

High-Capacity Sample Automation for Diamond MX

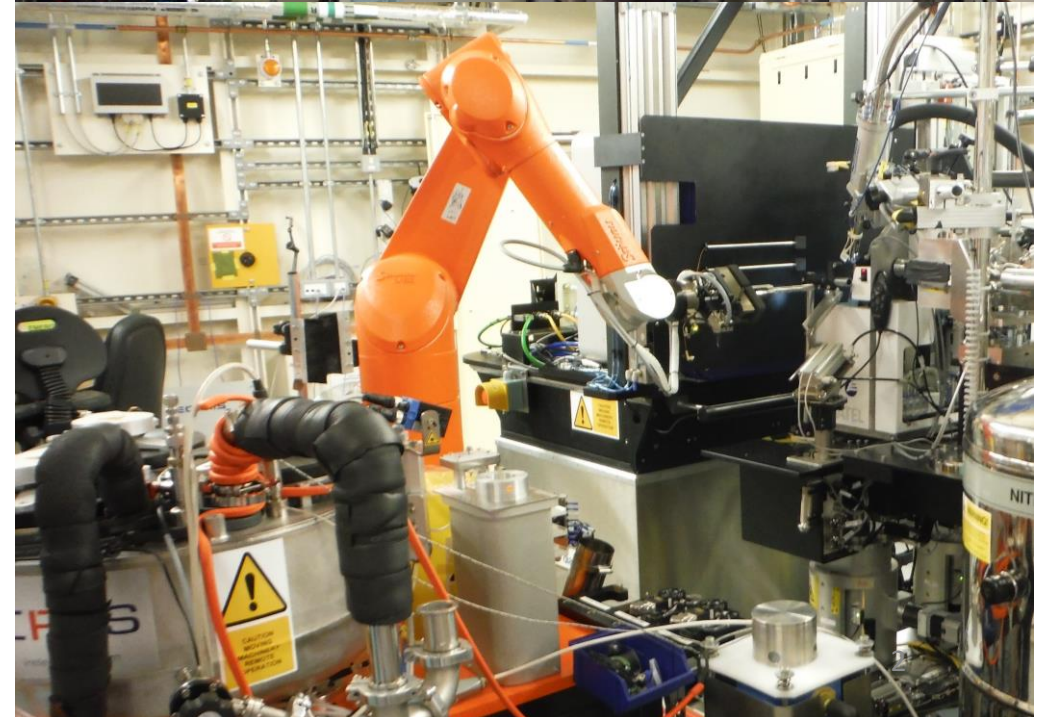
Mark Williams

Automation Scientist, Diamond Light Source

dls.mx

Pre-2015 Scenario

- I02, I03, I04:
 - Rigaku Actor system
 - Mitsubishi robot arm
 - 2 dewars, each with 5 unipucks of 16 samples
 - 160 samples total
- I04-1, I24:
 - Irelec CATS system
 - Staubli robot arm
 - 9 unipucks
 - 144 samples total

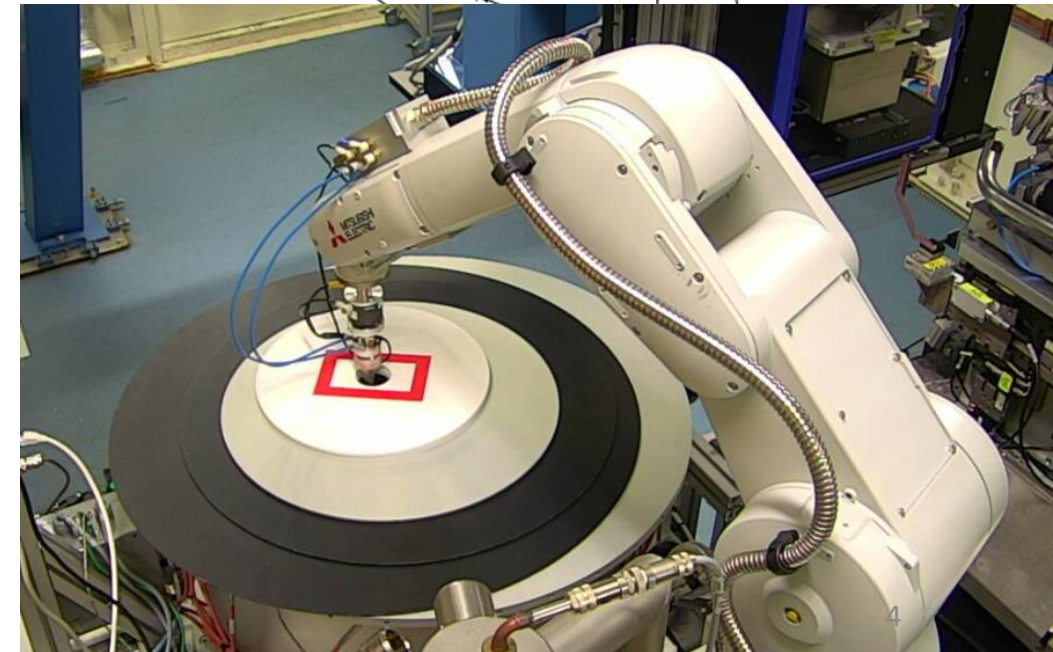
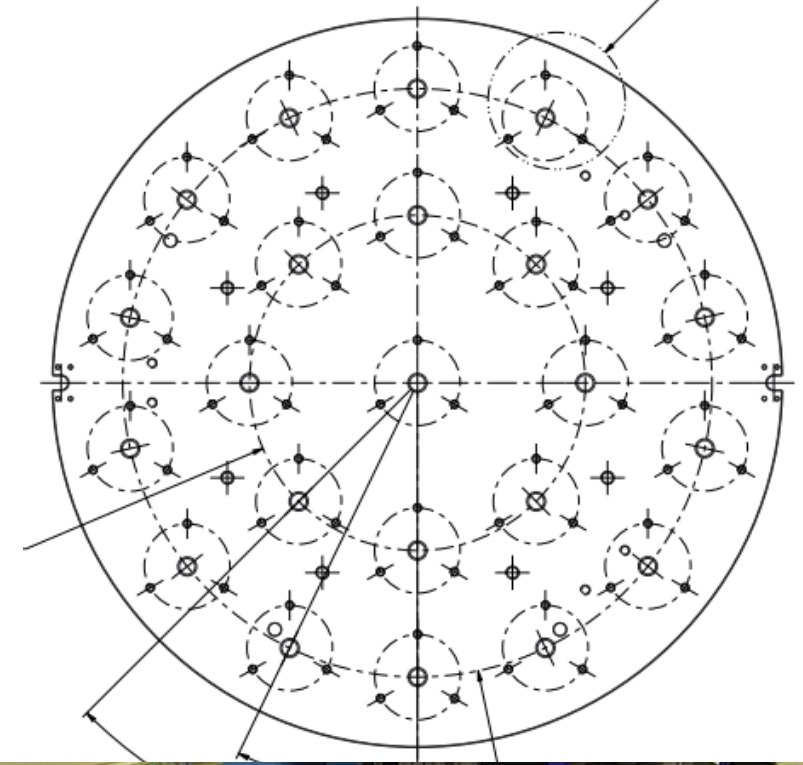


Pre-2015 Scenario

- 2 different robot systems to support
 - In house knowledge was wide but shallow
- 2 companies to deal with for upgrades and maintenance
- Improvements are slow and costly
- Very poor integration with Diamond software
 - EPICS completely bypassed
 - Dependent on API's provided by OEMs
- 30s+ exchange time
- 95s dry time
- Slow to recover from errors
- No space for capacity increases

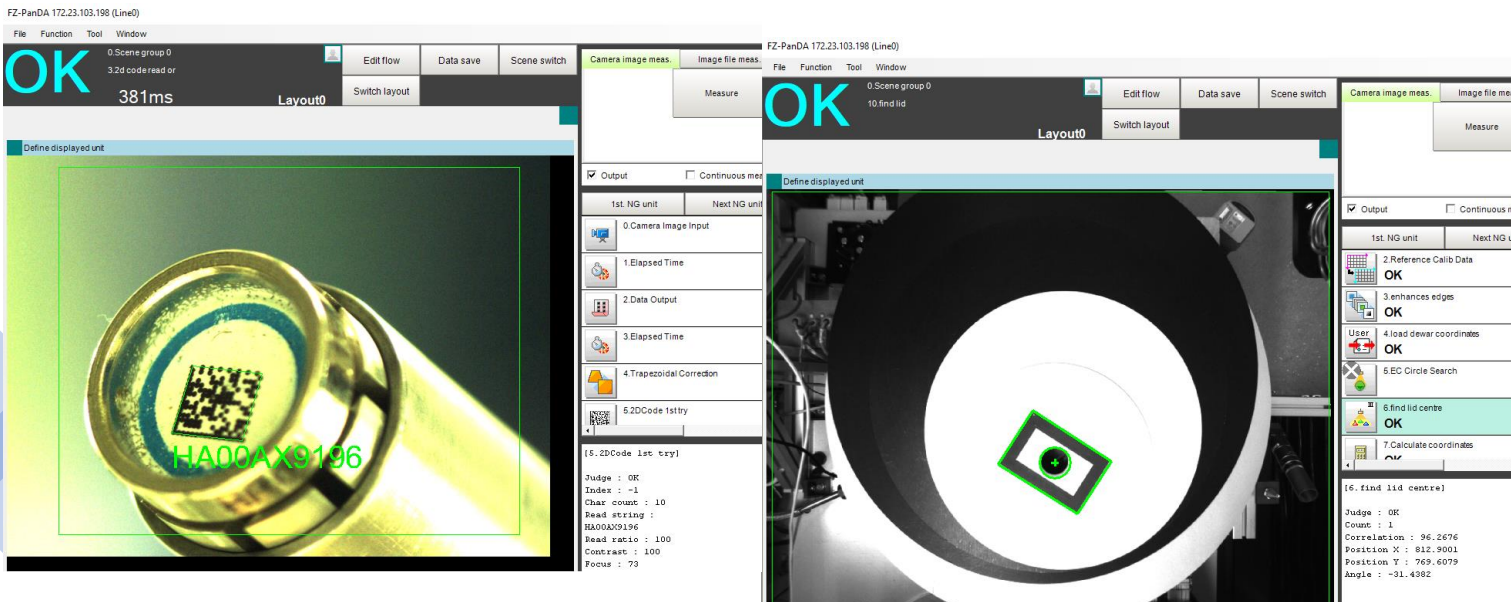
Improvements – Hardware - Stage 1

- First purchase – large Dewar
 - Manufactured by Cryotherm
 - Designed at DESY for 23 unipucks, 368 samples
- New longer robot arm needed
 - Used Mitsubishi arm procured, used with existing controller
- Omron PLC controller for all the I/O
 - Built up organically as new needs identified
- LN2 fill control box discarded
 - Dewar would overfill regularly
 - Brought control onto the PLC



Improvements – Hardware – Stage 1

- Overhead camera needed to locate hole in Dewar lid
 - Omron vision system controls
 - Added another camera to read pin barcodes



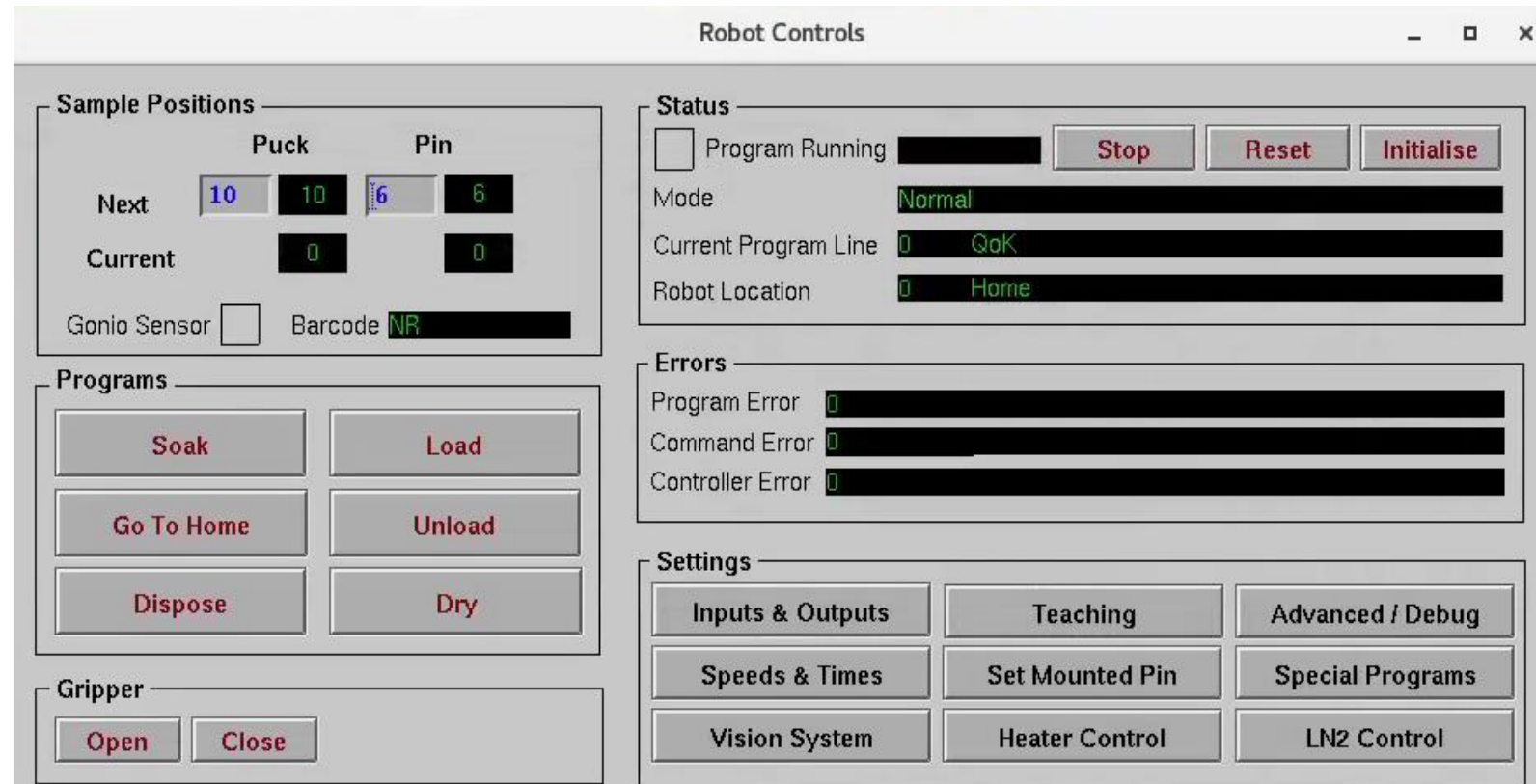
Improvements – Mitsubishi layer

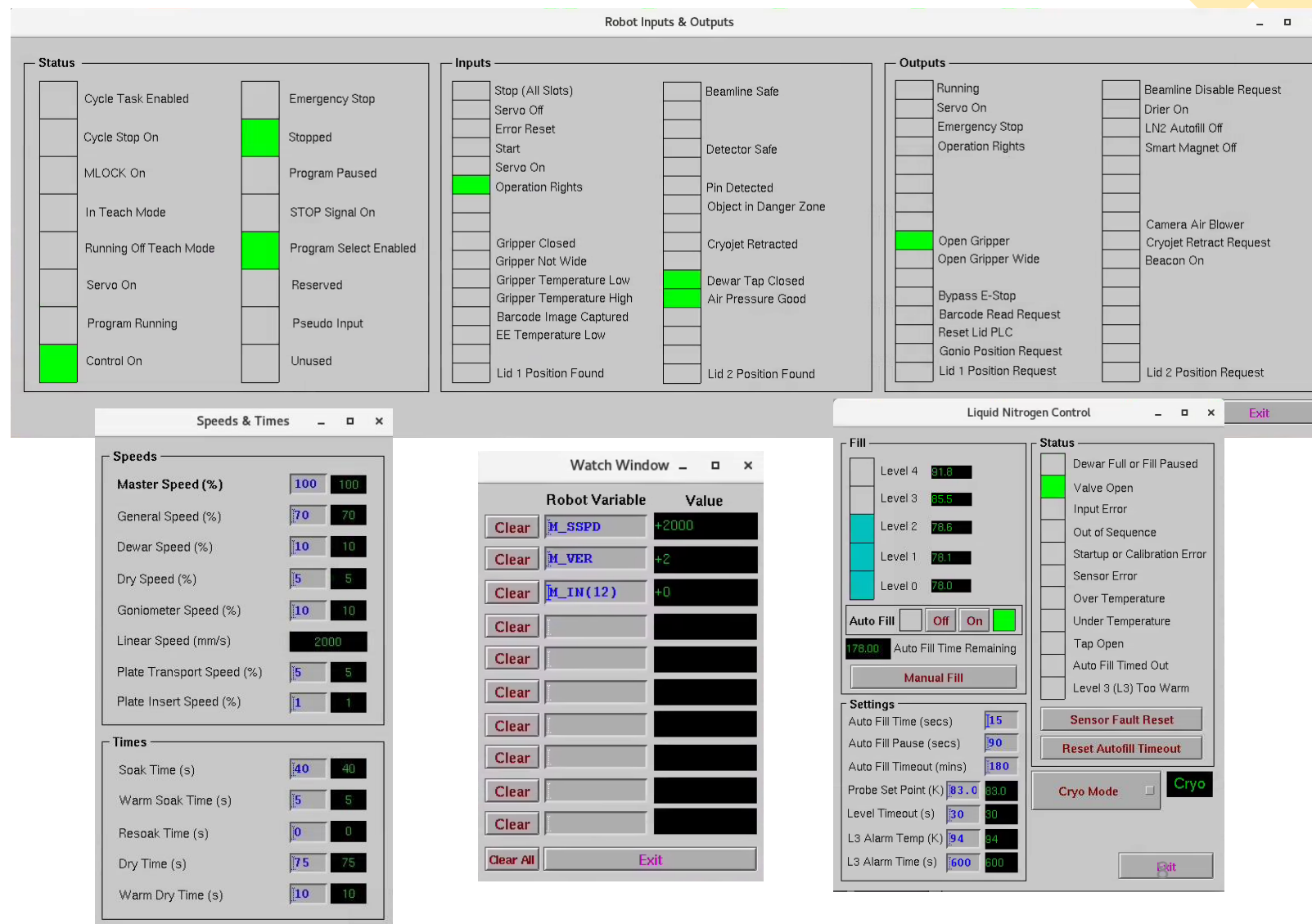
- Mitsubishi programs rewritten from scratch
 - MELFA BASIC V
 - Hierarchical structure
- All pin positions calculated once then stored
- Same code across multiple beamlines
 - Different setups accommodated via config program
- Movement speeds, times etc set as variables
- Knowledge in house

XYZ	X	Y	Z	A	B	C
P_PIN(1,13)	-573.130	-244.140	79.300	180.000	0.000	0.000
P_PIN(1,14)	-587.960	-244.410	79.300	180.000	0.000	0.000
P_PIN(1,15)	-600.570	-236.630	79.300	180.000	0.000	0.000
P_PIN(1,16)	-606.970	-223.260	79.300	180.000	0.000	0.000
P_PIN(2,1)	-659.810	-184.030	79.210	180.000	0.000	0.000
P_PIN(2,2)	-647.550	-176.770	79.210	180.000	0.000	0.000
P_PIN(2,3)	-636.860	-186.210	79.210	180.000	0.000	0.000
P_PIN(2,4)	-642.510	-199.270	79.210	180.000	0.000	0.000
P_PIN(2,5)	-656.710	-197.940	79.210	180.000	0.000	0.000
P_PIN(2,6)	-672.830	-178.390	79.210	180.000	0.000	0.000
P_PIN(2,7)	-663.350	-167.000	79.210	180.000	0.000	0.000
P_PIN(2,8)	-649.210	-162.540	79.210	180.000	0.000	0.000
P_PIN(2,9)	-634.910	-166.430	79.210	180.000	0.000	0.000
P_PIN(2,10)	-624.980	-177.440	79.210	180.000	0.000	0.000
P_PIN(2,11)	-622.600	-192.060	79.210	180.000	0.000	0.000
P_PIN(2,12)	-628.480	-205.660	79.210	180.000	0.000	0.000
P_PIN(2,13)	-640.770	-213.930	79.210	180.000	6 0.000	0.000
P_PIN(2,14)	-655.600	-214.230	79.210	180.000	0.000	0.000

Improvements – Epics layer

- Mitsubishi provided the communications protocol documentation
- StreamDevice used to bring into EPICS
- Rapid updating over TCP/IP Ethernet
- Basic top level GUI with main programs and status
- Knowledge in house





Improvements – Epics layer – Teaching Screen

- Controls for moving the robotic arm
- Can store positions from the robot arm
- Can manually edit positions (with care)
- Very fast, only loads / saves changed positions

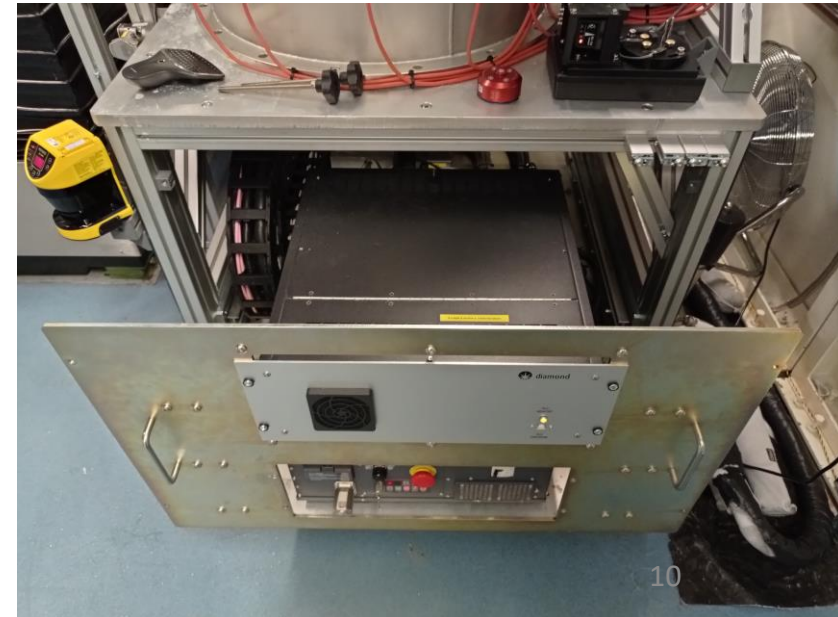
The screenshot shows a 'Teach Mode' window with the following sections:

- Program Control:** Includes buttons for 'Load Positions', 'Save Positions', and 'Undo All Changes'. A 'Large Mode' button is also present in the top right.
- Direct Execution:** Includes buttons for 'Servo On', 'Servo Off', and 'Reset Alarm'. Below these is a 'Master Speed (%)' control with a numeric input set to 10 and a green '10' display.
- Teaching:** This section contains a 'Position Name' field with 'P_HOME' entered. Below it are two rows of coordinate inputs (X, Y, Z, L1, F1, A, B, C) with numerical values. The top row shows values like X: -250.00, Y: 5.00, Z: 400.00, L1: 0.00, F1: 7.00, A: 180.00, B: 0.00, C: 0.00. The bottom row shows the same values but with some inputs highlighted in blue, indicating they are being edited. At the bottom of this section are 'Get Current Positions' and 'Set Positions' buttons.

At the very bottom of the window are two large buttons: 'Save & Exit' and 'Undo & Exit'.

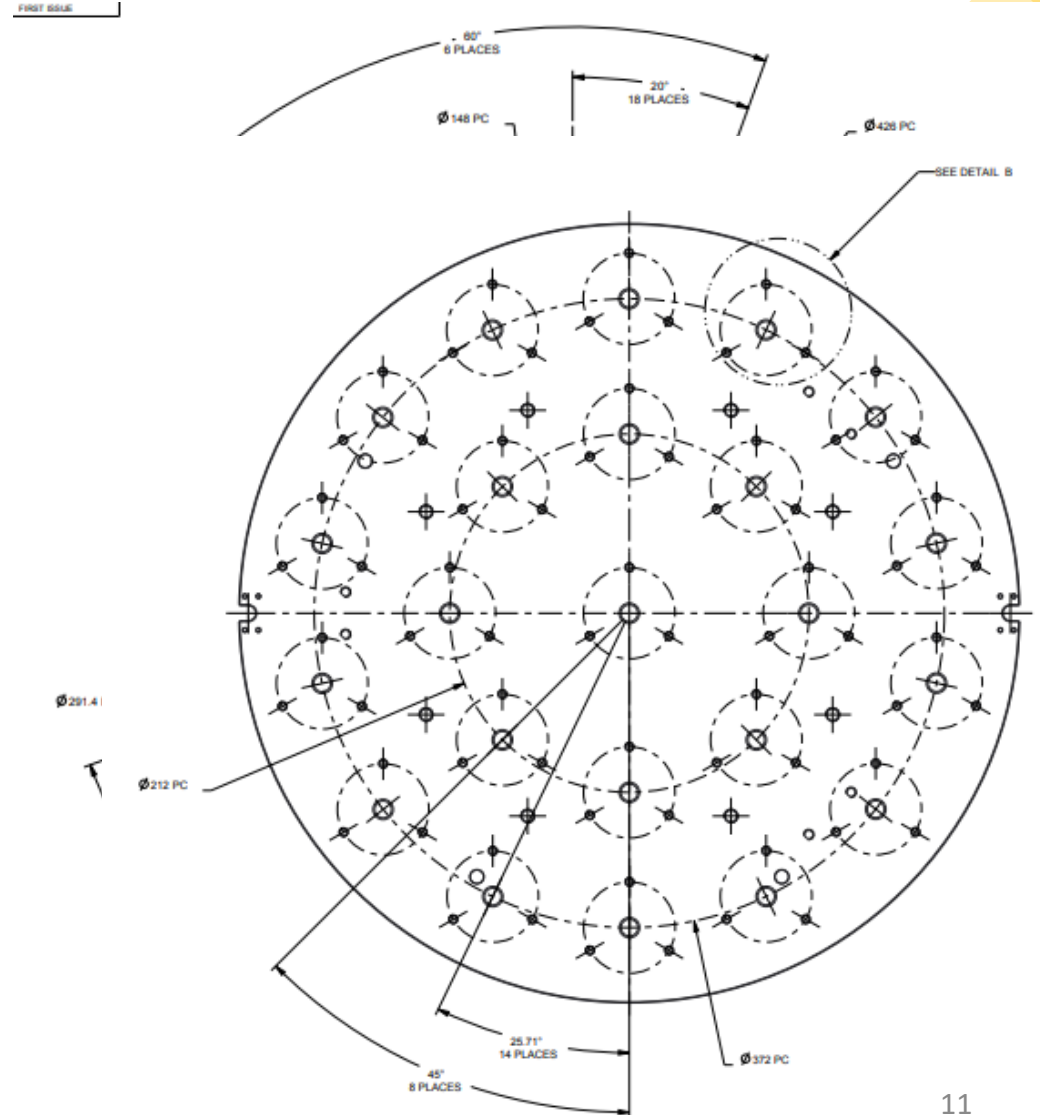
Improvements – Hardware – Stage 1 (ctd)

- Compressed air drier
 - Dry times reduced from 95s to 30s
- Whole system built onto a tabletop
 - Robot controller and PLC controller via accessible drawer
 - Electrical connectors all on one panel
- Keyence Laser scanner to stop robot if anyone approaches
 - Alternatively use the hutch locked signal
- Deployed on 103 Jan 2015



Improvements – Hardware – Stage 2

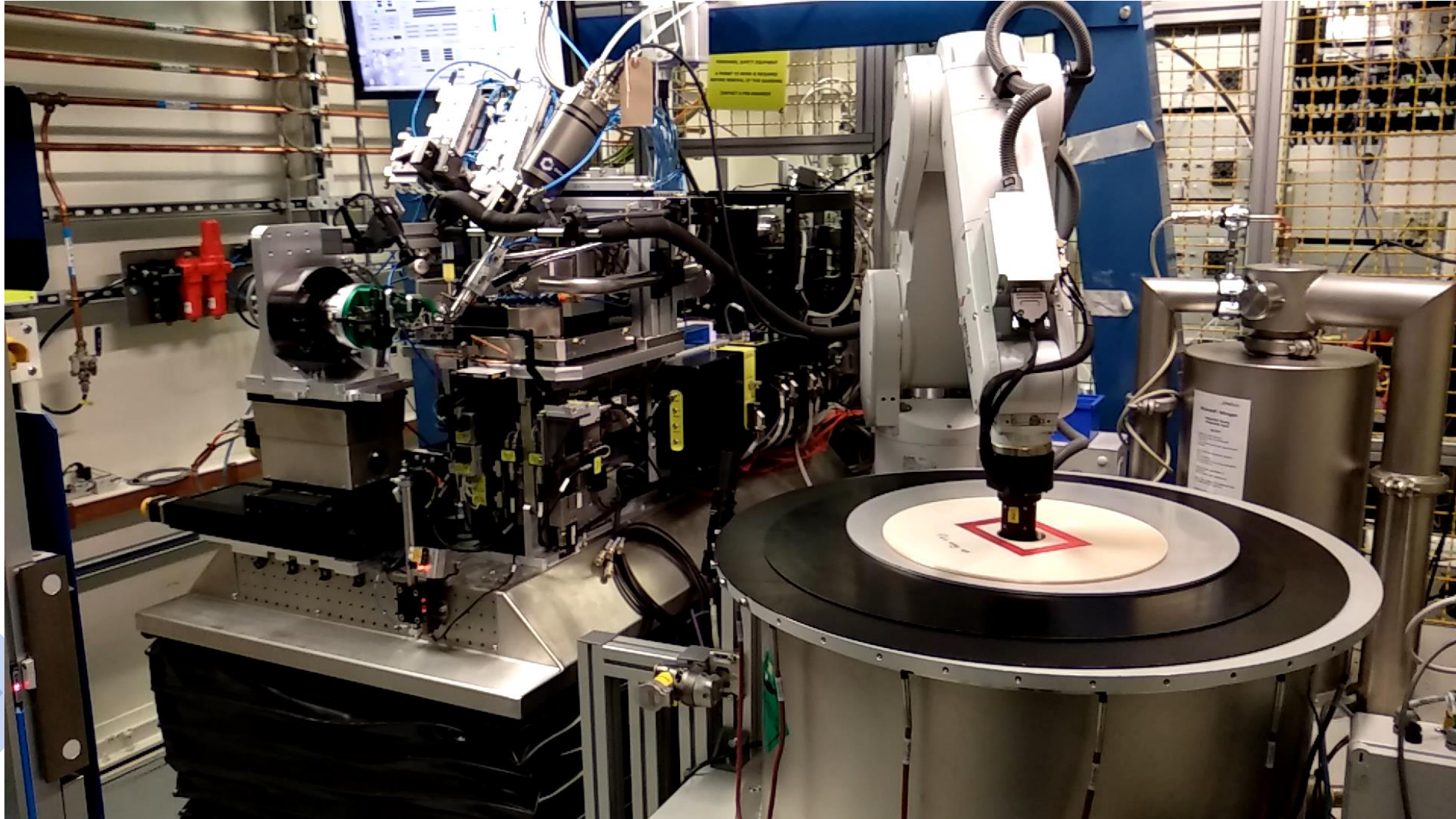
- Dewar baseplate redesigned to hold 30 pucks, 480 samples
- Larger Dewar bought to hold 37 pucks, 592 samples
- New model Mitsubishi arms bought
 - Have collaborative modes if needed
- Goniometer pin sensor integrated
- Air blower on barcode reader
- Dewar drain tap interlocked to LN2 fill



Current Situation - I03/I04/I04-1/I24 (MX)

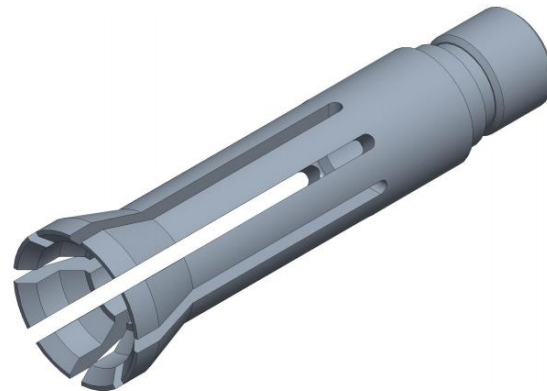
- Mitsubishi RV-7FLM Robot Arm
- Large Dewar with 37 pucks, 592 samples
- ~15s exchange time
- ~30s dry time, every 90 mins, done straight after a load
- SPINE pins only

Current Situation

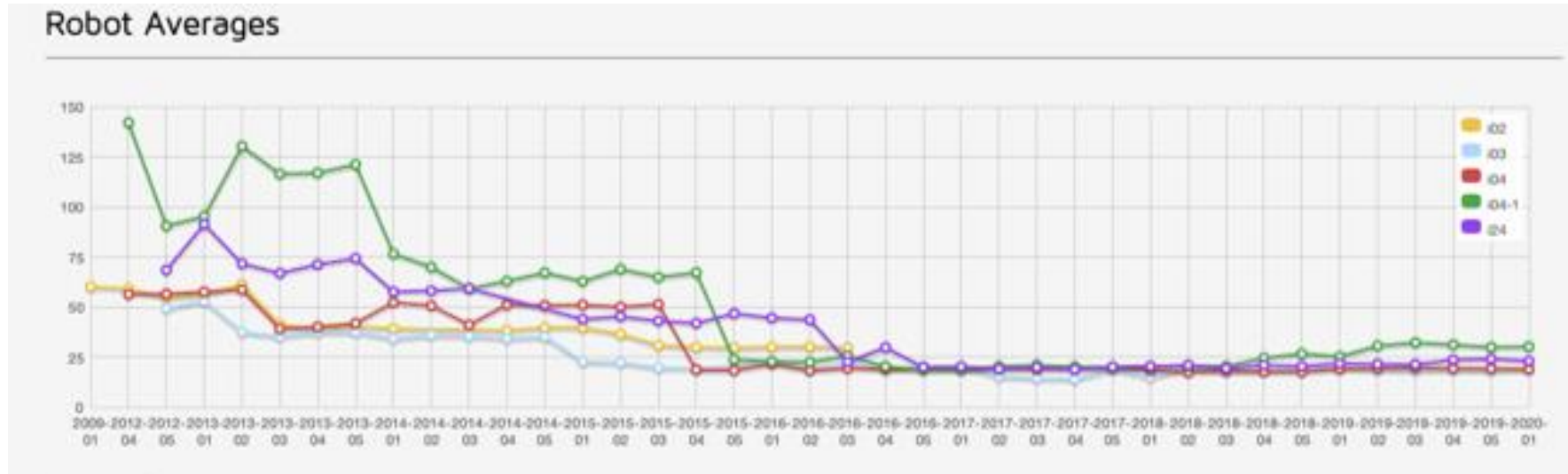


Gripper

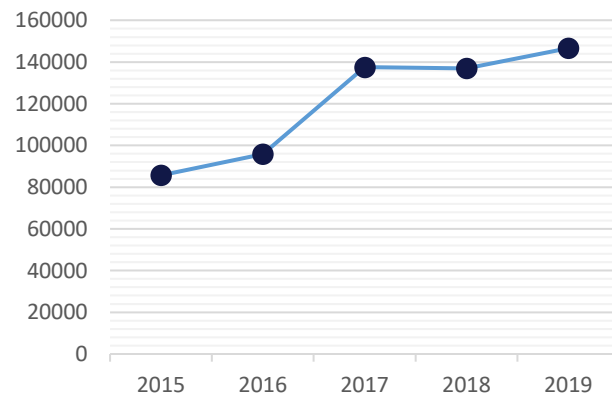
- Have used Rigaku grippers (manufactured by Oceaneering) since Diamond opened
- Simon Morton of ALS shared their gripper with us
- Slight modifications to use Schunk crash protection, now used on I03, I04-1 and I19
- Means we can now repair in house instead of returning to Rigaku



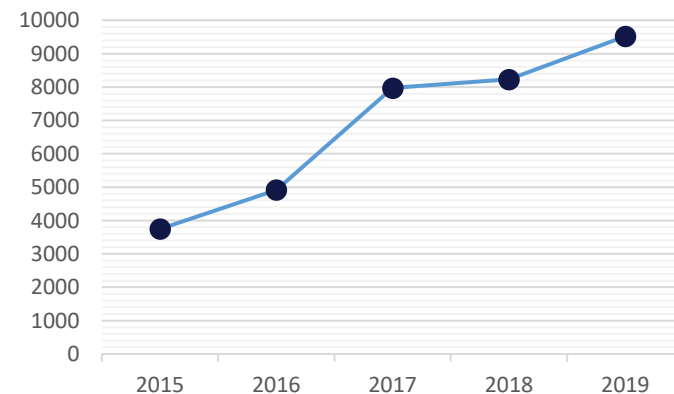
Exchange Times and Throughput



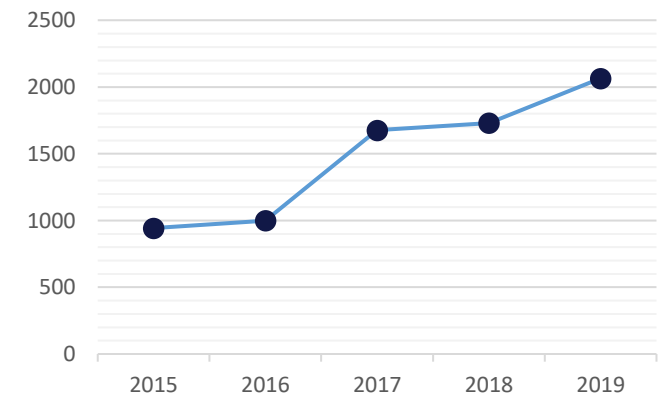
Sample loads per year



Pucks per year

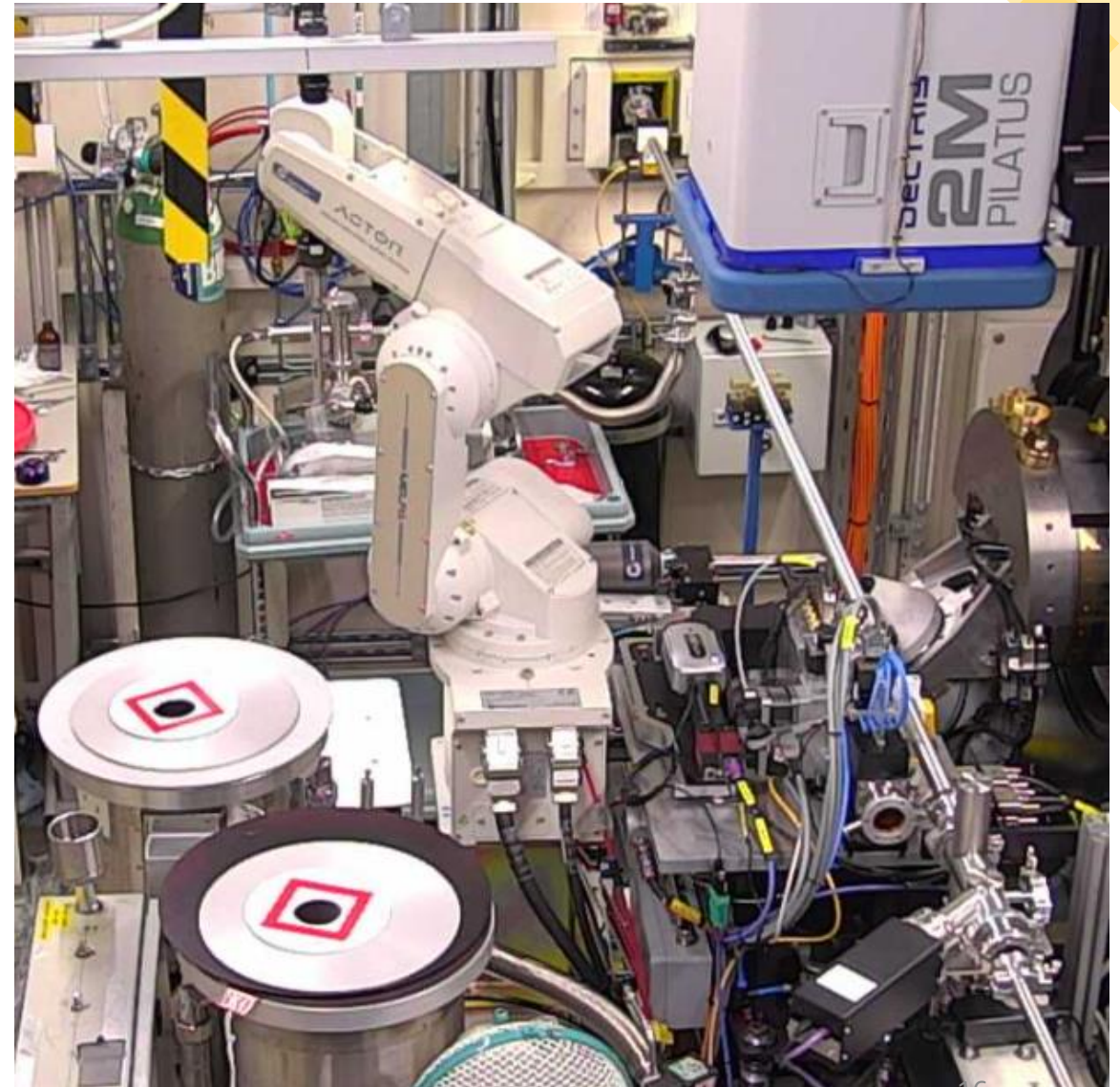


Dewars per year



Current Situation – I19

- Mitsubishi RV-6S Robot Arm (older model)
- 2 Dewars, each with 7 pucks, 224 samples
- Running same code on both Mitsubishi and EPICS levels



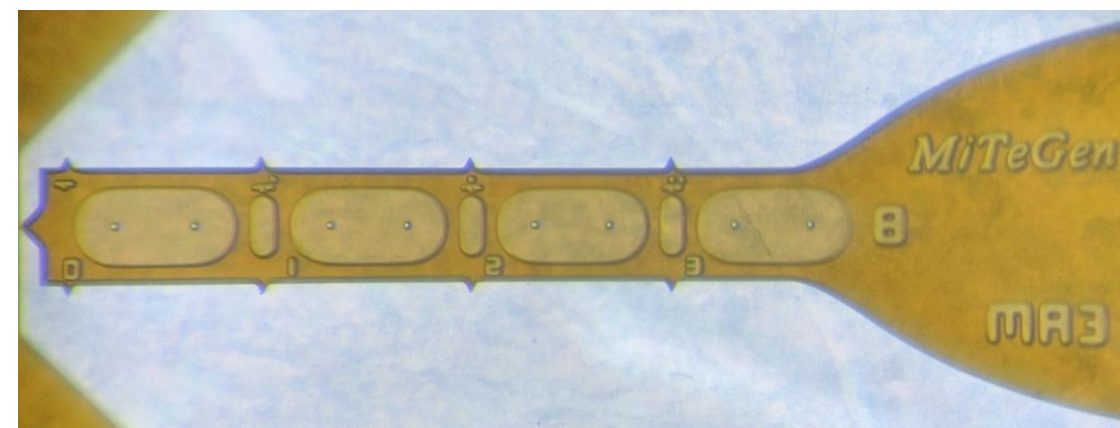
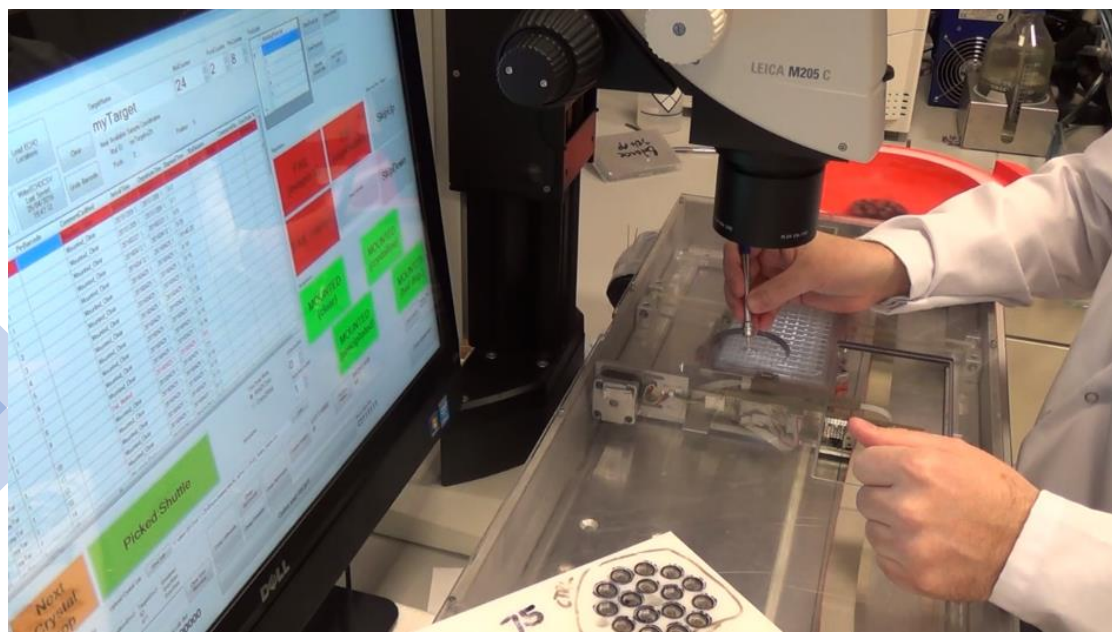
Current situation - VMXi

- Completely automated *in situ* beamline, samples in trays
- Mitsubishi RV-2FM Robot Arm
- Conveyor belt controlled by robot as 7th axis
- Moves between 2 Formulatrix Imagers and entry port into mini-hutch
- Different Mitsubishi code as much simpler
- Same EPICS control



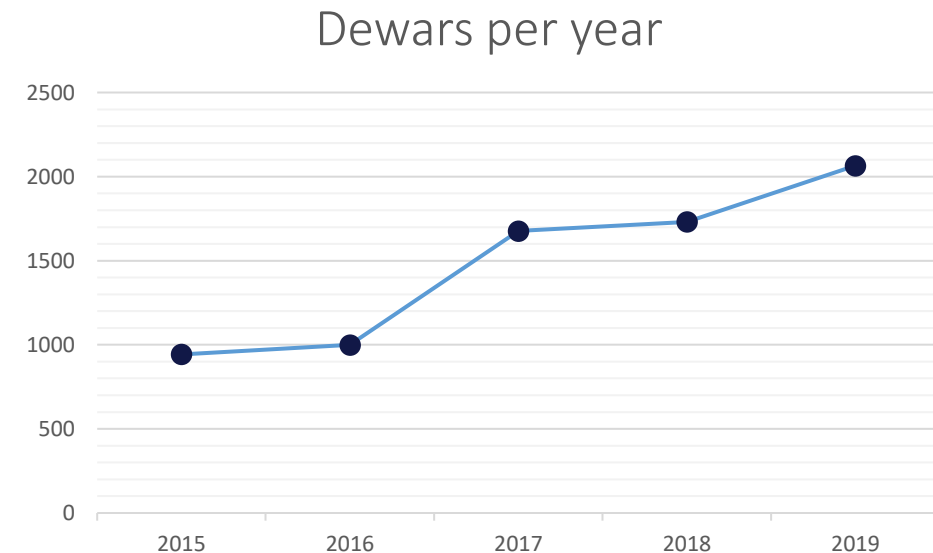
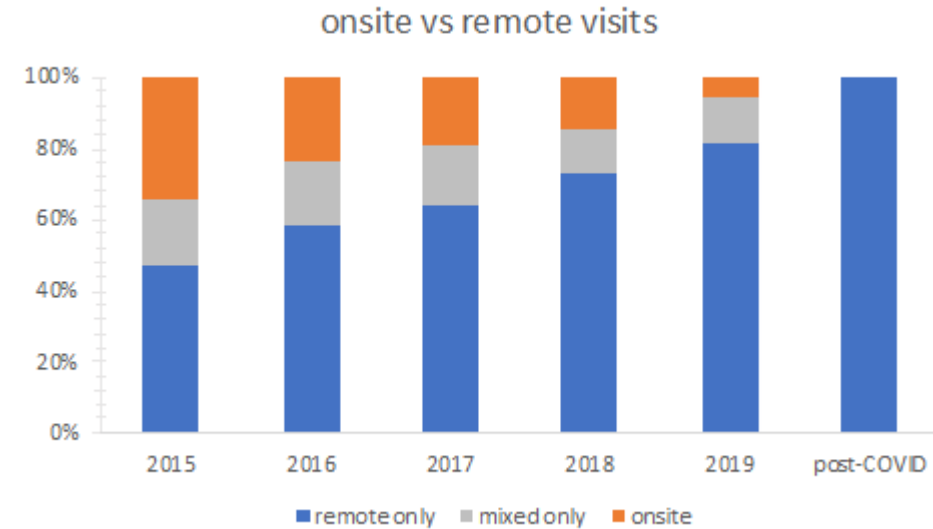
Current Situation - XChem

- Very high throughput Fragment Screening program
- Shifter helps user fish crystals at high speed (100 / hour) (oxfordlabtech.com)
- Dedicated I04-1 beamline for multiple days per week
- Multipin to be used in future to increase capacity



Logistics

- >70% visits fully remote in 2019
- Ever increasing shipments to Diamond
- Users needed an easier way to send Dewars
- Diamond needed an easier way to manage Dewars



Logistics

- Dewar shipping to Diamond can be booked through Synchweb/ISPyB
- Users can track the Dewar as we pull info from DHL API
- Staff can track all incoming Dewars

Create Airway Bill: To Facility

Shipment Details

Shipment: NR16818-33_06092017

Dewars: ☒ DLS-MX-1235 ☒ DLS-MX-1234 ← Tick the dewars you want to send

Weight: 36 Kg

DHL Account Number: Click to edit ☒ Use Facility Account ← Click Use Facility Account, then Accept the Terms and Conditions

Declared Value: 100 GBP

Package Description: Dry shipper - not restricted as per IATA special provision A152

Contact Details

Contact: Elizabeth Windsor

Contact Phone Number: 0123 123 7100 ← Check the details are correct

Origin: CAMBRIDGE-GBR



Destination: OXFORD-GBR

Date	Status	Location	Signatory
2021-03-09 12:01:00	Shipment pick up	CAMBRIDGE-GBR	
2021-03-09 20:00:00	Processed at location	CAMBRIDGE-GBR	
2021-03-09 20:24:00	Depart facility	CAMBRIDGE-GBR	
2021-03-09 22:43:00	Arrived facility	EAST MIDLANDS-GBR	

	Proposal ▲	Dewar ▲	Tracking No ▲	Origin ▲	Est Ship ▲	Est Arrival ▲	Updated ▲	Status ▲	Pucks ▲
+	sw24950	DLS-MX-0915	5847281930	Leeds - York Uk	3rd Mar	4th Mar	4th Mar 10:46	Delivered - Signed fo...	1
+	sw24950	DLS-MX-0252	2126193090	Leeds - York Uk	3rd Mar	3rd Mar	4th Mar 10:46	Delivered - Signed fo...	1
+	in20015	DLS-IN-0832	1033367823	Cambridge - Uk	9th Mar		10th Mar 12:44	With delivery courier	0
+	mx24948	DLS-MX-0521	7152245682	Newcastle - Durham Uk	10th Mar		9th Mar 11:27	pickup cancelled	4

Dewar Scanning

- Once on site, Dewar barcodes are scanned as they move around the ring
 - Stores-In → Dewar Storage → Beamlines → Dewar Storage → Stores-Out
 - Users can track Dewar around synchrotron



* m x 2 4 4 4 7 - 0 0 4 6 3 3 4 *

Auto Collect
This dewar contains 7 container(s) for automated data collection

Label	DLS-MX-0287
Shipping Name	MX2447-MANC-010221
Safety Level	Green
No. Parcels	2
Proposal	mx2447
Home Lab Name	LEYS
Local Contact	
Containers (7)	<div>DLS-0033DLS-257DLS-256</div> <div>DLS-0034DLS-0035DLS-403</div> <div>DLS-404</div>

Date	Status	Location
08-03-2021 16:53	at facility	tray-4d
05-03-2021 12:16	processing	i04
05-03-2021 12:16	processing	i04
05-03-2021 12:15	processing	i04
05-03-2021 12:15	processing	i04
05-03-2021 12:15	processing	i04
05-03-2021 12:15	processing	i04
05-03-2021 12:15	processing	i04
05-03-2021 12:14	processing	i04
05-03-2021 12:10	at facility	i04
05-03-2021 12:06	at facility	i04
03-03-2021 13:21	at facility	tray-4d
03-03-2021 10:36	at facility	stores-in
01-03-2021 15:12	pickup booked	
01-03-2021 15:12	awb created	

Dewar Store

- Stores over 100 Dewars
- Brings each to easy access height
- Barcode scanner to track each Dewar's location



Dewar Store



Dewar Organisation

- Dewar store has prompts to refill LN2, or prepare for dispatch
- Diamond staff are emailed the names and locations of Dewars the day before experiments

Scan Dewar and Rack

Barcode or FacilityCode

Scan the long barcode from the dewar case

Location

Scan the location e.g. RACK-A1

Submit Cancel

Find a Dewar

BarCode or FacilityCode

e.g. DLS-MX-####

Search Cancel

Dewars that need refilling

TRAY-9F

(Scan dewars back into the same position after refilling)

TRAY-1A:	TRAY-1B:	TRAY-1C: mx25233-0046307 2021-03-08T20:31:48 DLS-MX-0488 dispatch-requested	TRAY-1D:	TRAY-1E: mx19880-0046367 2021-03-10T10:09:05 DLS-MX-1013	TRAY-1F:
TRAY-2A:	TRAY-2B:	TRAY-2C: mx25587-0046394 2021-03-10T10:24:52 DLS-MX-0455	TRAY-2D: mx25402-0046382 2021-03-10T09:49:34 DLS-MX-0701	TRAY-2E: mx23853-32-i23-0045461 2021-03-08T09:58:00 DLS-MX-0930	TRAY-2F: mx19800-0046049 2021-03-10T10:24:39 DLS-MX-0134

Expected dewars tomorrow on i24 - Message (HTML)

File
Message
Help
Tell me what you want to do

Mark Unread
Find
Zoom

Expected dewars tomorrow on i24

no-reply@diamond.ac.uk
Thu 04/03/2021 16:00

To Williams, Mark (DLSLtd,RAL,LSCI)
Cc Owen, Robin (DLSLtd,RAL,LSCI); Axford, Danny (DLSLtd,RAL,LSCI); Horrell, Sam (DLSLtd,RAL,LSCI); Mazzorana, Marco (DLSLtd,RAL,LSCI); Bjorkelid, Christofer (DLSLtd,RAL,CEO)

Dear all,

[Here](#) are the dewars for tomorrow on i24:

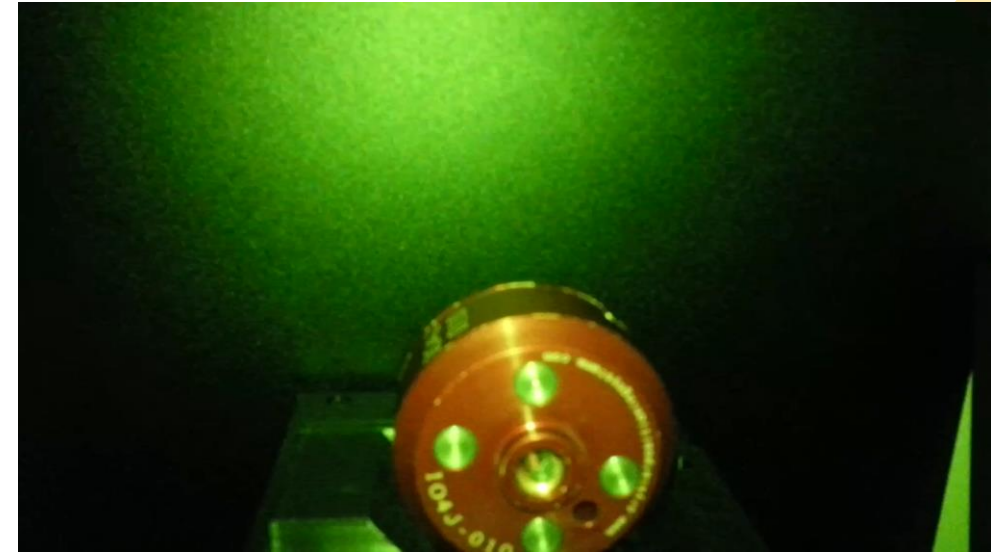
05 Mar 2021 12:00: in26517-11 - Christofer Bjorkelid
tray-12f -- DLS-IN-0082 -- at facility (in26517-11 Mar2021)
CPS-2167 (16 samples)
CPS-2164 (16 samples)
CPS-2165 (16 samples)
CPS-2168 (16 samples)
CPS-2169 (10 samples)
CPS-2166 (16 samples)

05 Mar 2021 18:00: in28224-3 - Christofer Bjorkelid
i24 -- DLS-IN-0206 -- processing (in28224_1)
CPS-4777 (16 samples)
CPS-3536 (16 samples)
CPS-3537 (16 samples)
CPS-3535 (16 samples)
CPS-3443 (16 samples)
CPS-3447 (16 samples)
None -- Immunocore3 -- sent to facility (in28224_1)

05 Mar 2021 19:00: sw24893-5 - Christofer Bjorkelid
tray-10a -- DLS-IN-0221 -- at facility (sw24893 R20210301)
CPS-3550 (16 samples)
CPS-3552 (16 samples)
CPS-3553 (16 samples)
CPS-3554 (16 samples)
CPS-3555 (16 samples)

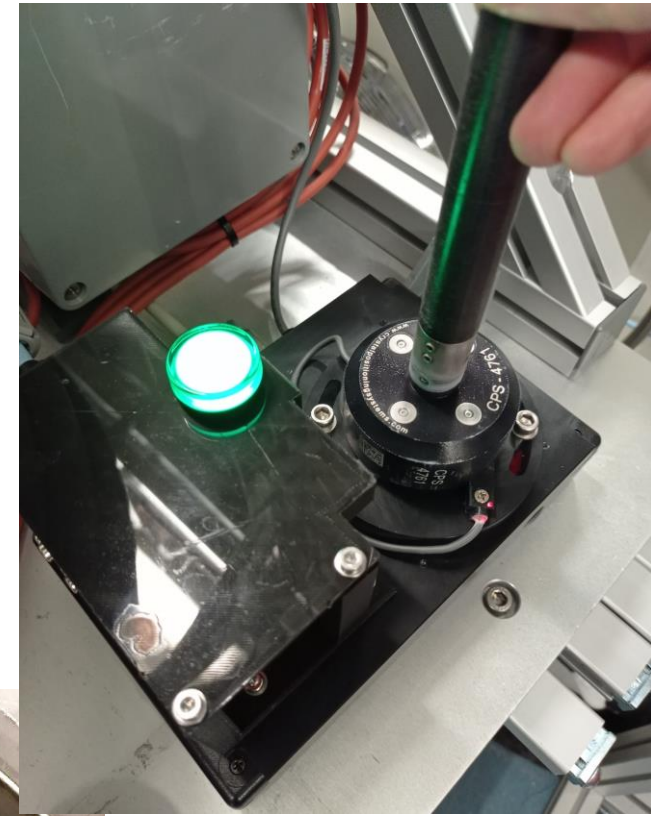
Puck Organisation

- Even before Covid, we often had pucks from multiple visits on the beamline simultaneously
- With responsive scheduling and limited staff on site, even more important to keep track of pucks and samples
- Pucks have been barcoded using a laser etcher for the last few years



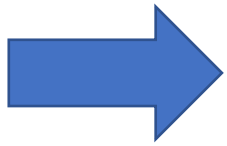
Puck Scanning

- Beamline staff scan the barcode, and a laser pointer instructs us where to load or unload the puck from
- Automatically assigns pucks to positions in ISPyB database
- Creates visits in unattended data collections mode

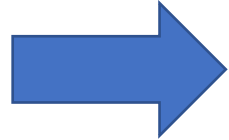


Future Work

- Diamond-II upgrade
- New endstations
- Faster detectors



Higher throughput



Higher capacity

Acknowledgements

- Diamond
 - Beamline Staff
 - Mechanical & Electrical Technicians
 - Controls Team
 - GDA Team
 - MPS Team
 - Engineering Team
- SLS
 - Katherine McAuley
- DESY
 - Alke Meents
 - Nico Stuebe
- ALS
 - Simon Morton



diamond

PAUL SCHERRER INSTITUT



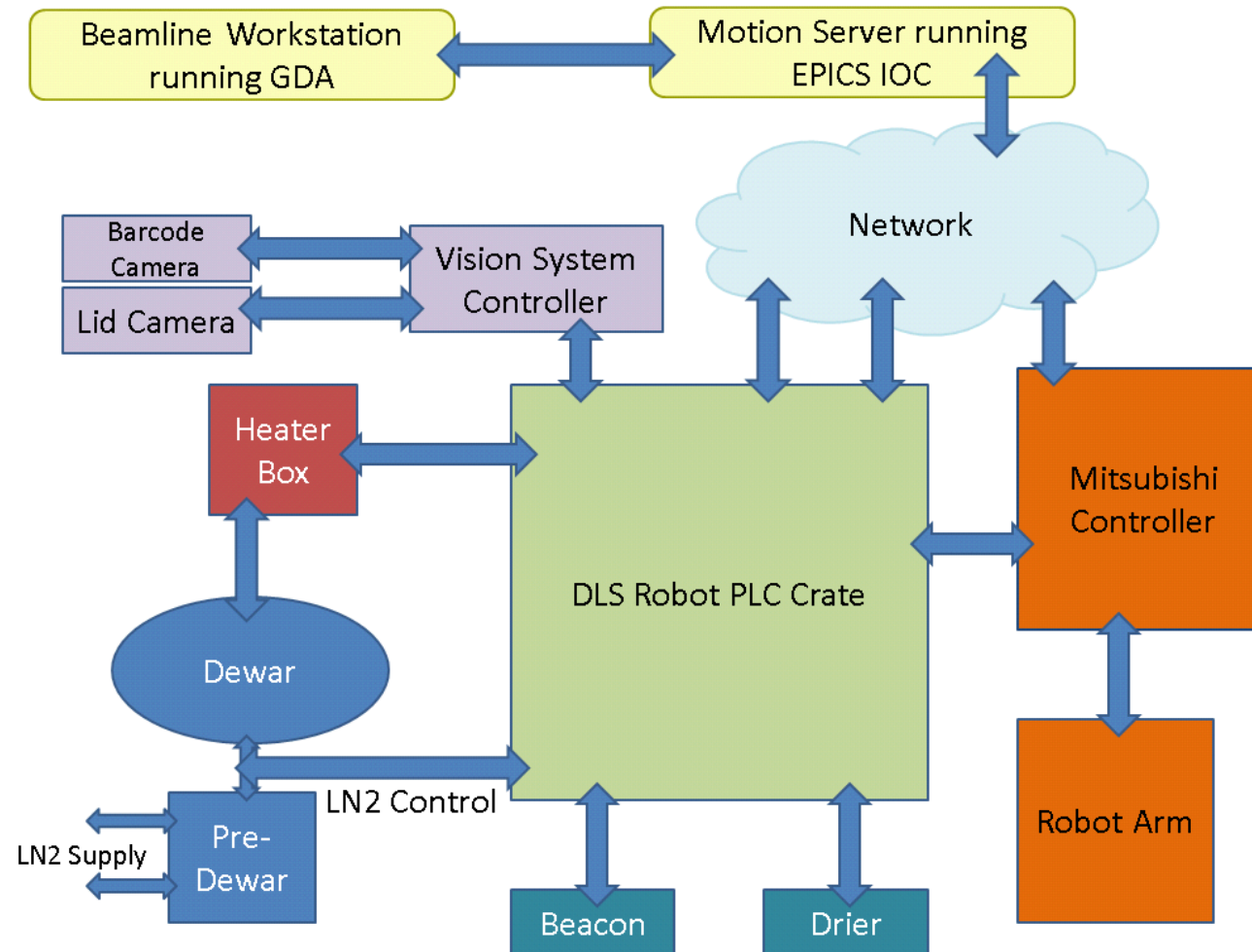
ALS

ADVANCED LIGHT SOURCE



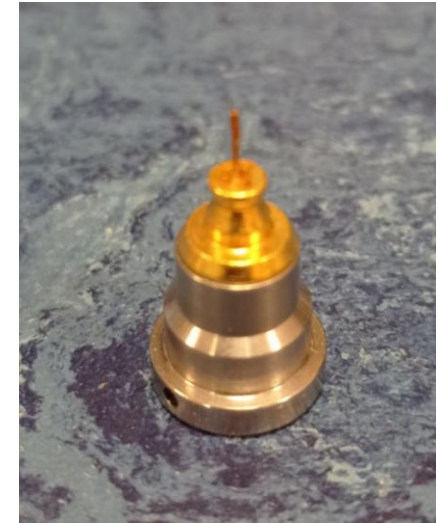


Improvements – Hardware – Stage 1



Current Situation – I23

- Low throughput in vacuum beamline
- Screen samples on I03
- Pins on adapter to make them SPINE compatible
- Heat conduction from goniometer is a problem



Current situation - VMXi

