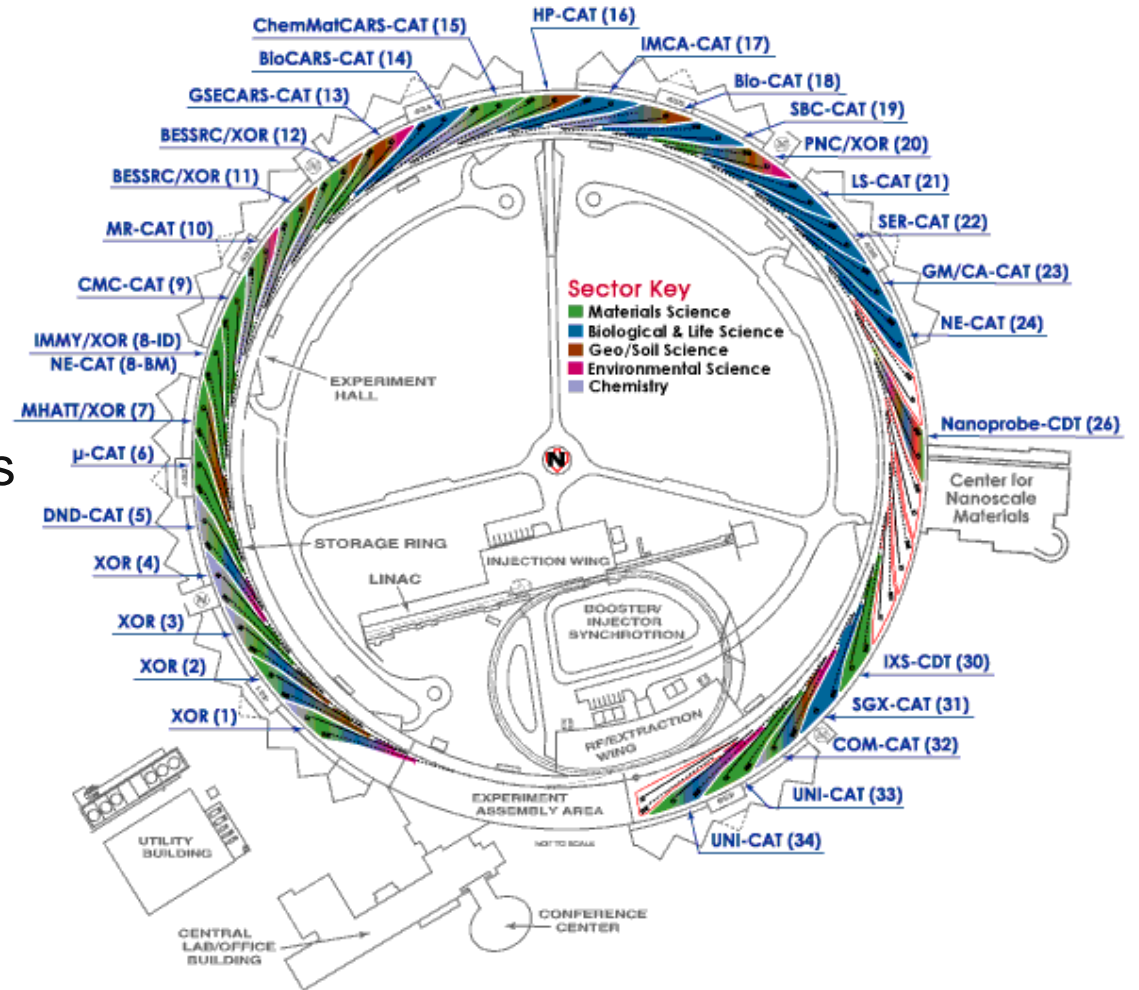
November 5, 2008



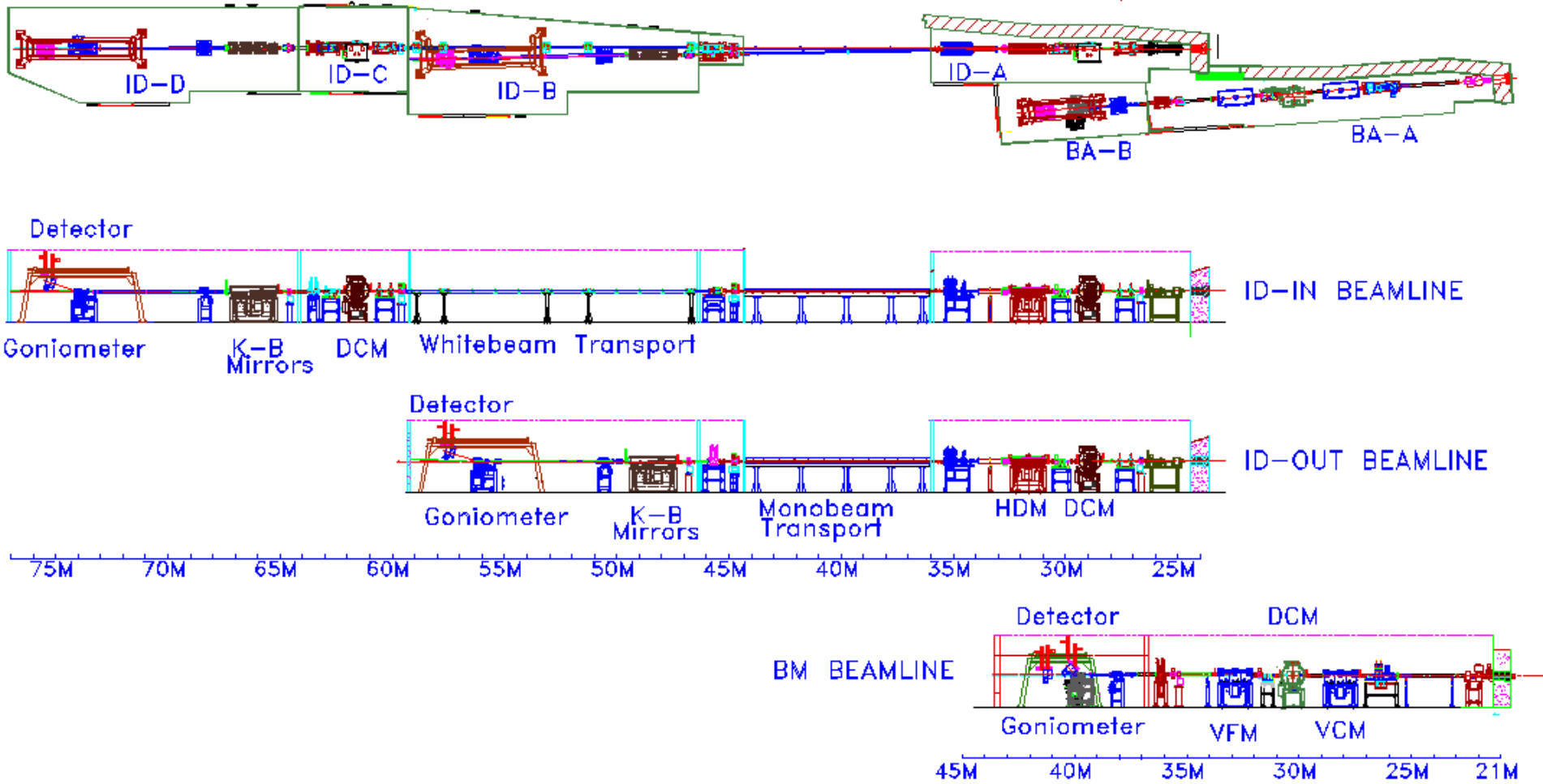
NOBUGS 2008

OUTLINE

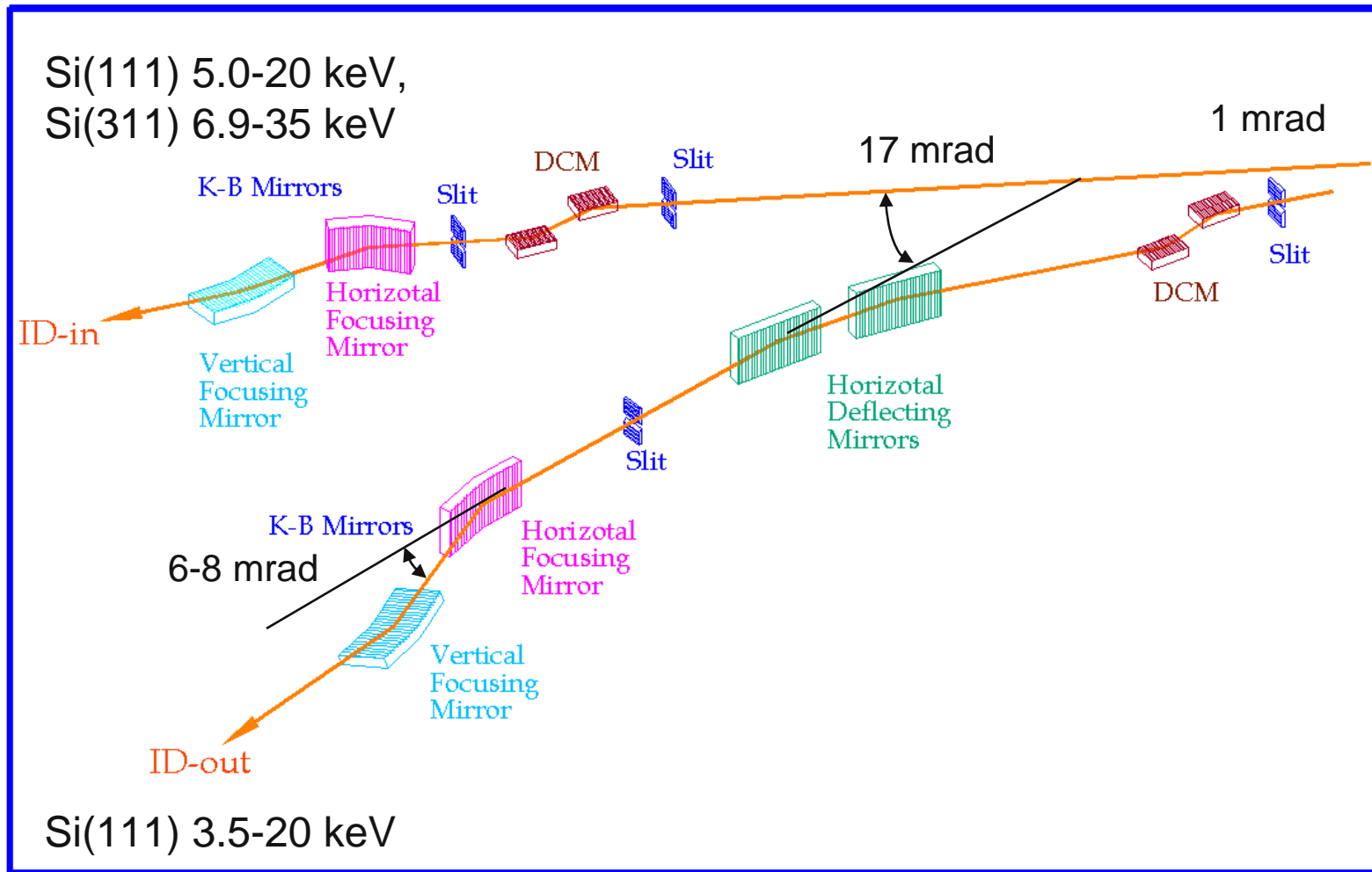
- GMCA Beamlines
- Sample automounters
- Recent hardware upgrades
- Server software
- Client software: MEDM
- Client software: BLU-ICE
- Conclusion
- Future improvements



GMCA beamlines

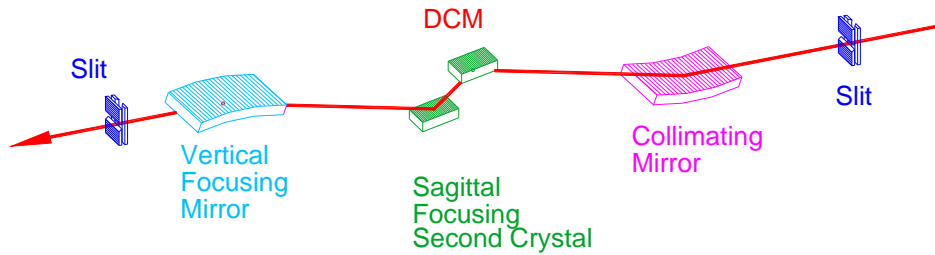


GMCA beamlines: ID

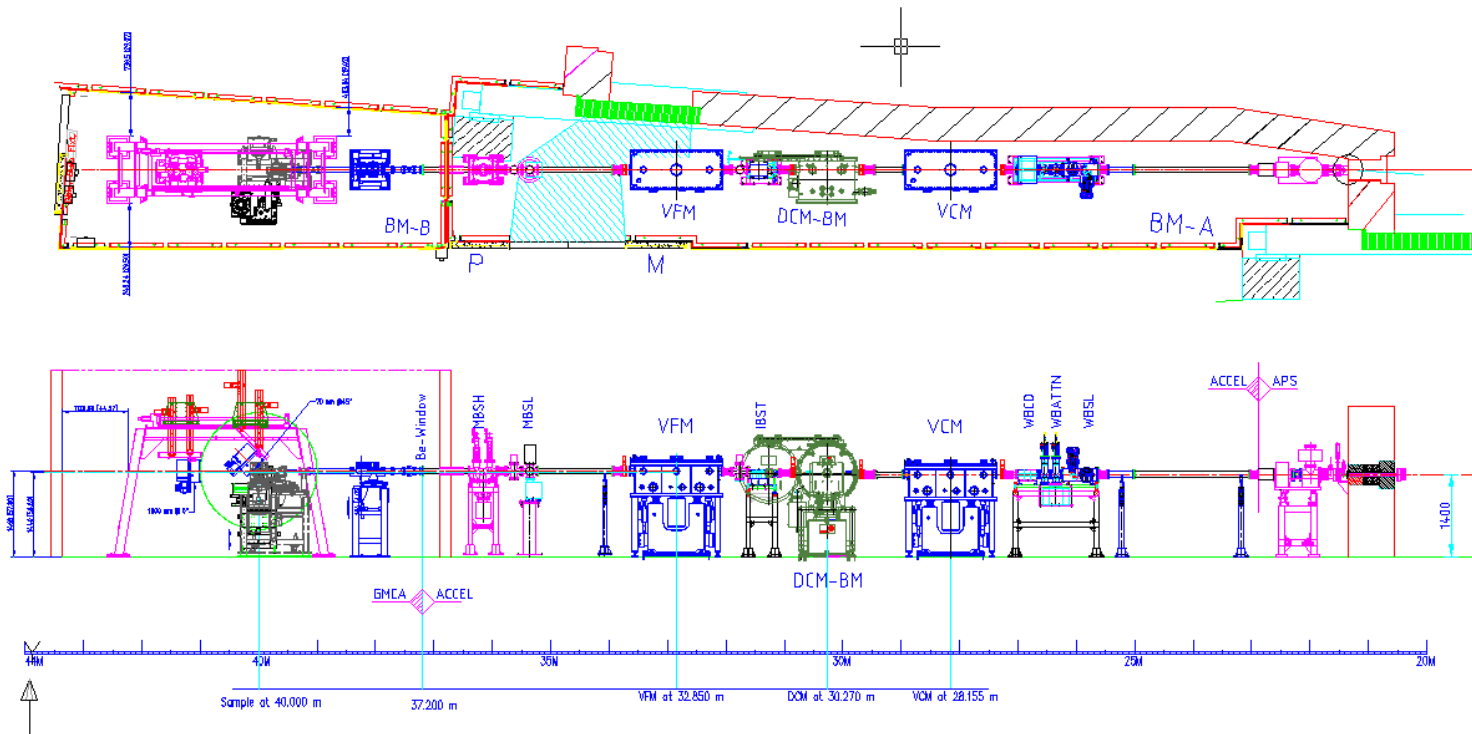


- Two ID beamlines from canted undulators

GMCA beamlines: BM

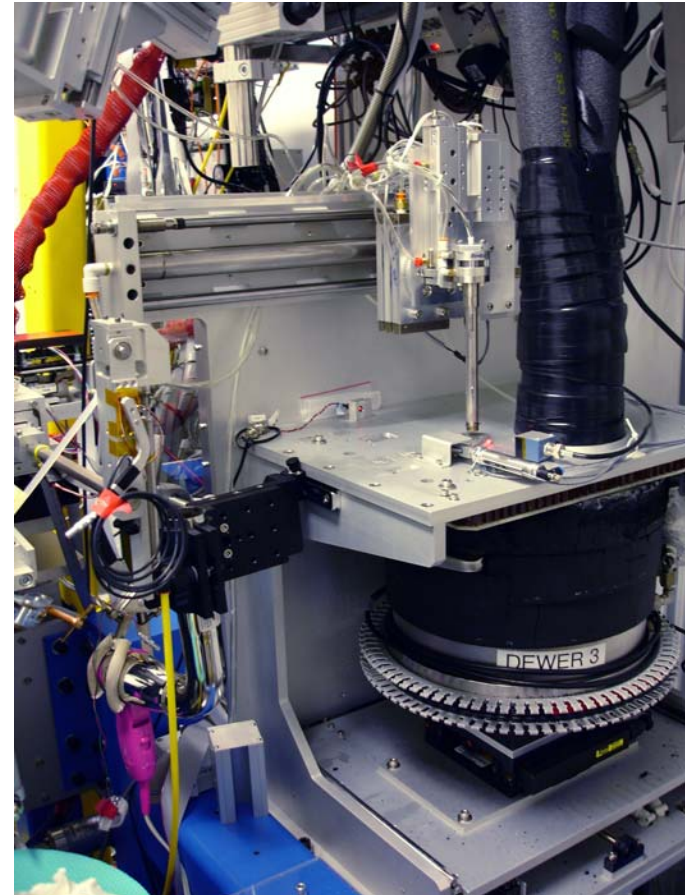
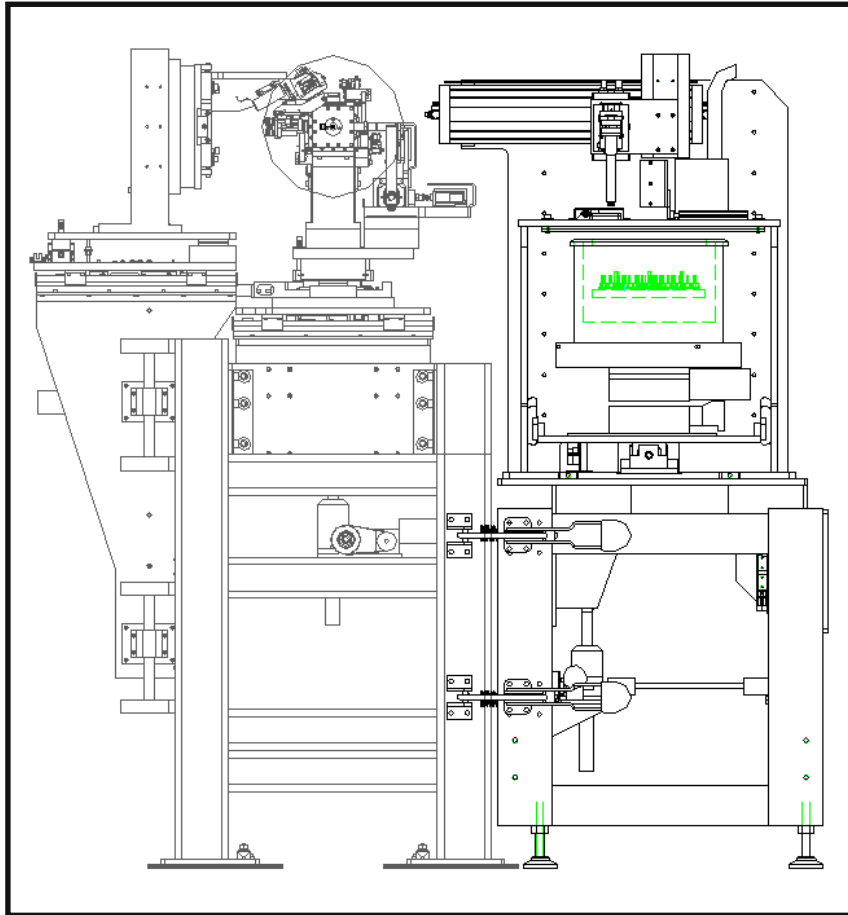


Energy Range: 3.5 – 25 keV
 Flux: $0.5 - 1.2 \times 10^{12}$ photons/sec/100mA
 Focal size: 110 x 150 microns
 Status: commissioning



Sample automounters

Modified LBNL/ALS robot design, collaborated with LR Design.



Recent hardware upgrades

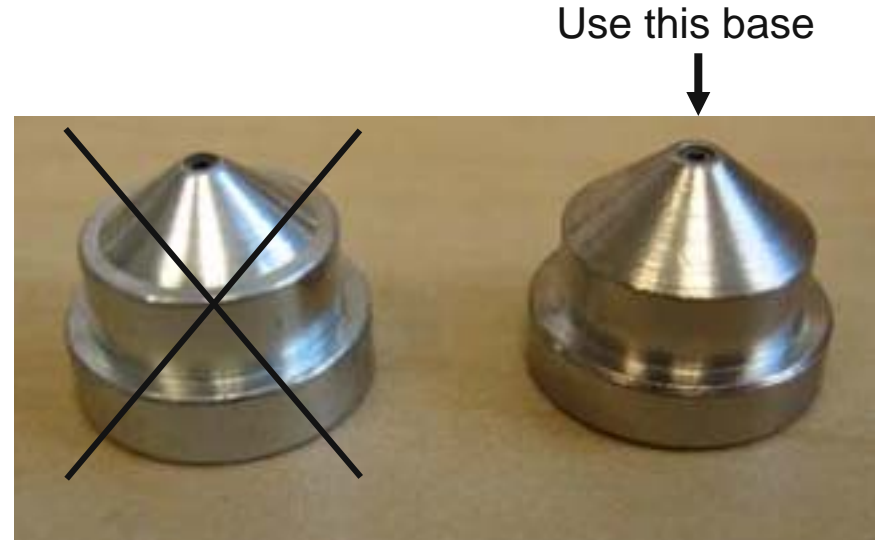


Greenish (background) – current cover over the foam Dewar, Argon filled honeycomb with G10 top and bottom

Blue (foreground) – previous cover over foam Dewar

- Improved Dewar Cover – Ice build-up after 45 minutes

Recent hardware upgrades

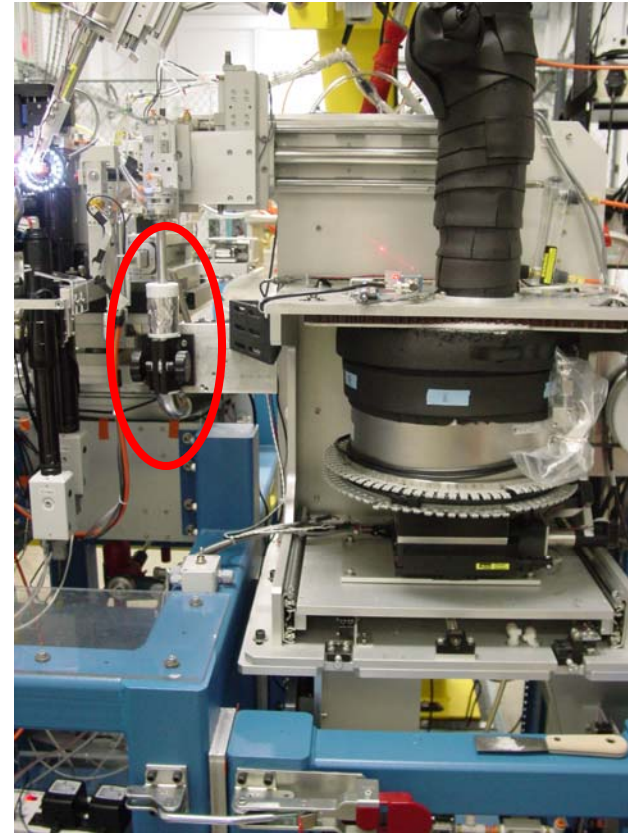
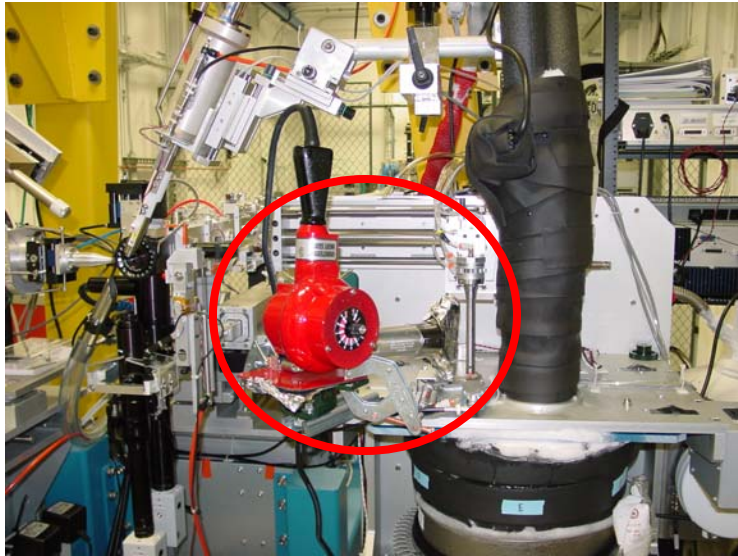


Original Hampton

ALS base

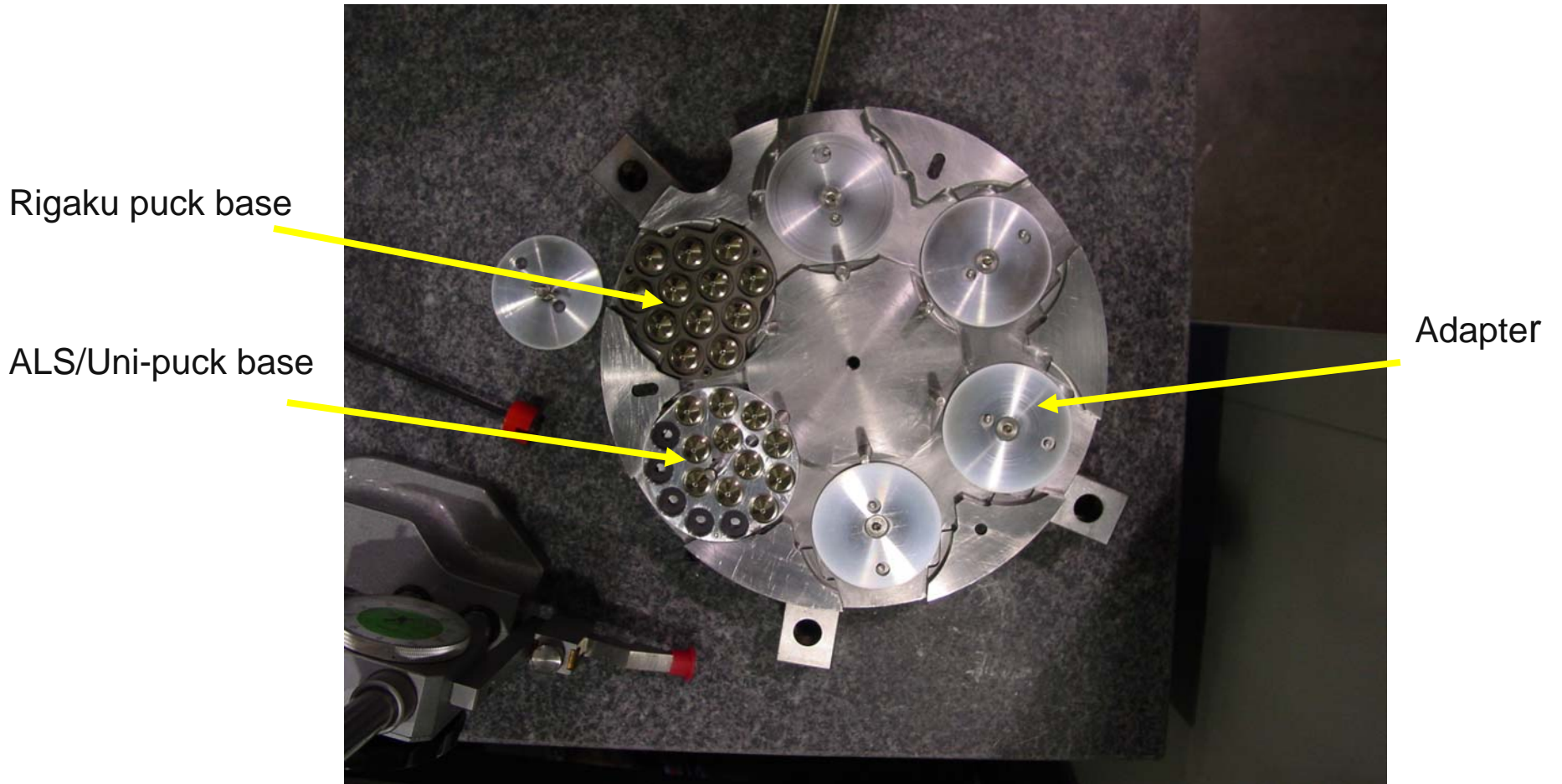
- ***Longer gripper with longer second translation stage allow to keep gripper cold between sample mounts***
- ***Restriction to ALS style Bases : Improved Reliability***

Recent hardware upgrades



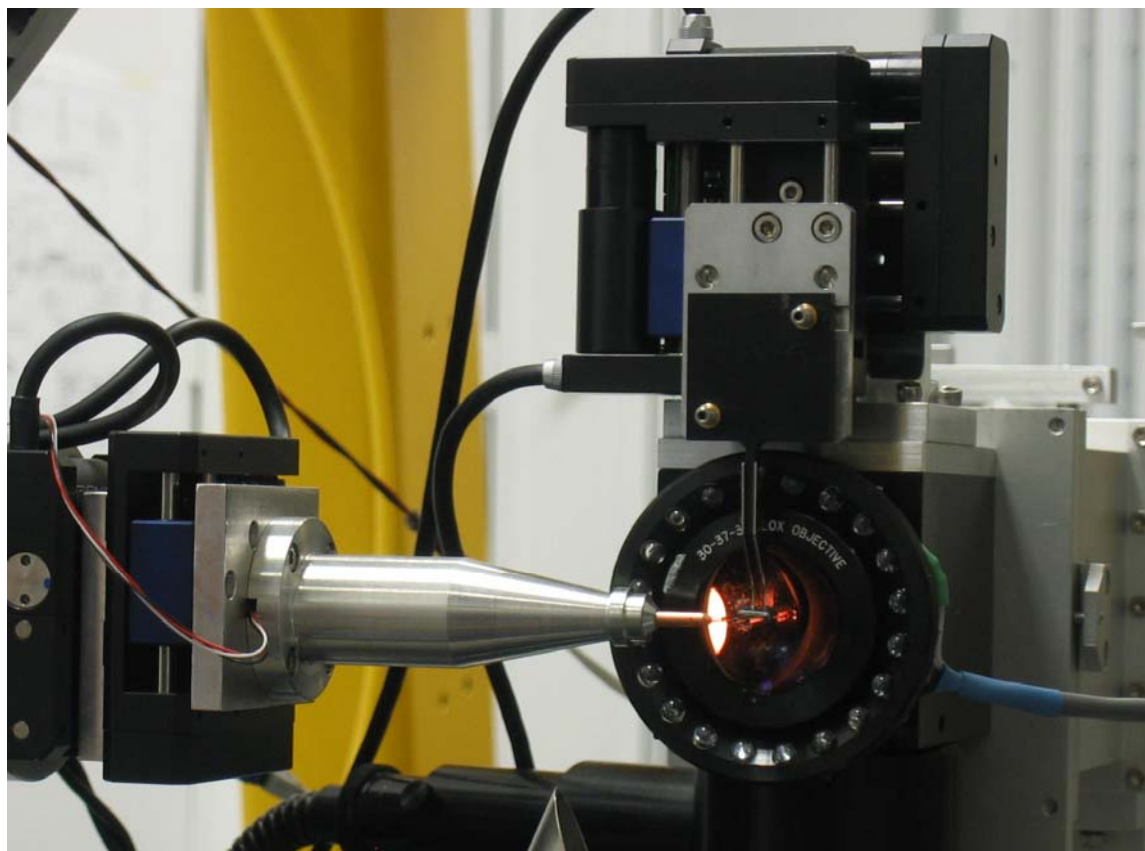
- Side dryer replaced by axial dryer

Recent hardware upgrades



- Universal baseplate for ALS and Rigaku pucks

Recent hardware upgrades



- Pin base sensor on the goniometer

Server software

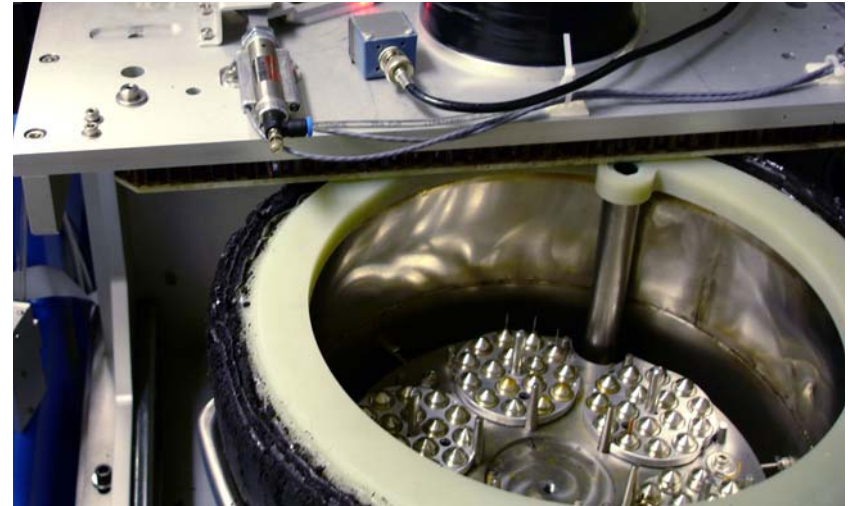
■ EPICS PV strings:

- Automounter command
- Automounter status
- Automounter status history (2 strings)
- Current sample mounted
- Mounted sample history (10 strings)

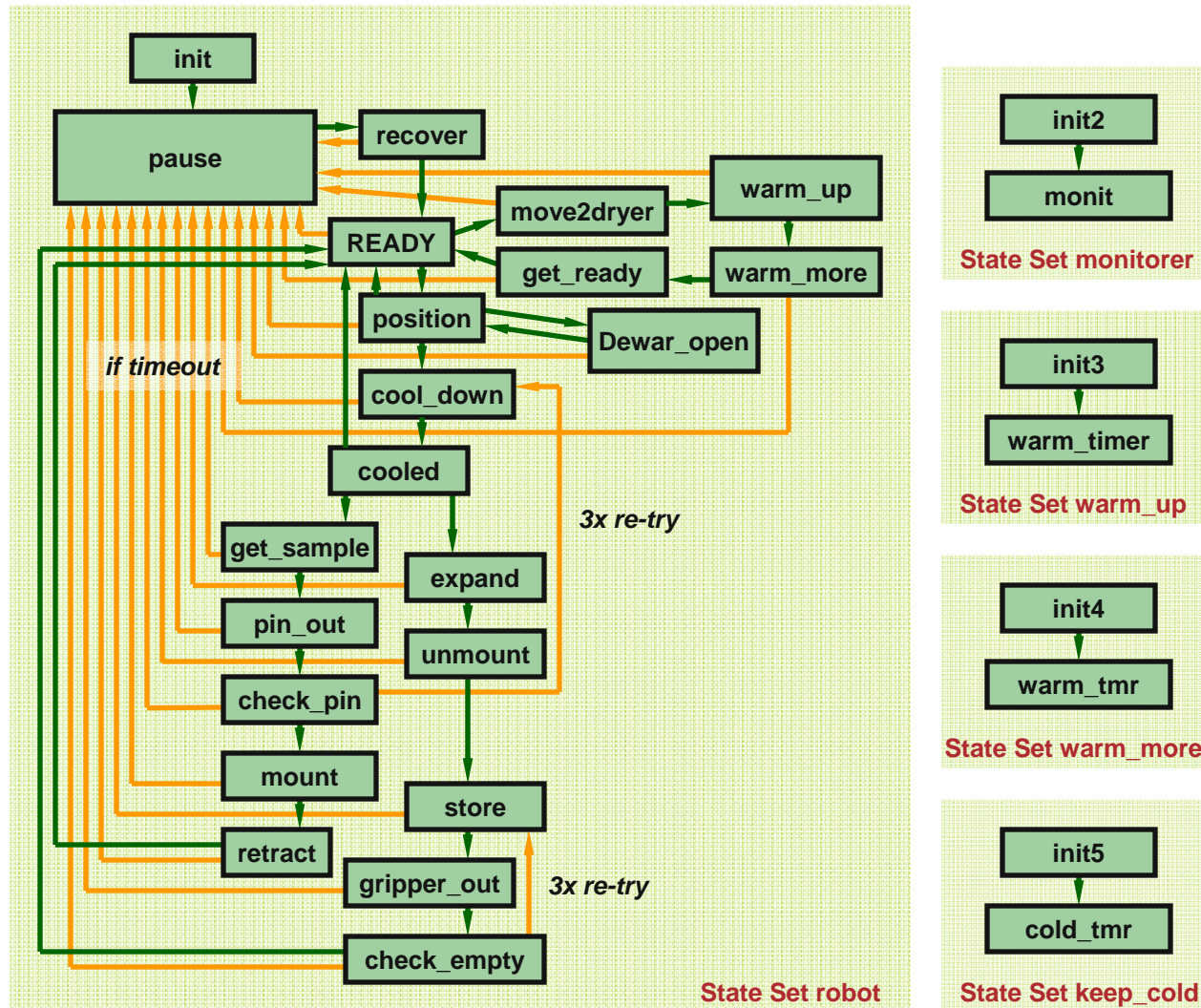
■ Commands

- **load** <Dewar_position> <puck_style> <sample #>
Dewar_position: {A | B | C | D | E | F}
puck_style: {R | A}
sample #: 1..12 for RigakuMSC ACTOR magazine,
1..16 for LBNL/ALS puck and UniPuck
- **unload**
- **unload reset**
- **warm-up**

- **Local switch causes control program to move Dewar between “load” and “home” positions**



Server software



■ Block diagram of the automounter server

Client software: MEDM screens

- Load / unload sample
- Sample mount history
- Robot parameters

The image displays three MEDM (Menu Driven Expert) screens for robot control. The top screen, **robot_A.adl**, shows a status window with the following text: `unload`, `mounted: none`, `00:30:25 starting Rd`, `00:32:46 warm_up, 1 s more`, and `00:32:49 SMR: ready`. Below the text is a large diagram of a 16-point sample mount with points labeled 1 through 16. A central 'U' icon is labeled 'UNLOAD'. The bottom right of the screen has a 'warm-up' button and a 'ready paused' indicator. The middle screen, **robot_R.adl**, shows a similar status window with the same text as robot_A.adl. Below the text is a diagram of a 12-point sample mount with points labeled 1 through 12. A central 'U' icon is labeled 'UNLOAD'. The bottom right of the screen has a 'warm-up' button and a 'ready paused' indicator. The rightmost screen, **robot_par.adl**, is titled '231i Robot Parameters'. It features a 'ready' button (highlighted in yellow) and a 'paused' button. Under 'gonio mount position', there are input fields for 'horizontal' (9.200 mm) and 'yaw' (0.000 mrad). Under 'timers setup', there are input fields for 'pin-base heating@gonio' (120.0 s), 'gripper extra warmup' (10.0 s), and 'keep gripper cold' (1200.0 s). Under 'sensors setup', there are input fields for 'warm-up temperature' (9.500 V), 'cool-down temperature' (2.000 V), and 'no_pin' (0.500 V). A 'puck type' dropdown menu is set to 'ALS'. At the bottom, there are 'Save 231:ioc2' and 'More' buttons.

Client software: MEDM screens

- Digital I/O
- Analog I/O
- Motion control

digital_IO_pmac24_comment.adl (on bl1d1380uj)

23i:pmac21:acc65e: digital I/O

Outputs				Inputs			
0	long horiz.	Off	On	0	long hor. OUTB		
1	pryo-jet UP	Off	On	1	long hor. INB		
2	long vert.	Off	On	2	low: o-jet UP		
3	short horiz./vert.	Off	On	3	low: o-jet DOWN		
4	rotate horiz.	Off	On	4	long vert. UP		
5	grip	Off	On	5	long vert. DOWN		
6	lid open	Off	On	6	short h/v OUTB/UP		
7	blow	Off	On	7	short h/v INB/DOWN		
8	suck	Off	On	8	gripper HORIZ		
9	dryer on	Off	On	9	gripper VERT		
10		Off	On	10	lid OPEN		
11		Off	On	11	lid CLOSED		
12		Off	On	12	req: Dewar to OPEN		
13		Off	On	13	req: Dewar to CLOSE		
14		Off	On	14	no pin on the gonio		

8_ADCs_comment.adl (on bl1d1380upper.gmca.aps.anl.gov)

23i:pmac21:59e ADC

1	9.555	Gripper RTD sensor
2	10.000	Pin base laser sensor
3	0.005	ACC-59E analog in
4	0.000	ACC-59E analog in
5	0.000	ACC-59E analog in
6	0.000	ACC-59E analog in
7	0.000	ACC-59E analog in
8	0.000	ACC-59E analog in

Backup Restore

/home/gmca/epics/stdApp/burt/231_8ADC_pmac21.snap

Move3_large_limits.adl (on bl1d1380upper.gmca.aps.anl.gov)

Robot XYZ position Assembly 23i:RB:Rd:

positioned **Positioned**

execution **Idle**

ready **Ready**

motion **Position**

homed **Homed**

23i:RB:RX: Dewar X (mm) ActPos **-0.000**

23i:RB:RY: Dewar Y (mm) ActPos **-0.000**

23i:RB:RZ: Dewar Z (mm) ActPos **-6.327**

RqsPos 0.000 0.000 -6.327

Tweak < 100.000 > < 0.100 > < 0.100 >

Memory 0.000 0.000 34.162

store recall store recall store recall

Limits -5.000 300.000 -31.000 69.000 0.000 0.000

Act->Rqs

Move1_large_limits.adl (on bl1d1380u)

Robot rotation Assembly 23i:RB:Rr:

positioned **Positioned**

execution **Idle**

ready **Ready**

motion **Position**

homed **Homed**

23i:RB:RA: robot phi (degr) ActPos **0.001**

RqsPos 0.000

Tweak < 30.000 >

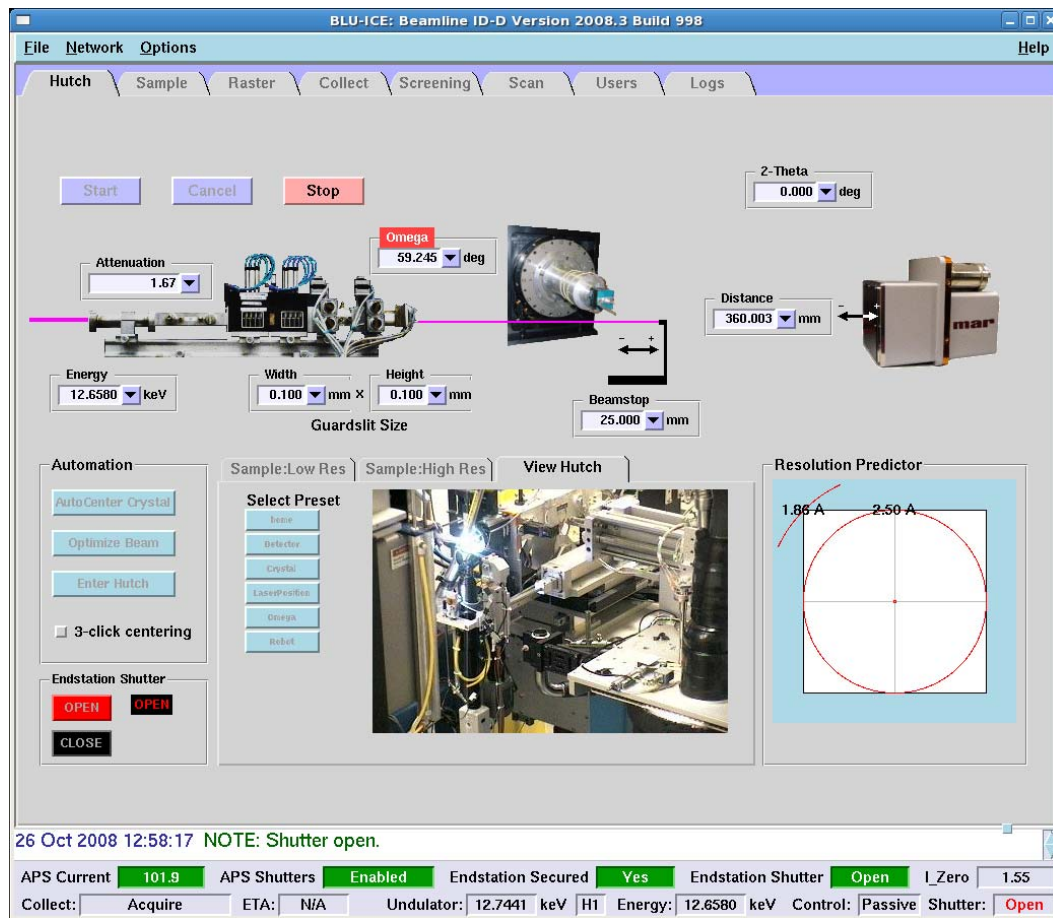
Memory 0.000

store recall

Limits -240.000 120.000

Act->Rqs

Client software: Blu-Ice



SSRL's Blu-Ice GUI adapted to EPICS control environment

- Single window GUI
- Multiple tubs
 - Hutch
 - Sample
 - Raster
 - Collect
 - Screening
 - Scan
 - Users
 - Logs

Client software: Blu-Ice

BLU-ICE: Beamline ID-D Version 702

File Network Options Help

Hutch Sample Collect **Screening** Scan Users Setup

Spreadsheet: Distance: mm B-warmup: sec

Automounter status
 Current: cool_down, 9.971V > 2.500V
 -1: unloading current sample
 -2: ready
 Command: load A 2

None	Load	Port	ID	Protein	Comment	Directory	Freezing
0	<input type="checkbox"/>	A	1	Protein1		Dir1	
1	<input type="checkbox"/>	A	2	Protein2		Dir2	
2	<input type="checkbox"/>	A	3	Protein3		Dir3	
3	<input type="checkbox"/>	A	4	Protein4		Dir4	
4	<input type="checkbox"/>	A	5	Protein5		Dir5	
5	<input type="checkbox"/>	A	6	Protein6		Dir6	
6	<input type="checkbox"/>	A	7	Protein7		Dir7	
7	<input type="checkbox"/>	A	8	Protein8		Dir8	
8	<input type="checkbox"/>	A	9	Protein9		Dir9	
9	<input type="checkbox"/>	A	10	Protein10		Dir10	
10	<input type="checkbox"/>	A	11	Protein11		Dir11	
11	<input type="checkbox"/>	A	12	Protein12		Dir12	
12	<input type="checkbox"/>	A	13	Protein13		Dir13	
13	<input type="checkbox"/>	A	14	Protein14		Dir14	
14	<input type="checkbox"/>	A	15	Protein15		Dir15	
15	<input type="checkbox"/>	A	16	Protein16		Dir16	
16	<input type="checkbox"/>	B	1	Protein17		Dir17	

Task list
 Mount Next Crystal
 AutoCenter Crystal
 Pause4Center
 Collect Image:
 Collect Image:
 Collect Image:
 Pause4Inspection
 Analyse with Web-Ice

Sample status
 Mounted: A 1

 Mount history:
 -0: A 1
 -1: F 4
 -2: F 3
 -3: F 2
 -4: F 1
 -5: C 1
 -6: B 10
 -7: B 9
 -8: B 8
 -9: C 16
 Puck type: ALS

Directory:

12 Feb 2008 10:34:31 NOTE: Crystal list updated

Collect: ETA: Undulator: keV Energy: keV Control: Shutter:

Screening tab

- Sample spreadsheet
- Task list
- Automounter status
- Sample status
- Activity log

Conclusion

Beamline	Fall 07	Winter 08	Summer 08
23ID-D, % of users (ALS pucks)	44%	45%	56%
Groups Scheduled	34	33	34
Robot Users	15	15	19
23ID-B, % of users (Rigaku/ALS pucks)	3%	21%	21%
Groups Scheduled	30	29	34
Robot Users	1	6	7
Combined Total (%)	25%	34%	38%
Robot user/Total	16/64	21/62	26/68

- Summer 2008 Trimester
 - D-hutch robot – 98.8% success rate for 1916 samples mounted.
 - B-hutch robot – 94.4% success rate for 144 samples mounted.
- Since December 2006, when the first sample automounter was commissioned, there has been a steady growth in the number of research groups that use it. In the most recent run 2008-02 (June 10 through August 12) the 23ID-D beamline automounter was used by 56% of the research groups with a 99% success rate in sample mounts and dismounts.

Future improvements

- Replace pneumatic driven stages by servo-motor driven stages
 - easy switching between different pin lengths
 - reduce level of vibrations
 - reduce time per sample mount / dismount

- Develop a new gripper with an electromagnet
 - more reliable: no moving parts

- Automate alignment procedure by using gripper-held sensors
 - faster and more precise alignment

- Add a bar code reader
 - sample identification convenience

Thanks to

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- Thomas Earnest
- Jim O'Neill

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NIGMS, NCI

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