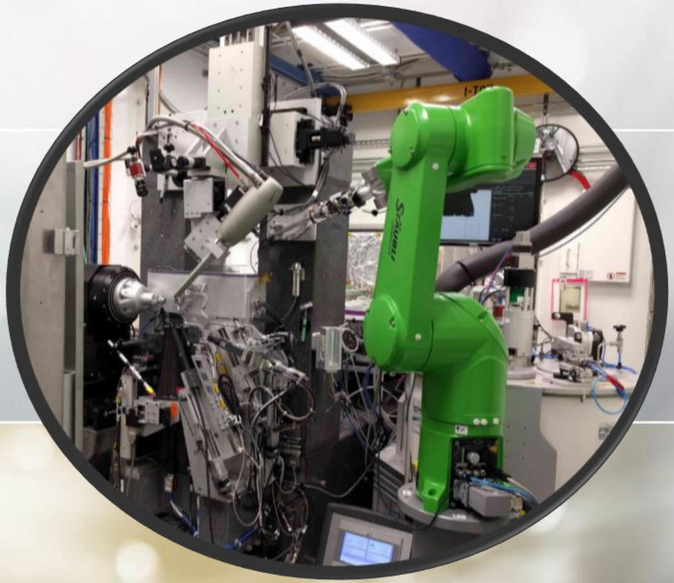
National Synchrotron Light Source II

Automation for macromolecular crystallography at the National Synchrotron Light Source II



NSLS-II MCE2021 workshop
March 16, 2021

Edwin O. Lazo

U.S. DEPARTMENT OF ENERGY | Office of Science

BROOKHAVEN NATIONAL LABORATORY

Team

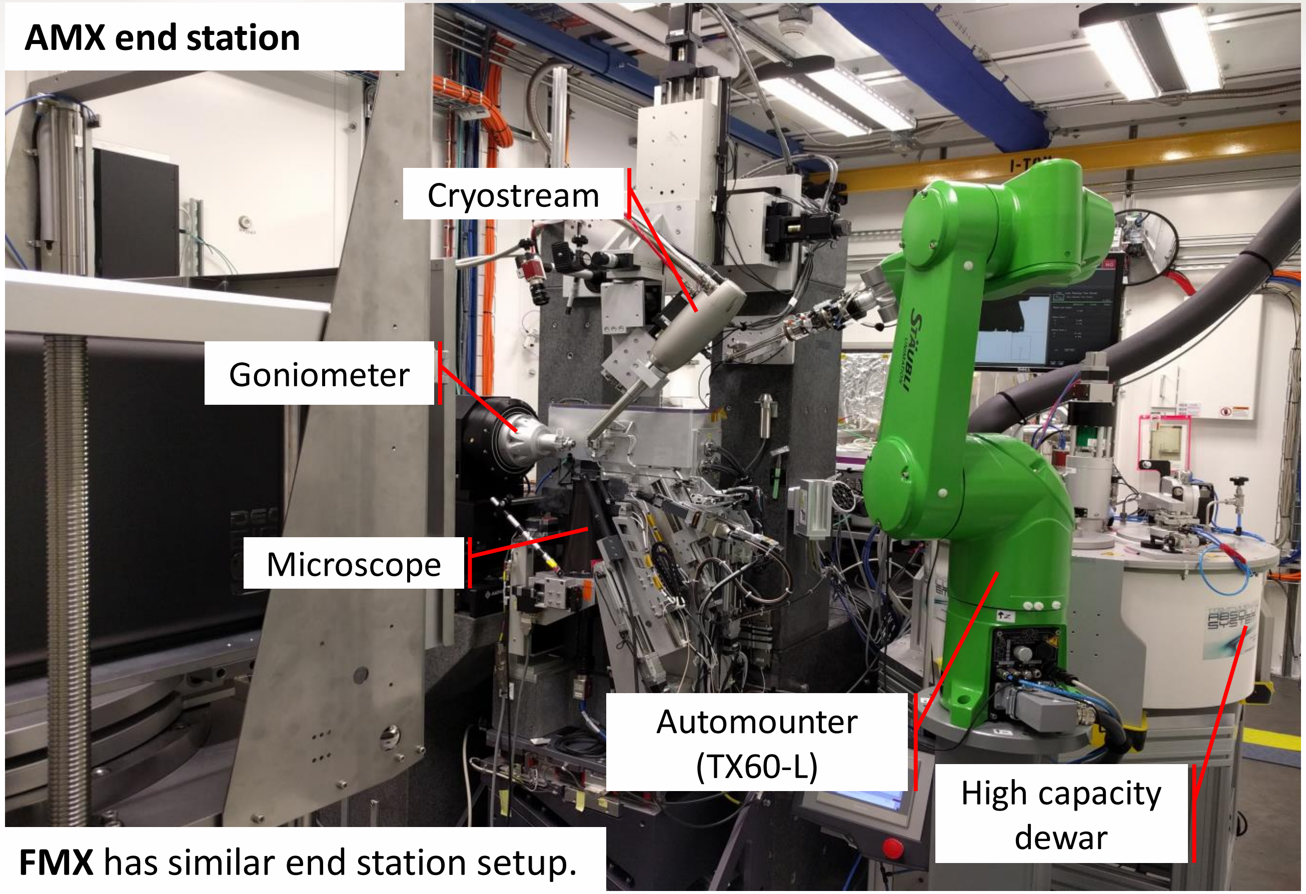
Sean McSweeney

AMX/FMX-
Jean Jakoncic
Martin Fuchs

Support-
Thomas Langdon

Facility-
William Jew
Peter Ratszke
Philip Marino
Leonard Pharr
Michael Santana

MX beamlines



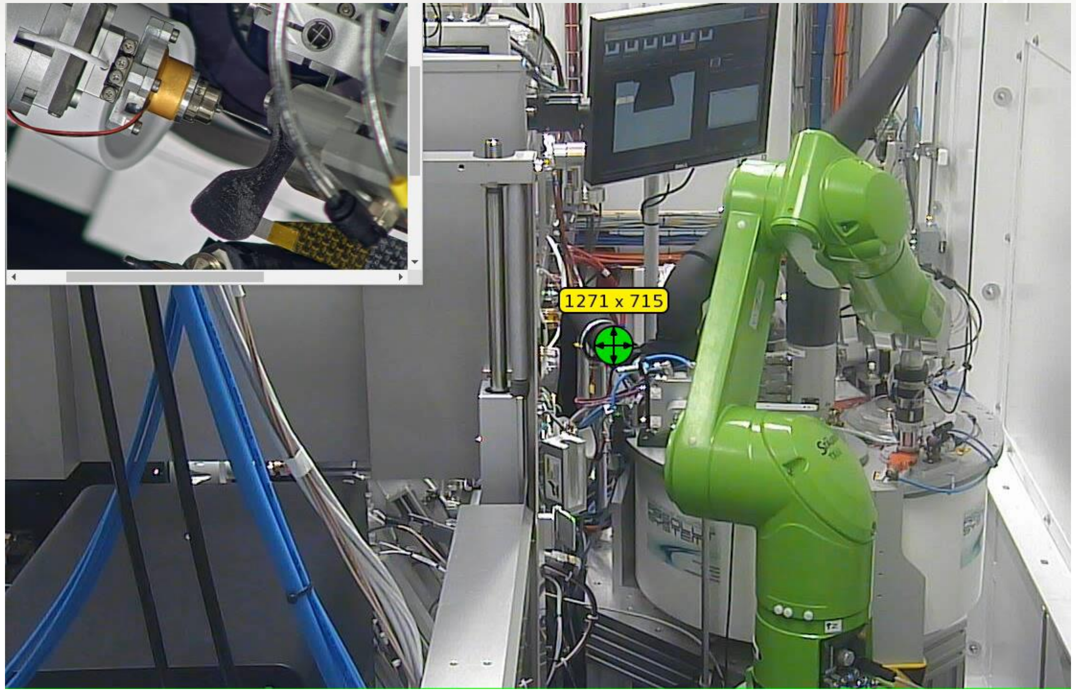
FMX has similar end station setup.

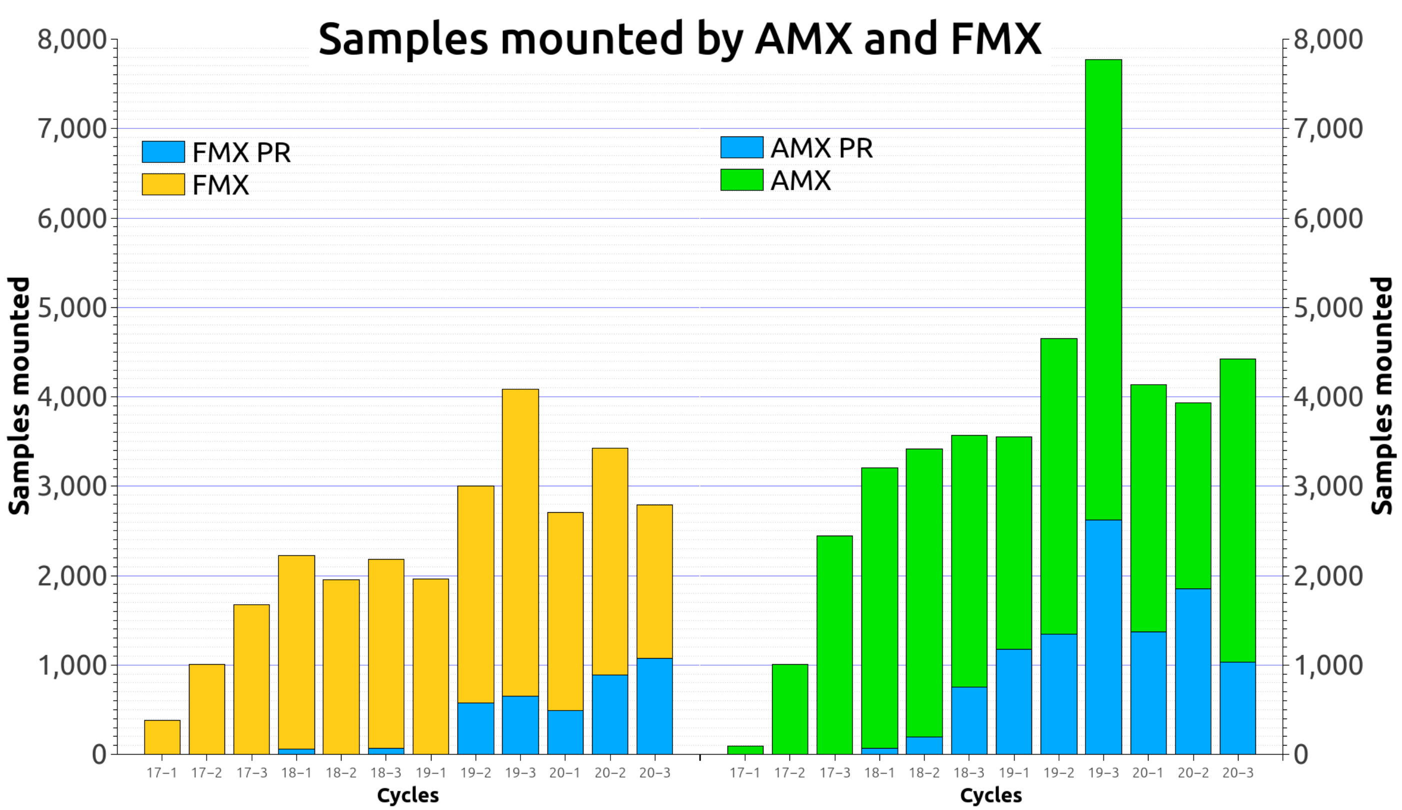
- 2 beamlines in the same sector (17-ID)
- First light Nov. 2016
- General user operations since Jan. 2017

	AMX	FMX
Flux (ph/s) at 12.7 keV	$5x10^{12}$	$3.6x10^{12}$
Spot size HxV (μm^2)	7 x 5	1.5 x 1 to 10 x 10
Detectors	Eiger 9M	Eiger 16M

Requirements: Robustness, speed, & easy to maintain
Challenges: Liquid nitrogen

Sample exchange time and reliability





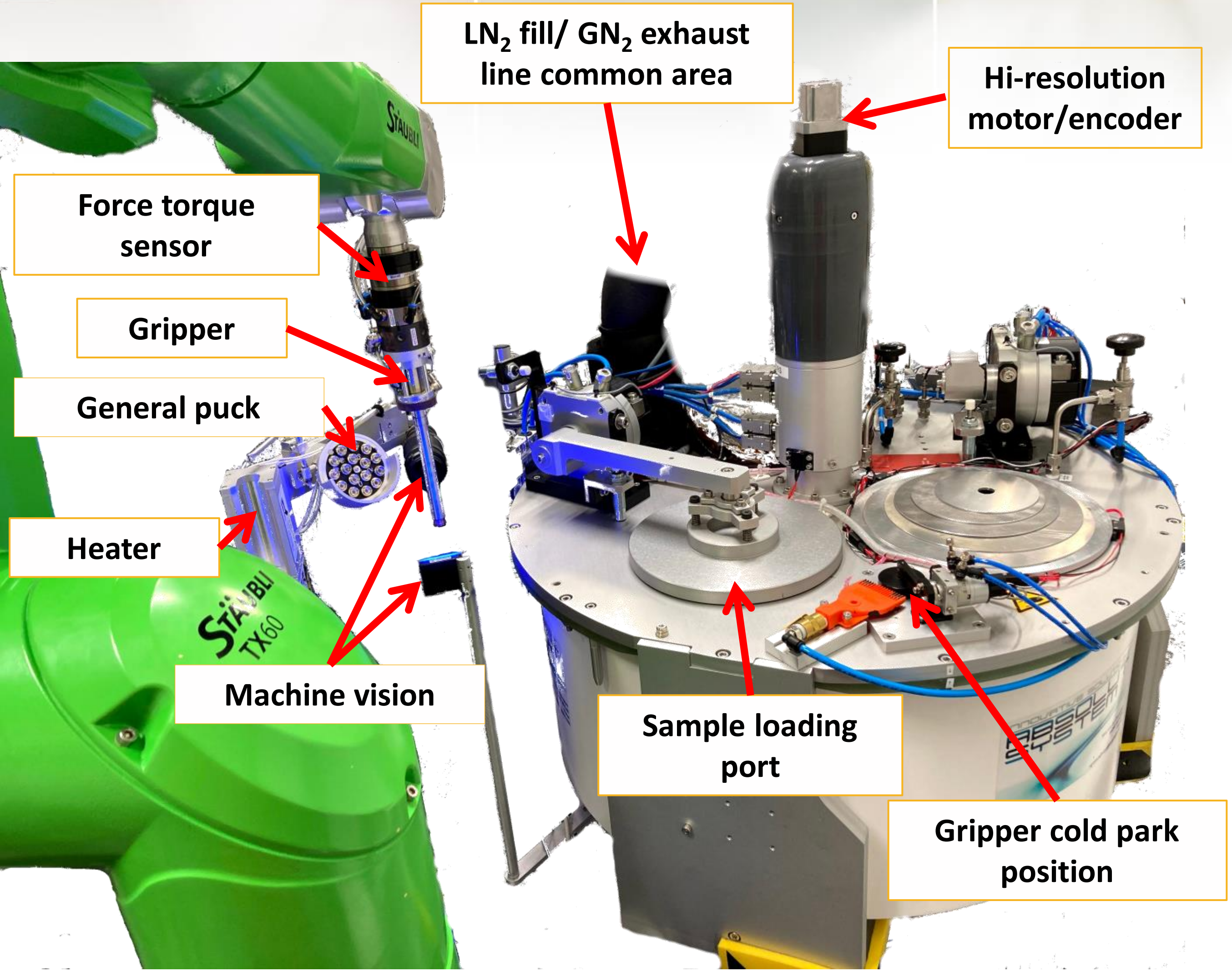
Enables:

Remote access and fully automated data collection

Reliability and sample throughput: (by both MX robots)

- Reliability: 99.95%
- Sample rate: 100 mounts/h excluding centering & data collection (currently <35s or 1000 mounts / 10h)
- 144 mounts/ hr (goal <25s or 1000 mounts / 7h)

MX Automounter at NSLS-II



24 Unipuck Dewar (Existing design from ESRF modified for unipucks)

Specifications

- Stäubli 6-axis arm, dewar, force torque sensor, in-house gripper
- In-house control system & diagnostics
- Optimized for Unipucks and Spine
- In operations since March 2017 (FMX) & April 2017 (AMX)
- Project began Nov. 2014, first mount March 2017 (~2.5 y)

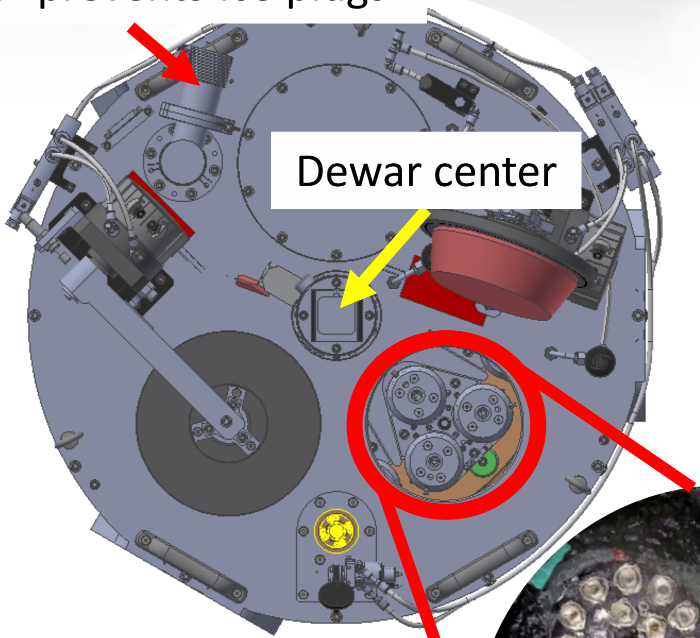
Diagnostics

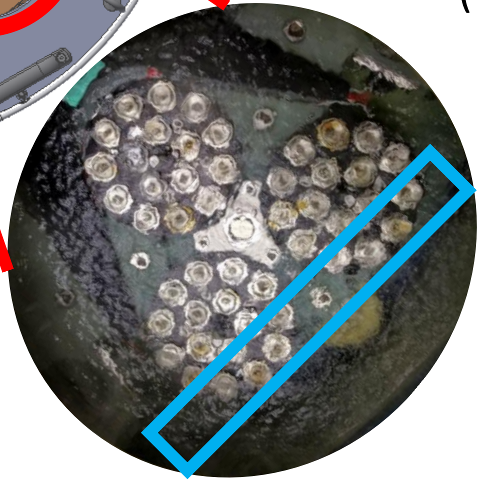
- Force torque sensor
- Hall sensors
- Machine vision
- Temperature sensors
- Limit switches
- Smart magnets
- Encoders
- Proximity sensors
- Alarms
- Hutch door sensors
- Experimental state machine (software)
- LN2 sensors

Dewar customizations & upgrades

Dewar can be controlled remotely

Heater- prevents ice plugs





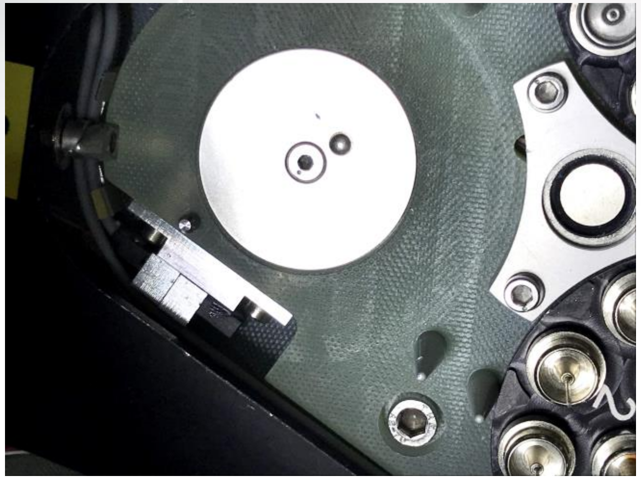
Reduced port diameters to reduce ice in dewar

Hi-res encoder
+/- count 1 (each count=5.6 µm)

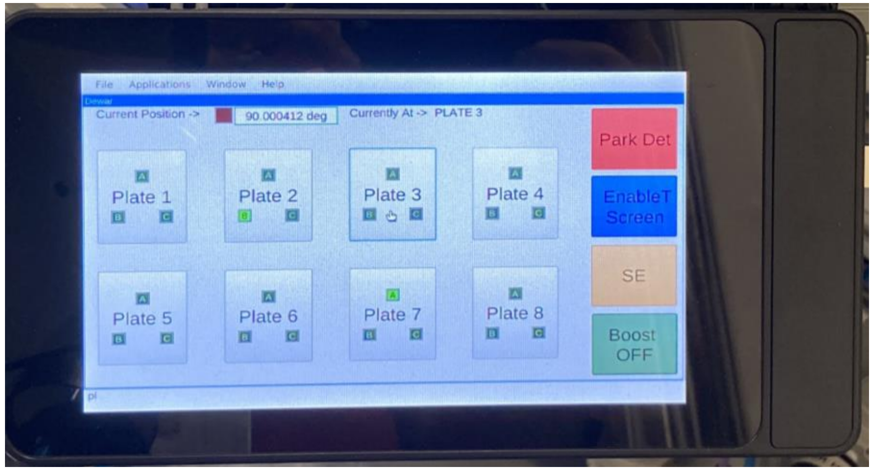
Clips/ Pins

Magnets- increased holding force to 20 N

Modified plates- dewar survey (+/-26 µm) instrument accuracy (+/- 28 µm).



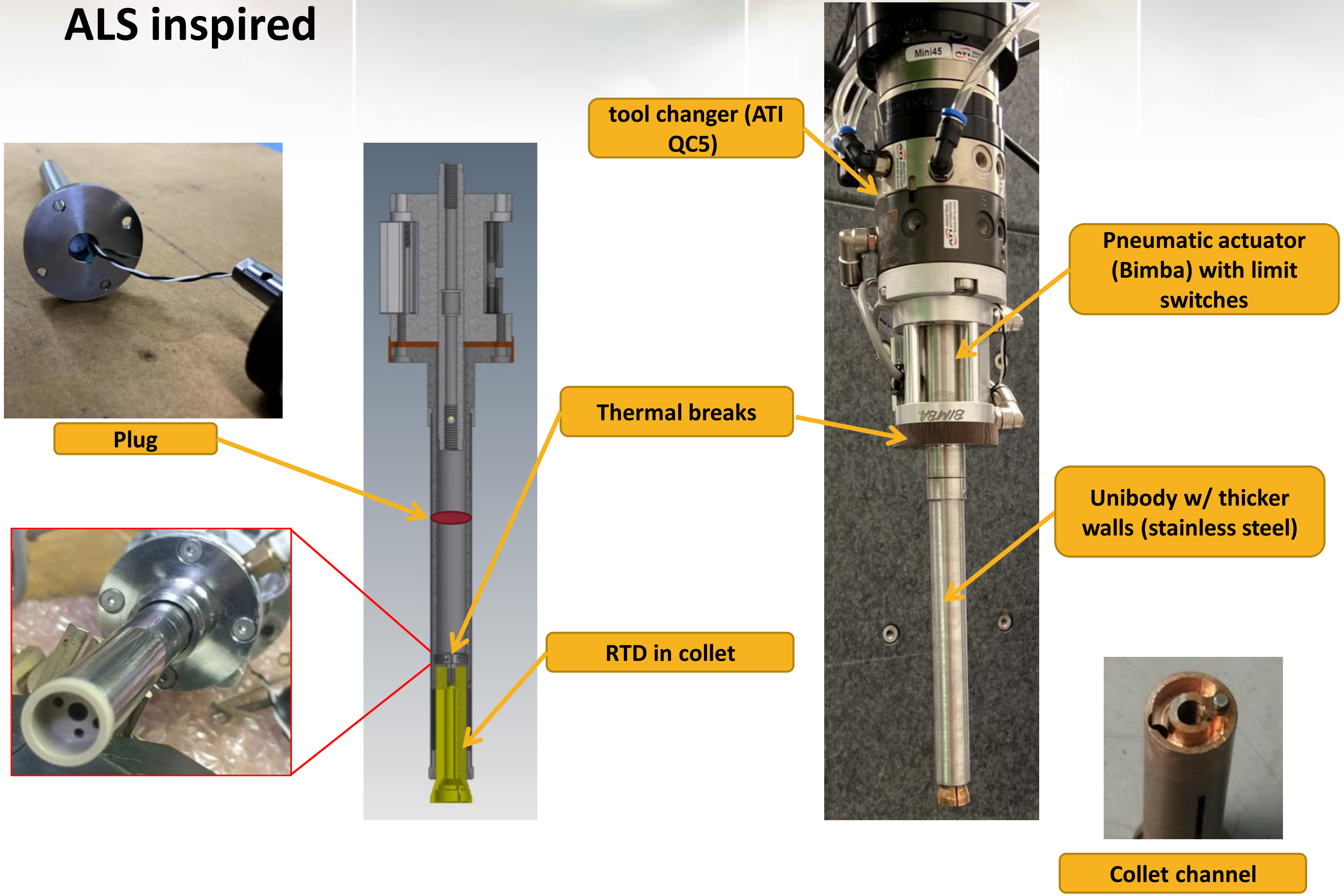
Puck sensors- Hall sensors (Grace Shea-McCarthy)



In hutch controller (NSLS-II delta tau / Rasp-Pi)

3 prong pneumatic dry mounting gripper

ALS inspired

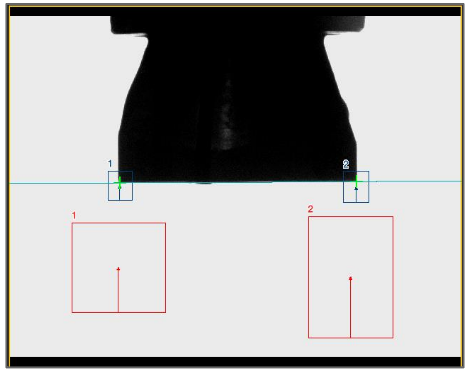


Due to upgrades-
Reduced cool down time by 58s
Increased warm up time by 17s
Durable- 24,000 & counting

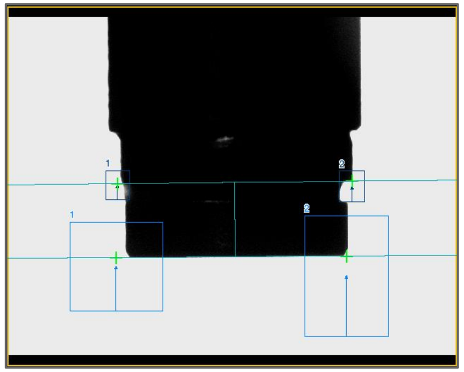
Gripper limitations-
At a rate of 20 samples/h gripper will begin to fail after ~120 mounts (7.5 Unipucks)

John Lara

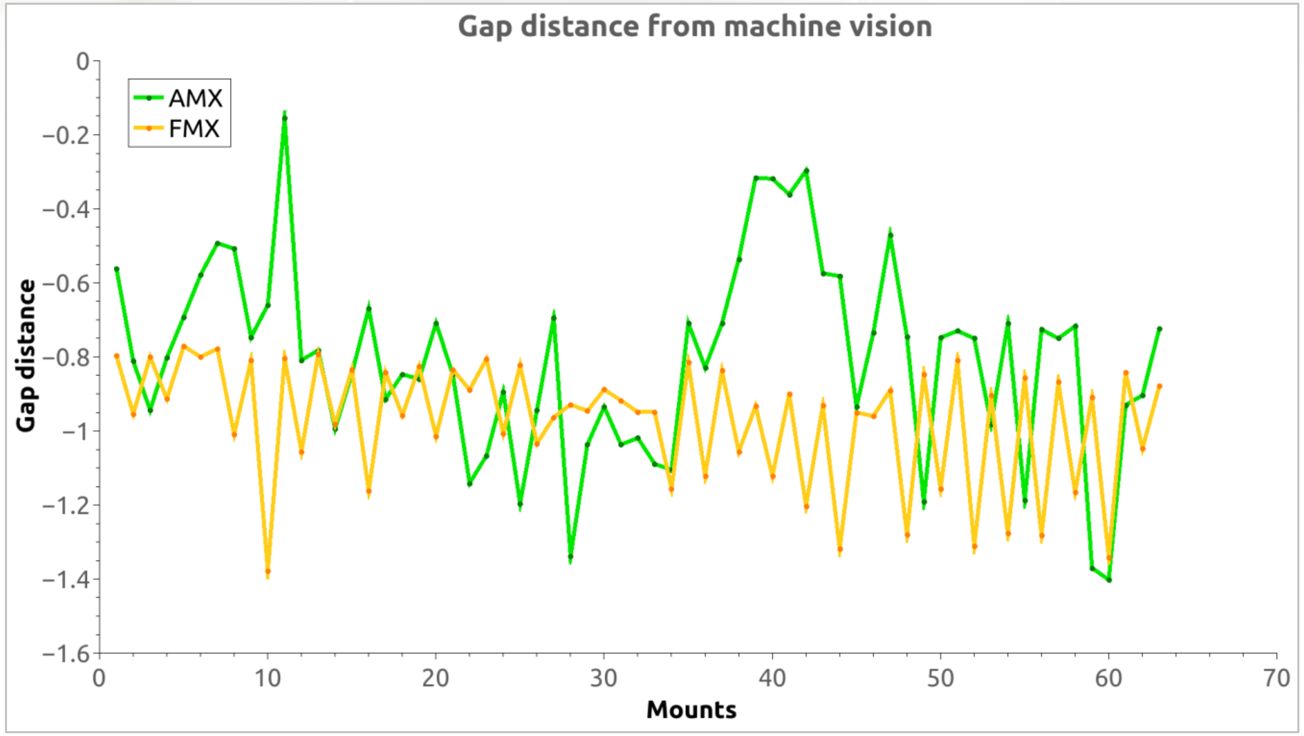
Keyence machine vision



No sample



Sample on



Machine vision for sample tracking & robot mount position calculations

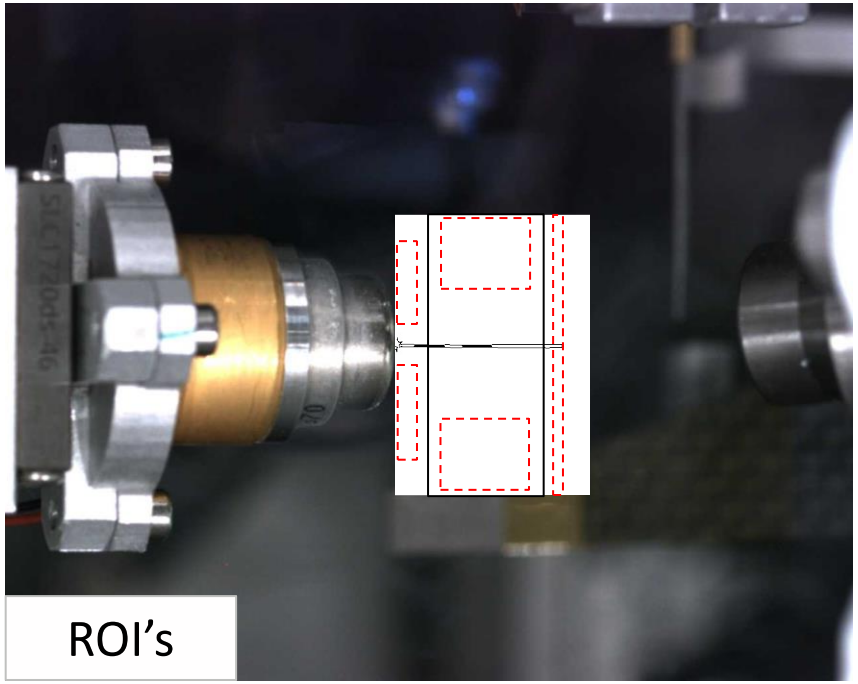
Gap range: 0.2 to 1.5mm

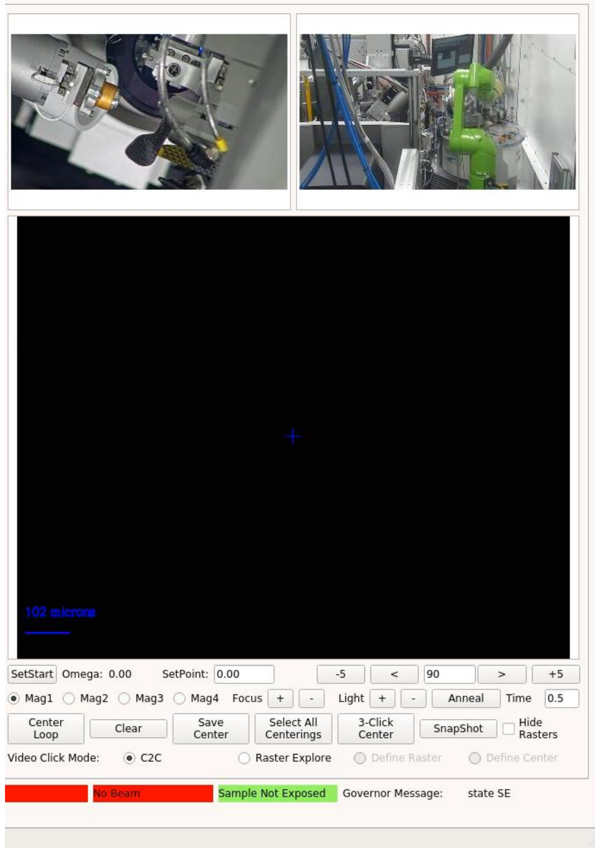
In-house machine-vision based pin positioning

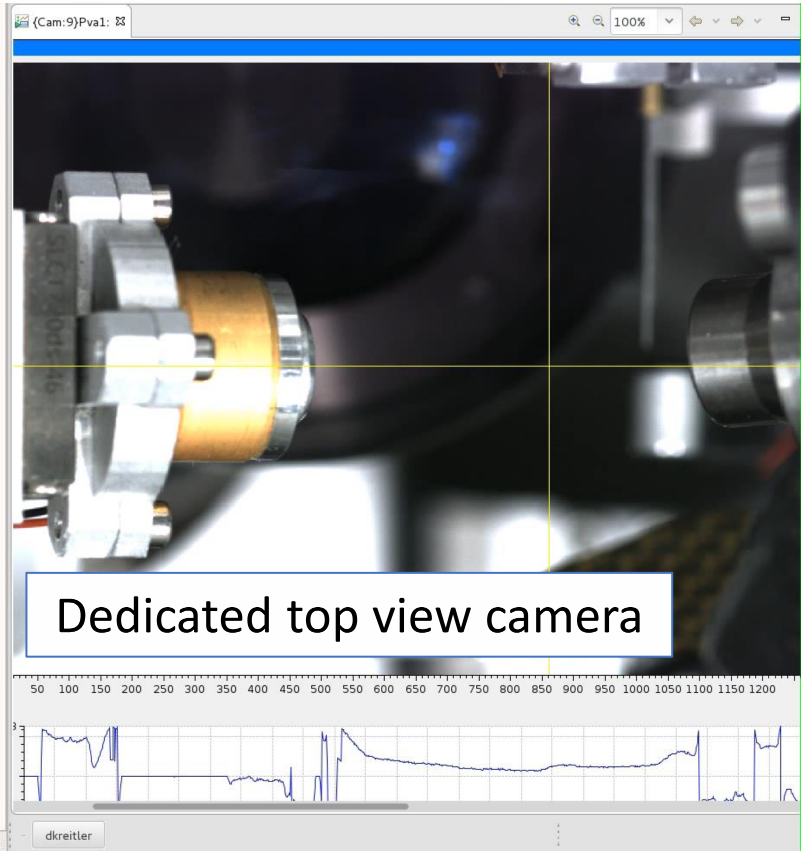
Steps after robot mount

- Pic at 0 deg
- Pic at 90 deg
- Calculations
- Gov moves Gonio X, pin Y, pin Z

Increases throughput

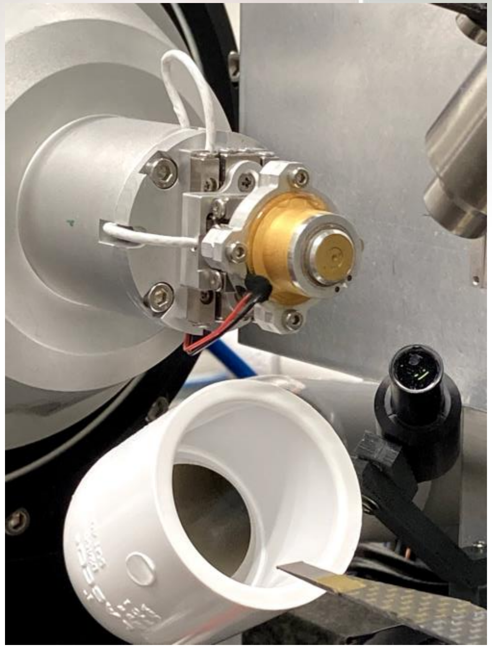






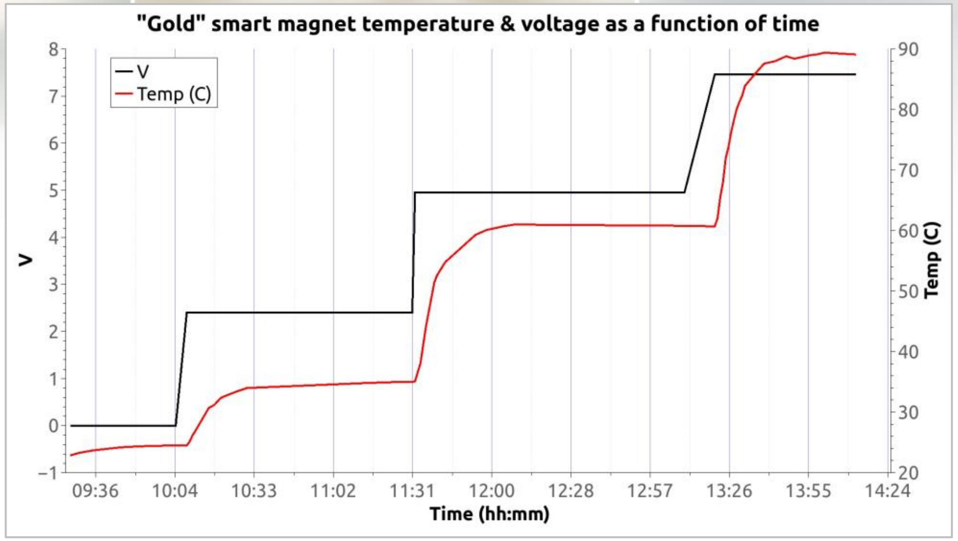
Samuel Clark & Herbert Bernstein

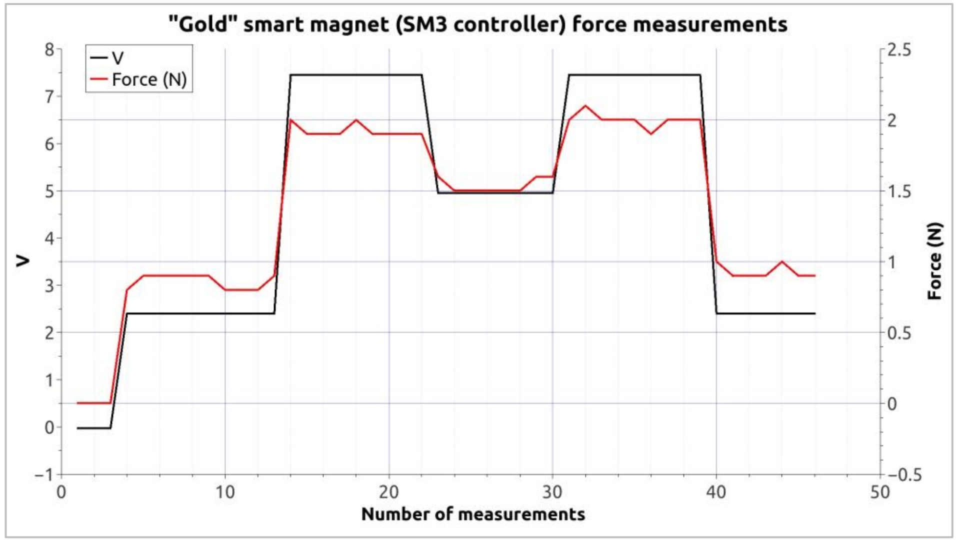
Smart magnet



New smart magnet
still does sample detection

smaller diameter (9.52 vs 9.6mm)





Can reach 90 °C

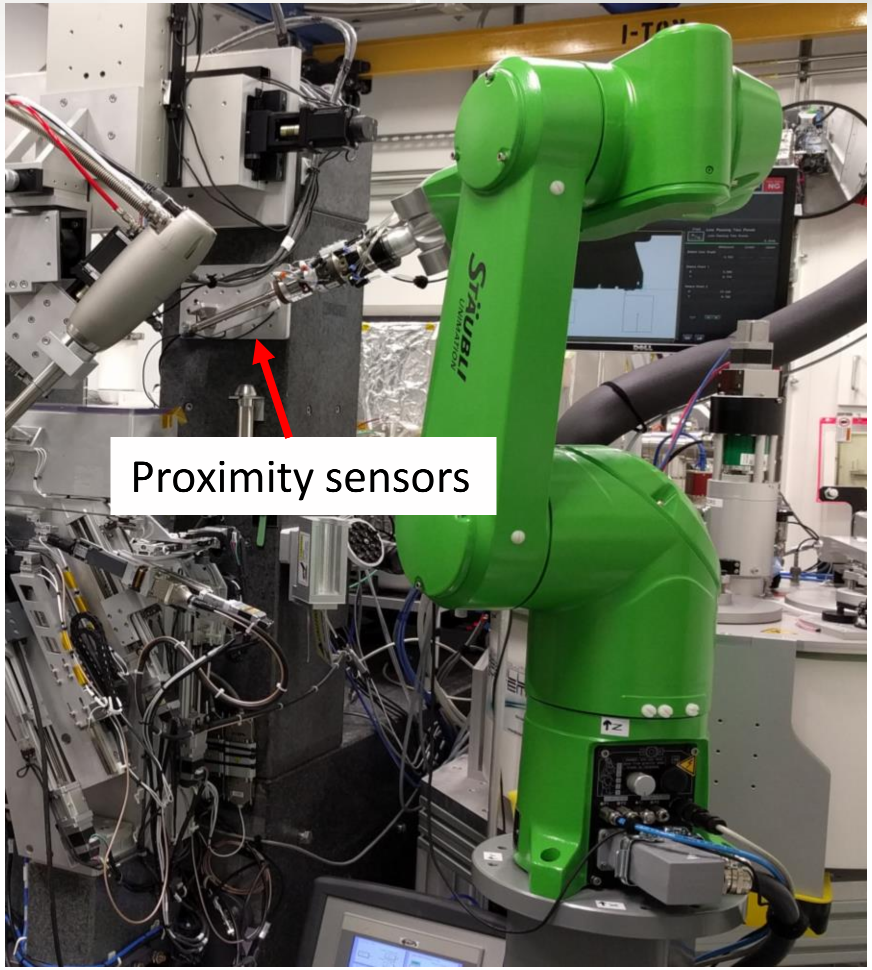
Previous 34 °C

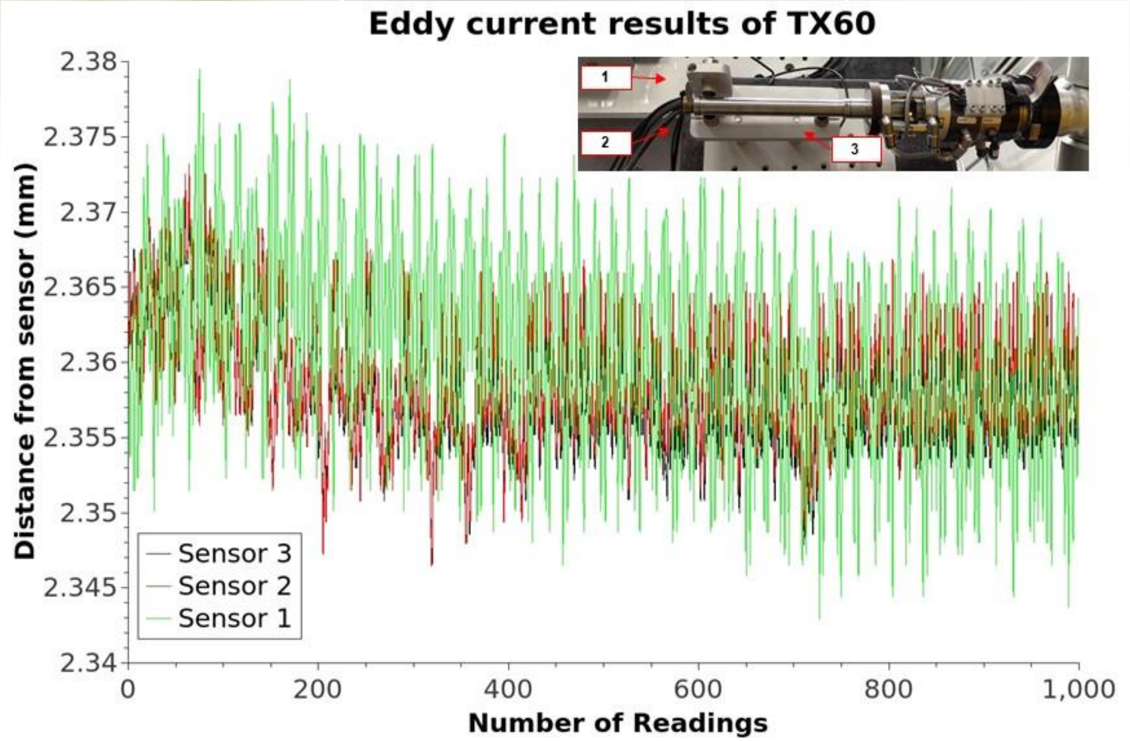
Reduces pause by 15s

Increased holding force ~2 N

Previous ~1.4 N

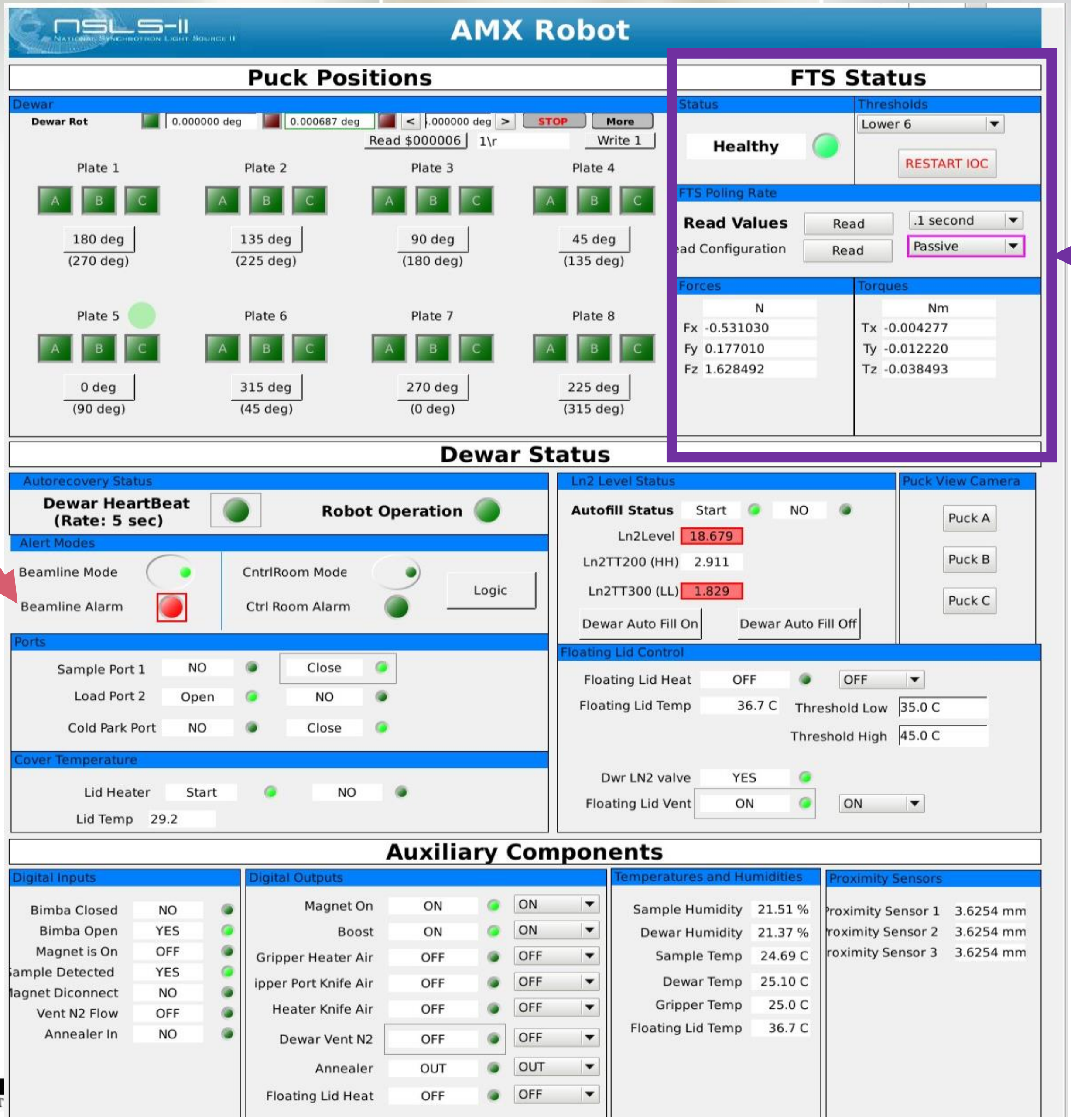
Proximity Sensors





- Robot repeatability: <30 µm
- Robot temp raises 7 °C affects gonio position by ~45um X-direction
- Check's robot performance during maintenance periods

MX Diagnostics and Alarms- EPICS



In-house force torque sensor driver

Bruno Seiva-Martins

Beast alarm system

Identifies 3 conditions:

- Equipment failure
- Sample safety
- Robot issue

Kun Qian, Stu Myers, Grace Shea-McCarthy

Throughput: Present & Future

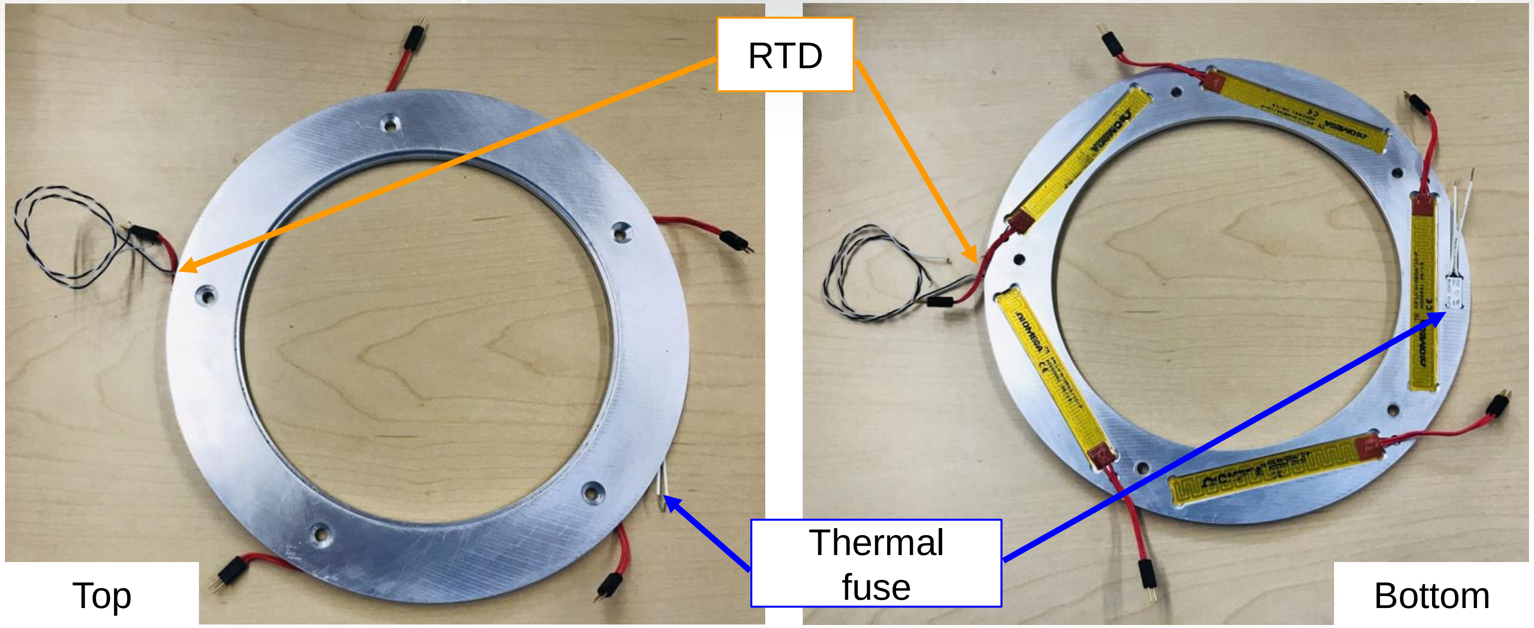
Beamline components, data processing SW, parallel codes + sample automation improvements .... has allowed to achieve these throughputs:

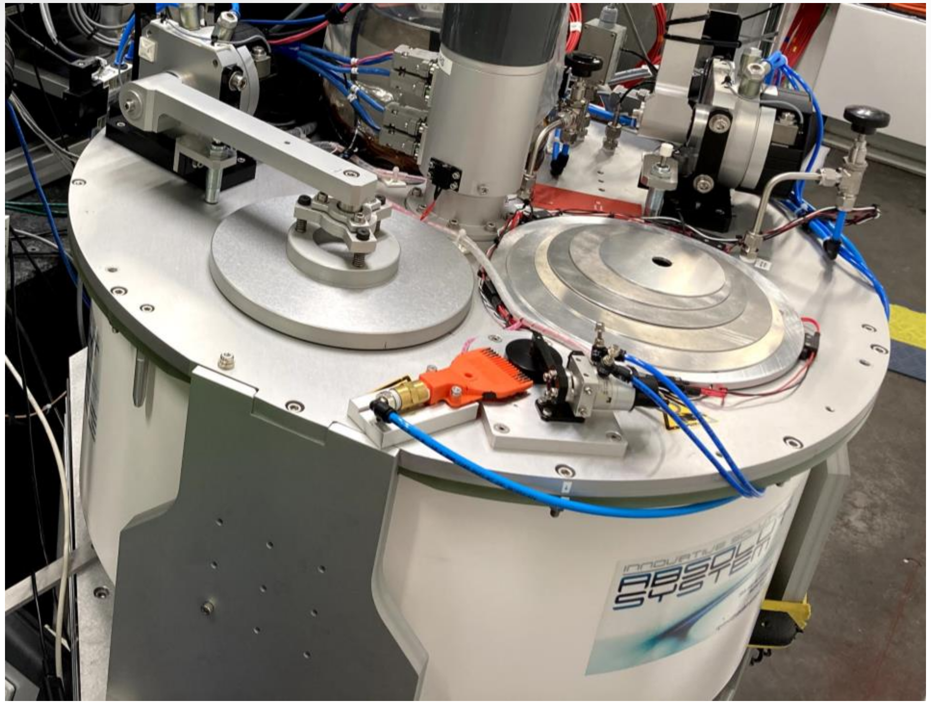
- **16 samples / H** using x-ray centering and **25 samples / H** using loop centering BUT gripper failure rate increases at > 20 sample / H

- **Faster sample exchange** will bring more samples / H

- Long term : **1000 samples / D while maintaining robustness**!!! Requires new SW and HW tools

Floating Lid (under development)





Floating lid at AMX

Hardware tested for 10 months no issues

Hurdles to overcome:

- Need to see inside dewar
- Robot needs to know where opening is on first mount

Motivation: With current lid, the faster we go, the faster ice accumulates in dewar

Kun Qian/Steven Antonelli

More diagnostics & “smart” software

- Trained control room staff to recover from known documented issues (while planning for an autonomous application)

Updates / Upgrades of the application

- Puck sensors use to detect if puck dislodged
- Puck sensors along with QR reader to scan pucks into data base
- Puck visualization- to detect if sample is safe to pick up

5 Years from now

Thoughts?

And with that I would like to thank you for your attention

Extra material

5 Years from now what I think

Monitoring services

- Ability to recover from errors without human intervention (e.g. motor out of place when robot is trying to mount)

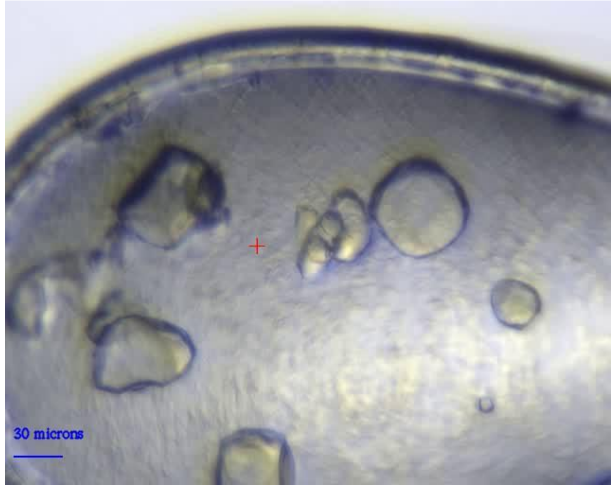
Higher throughput

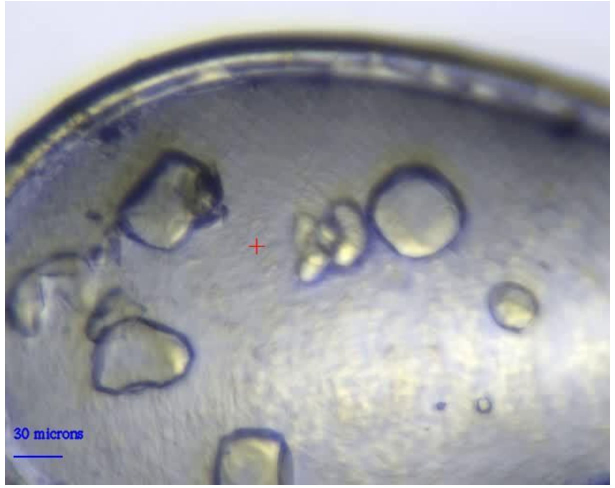
- New gripper required at > 20 samples / H (**NOTE THAT** loop centering is already > 25 samples/ H)
- Software optimization (run things in parallel)

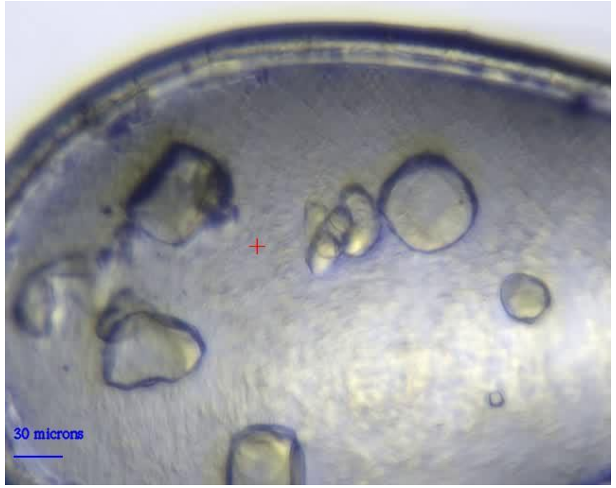
Robot Software Development Kit: (RoboDK?)

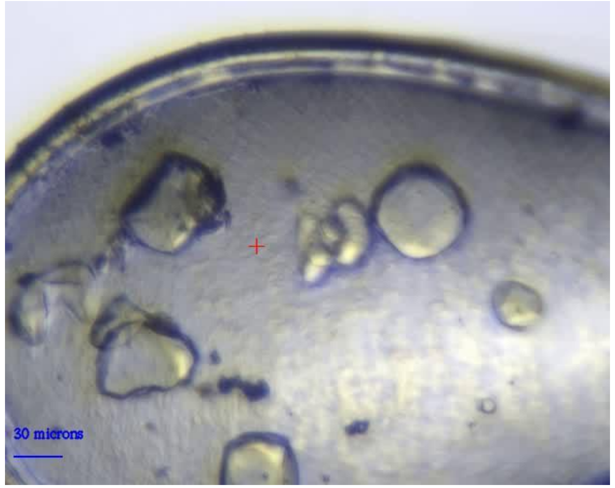
- Able to write robot code in different languages (e.g. Python)
- Easier to support different robots
- Enables better collaboration

Gripper unmount performance: preliminary results







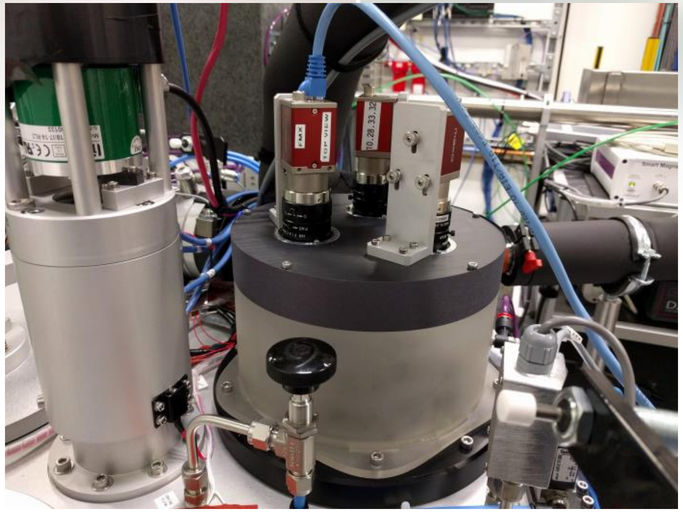


Unmounts: 0	**1**	**2**	**4**

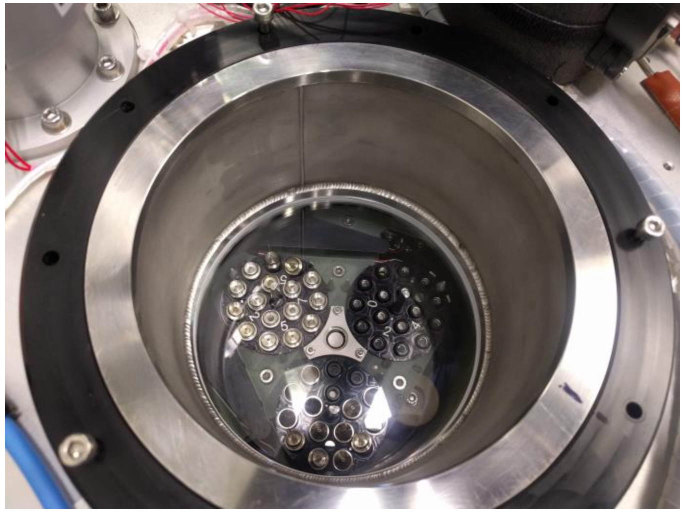
Gripper was not warmed up during this test. No X-rays available

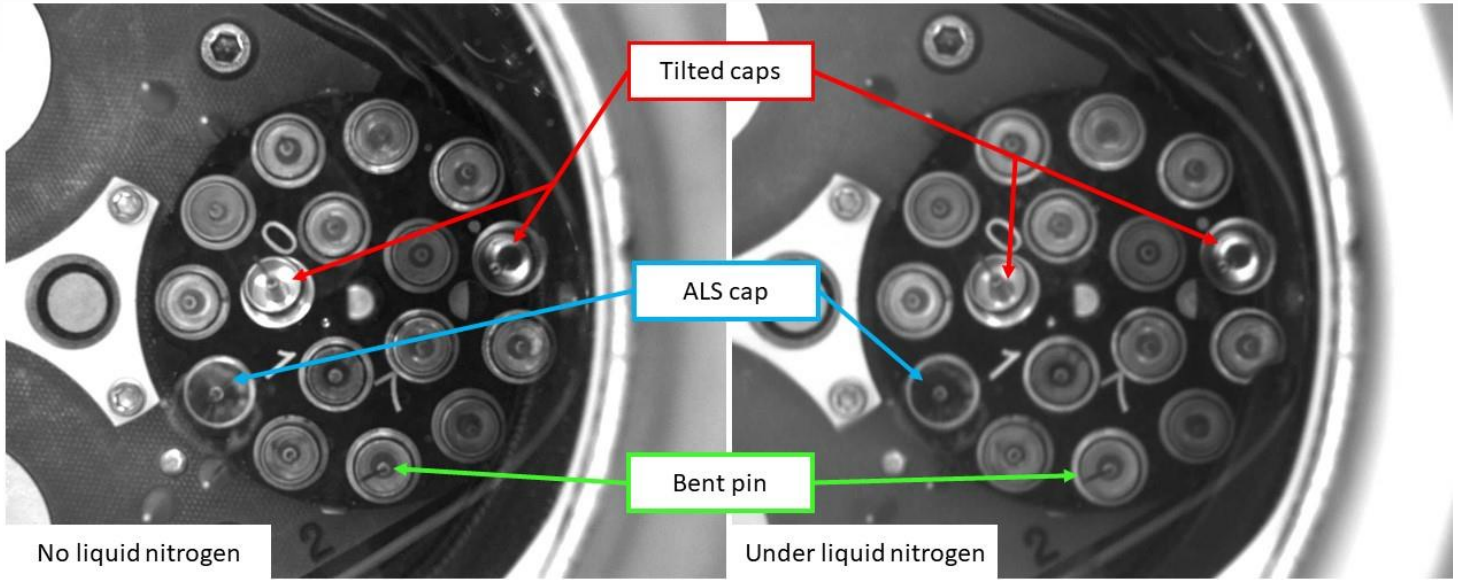
Note: First mount was done by hand

Puck Visualization (under development)



Hardware

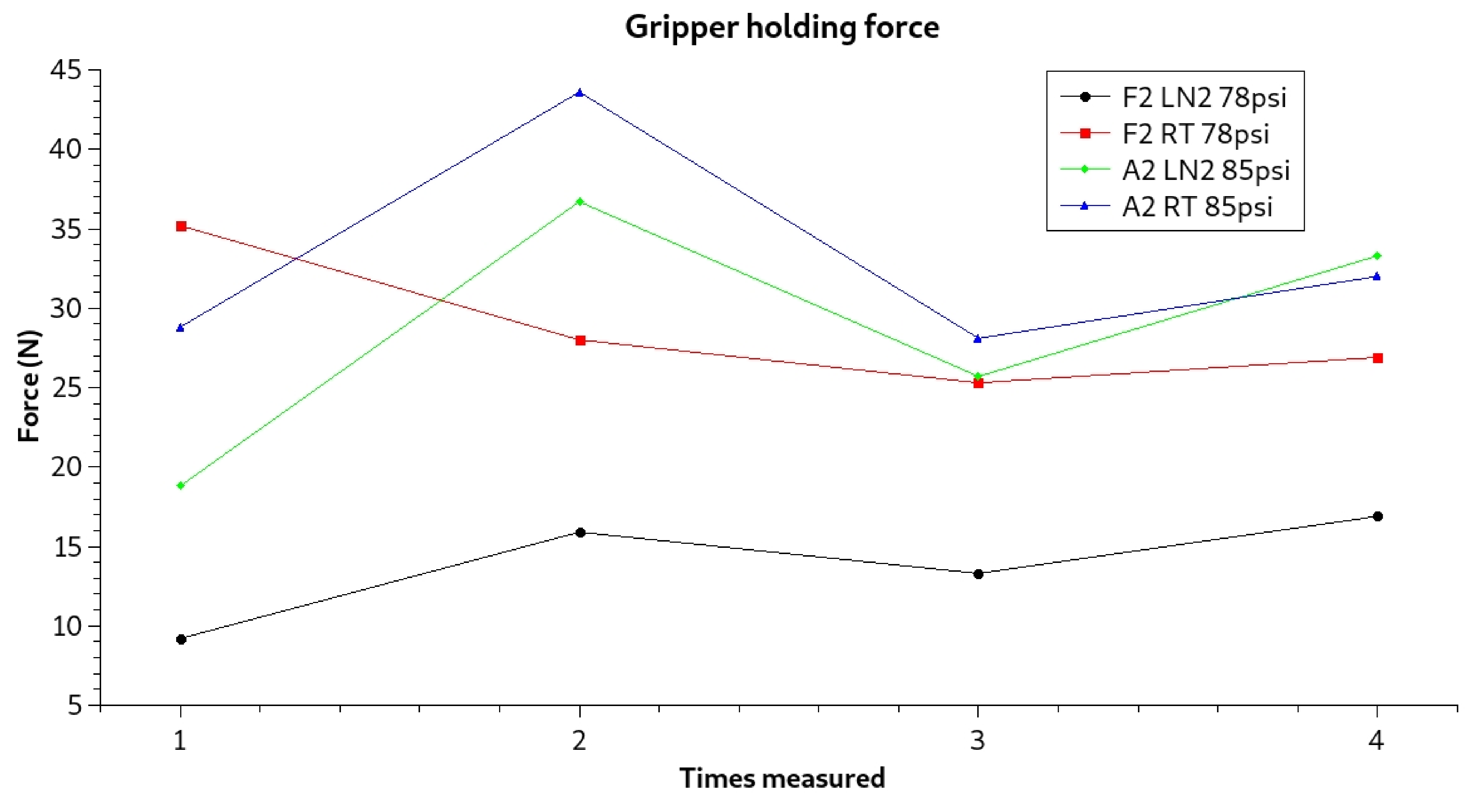




Detect samples under LN2, determines if sample is safe to pick up.

ML (TensorFlow) to train model.

Samuel Clark/Herbert Bernstein
Racheal Ng/Stephen Antonelli



Common conditions:
Manual
Robot speed 100%
0mm gap

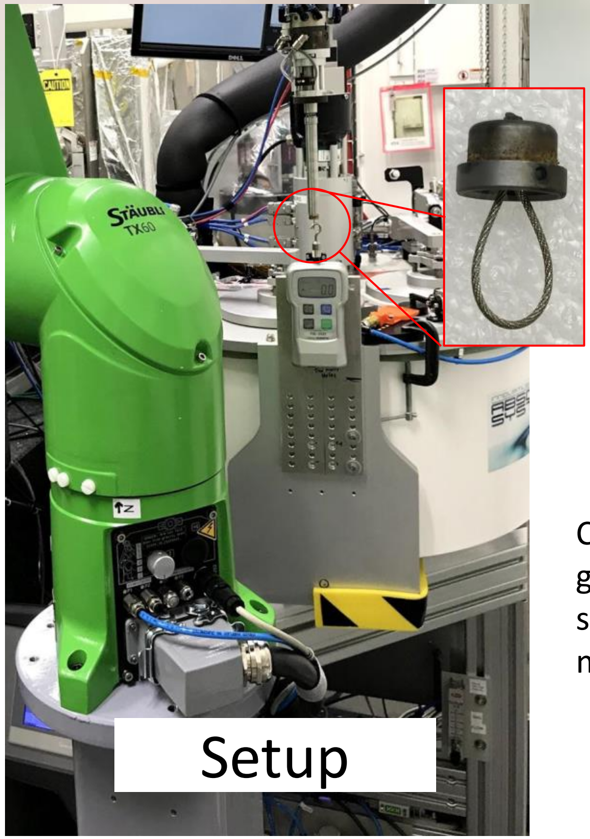
Avg. Force

A2-RT	33N
A2-LN2	29N
F2-RT	29N
F2-LN2	14N

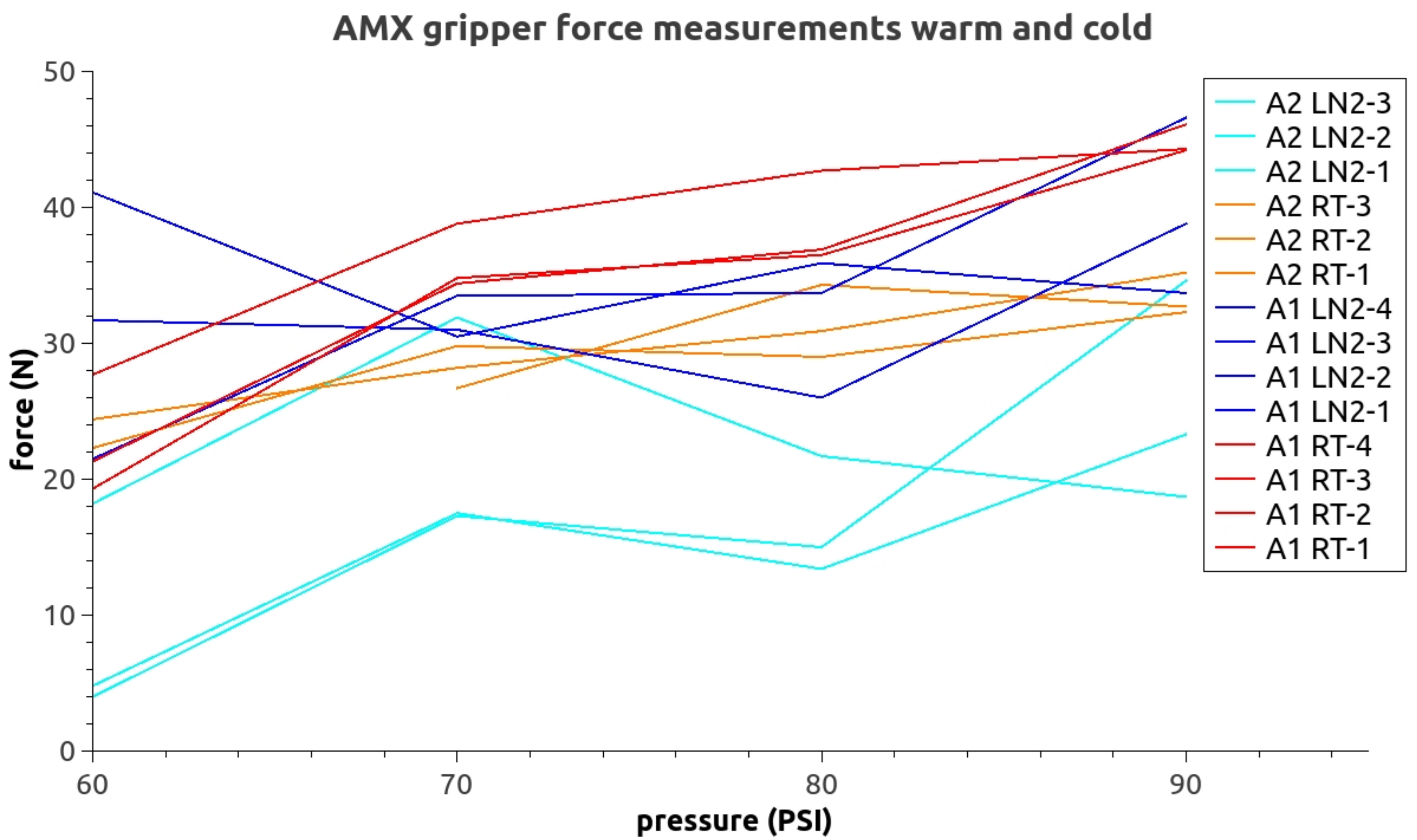
F2 gripper has weaker holding force than A2 gripper, psi?

Graph is in here: /media/elazo/MyPassport/Nextcloud/Gripper/2020-10-16_gripper_forceMeasurements
Password: gripperforce

Force characterization on AMX grippers



Conditions: 0mm gap, 100% robot speed in manual mode



Avg. force required to pick cap from puck:
RT **2.8N**
LN2 **2.9N**

Average forces from grippers

A1-RT	22.6N @ 60 psi	36N @ 70 psi	38.7N @ 80 psi	44.9N @ 90 psi
A1-LN2	31.4N @ 60 psi	30N @ 70 psi	31.9N @ 80 psi	37N @ 90 psi
A2-RT	23.4N @ 60 psi	28.2N @ 70 psi	31.4N @ 80 psi	33.4N @ 90 psi
A2-LN2	9N @ 60 psi	22.2N @ 70 psi	16.7N @ 80 psi	25.5N @ 90 psi

A2 gripper weaker than A1 in both warm & cold. In general higher pressure higher gripping force.

Raw data is here.
Graph is in /home/elazo/Dropbox/Gripper/2019-09-01_AMX_gripper_forceMeasurements