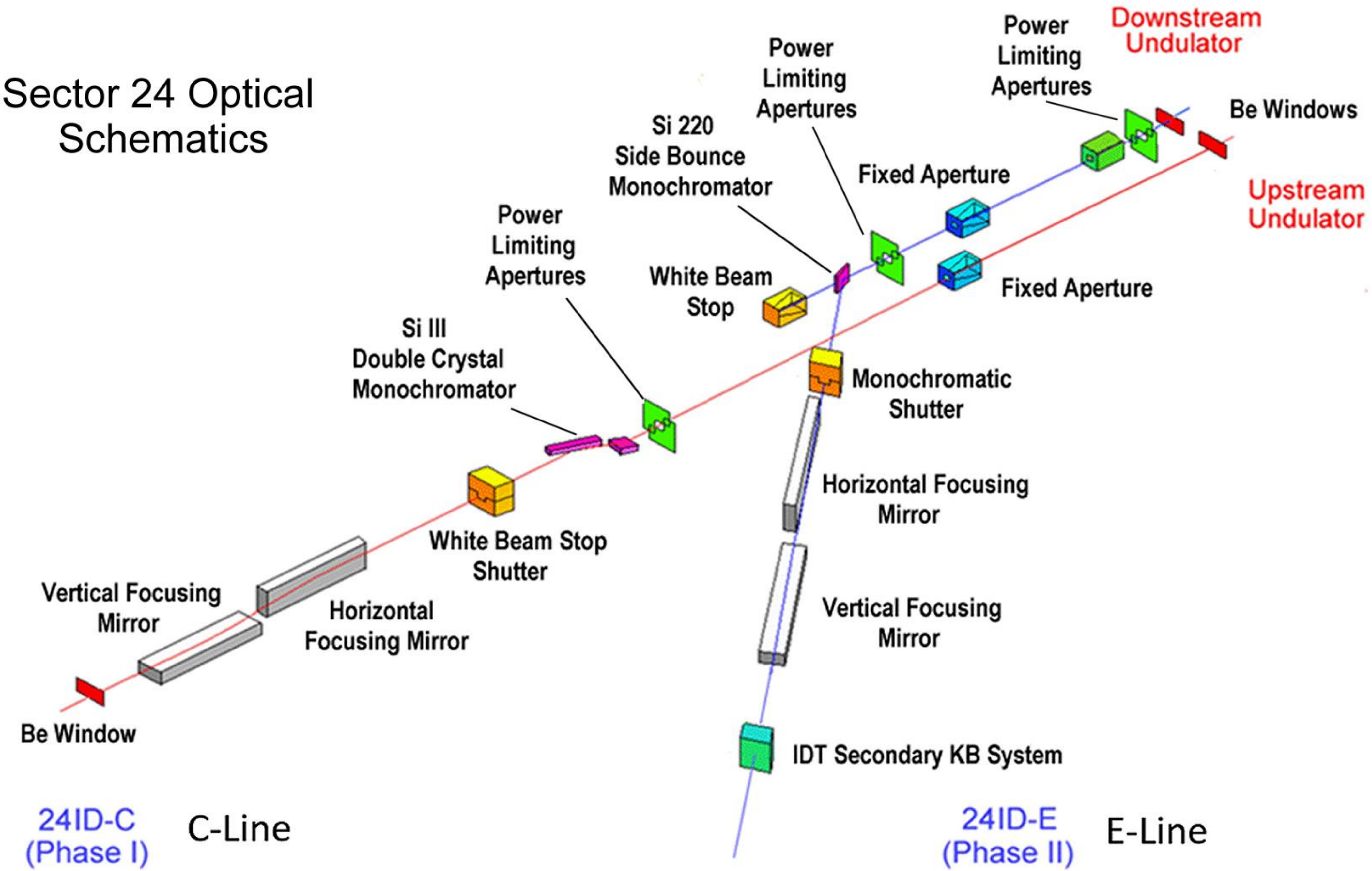
New End Stations at NE-CAT:
MD3UP Microdiffractometer & 30 Puck ALS-style Loader.

Malcolm Capel, Deputy Director NE-CAT, APS
Dept. Chemistry & Chemical Biology
Cornell University

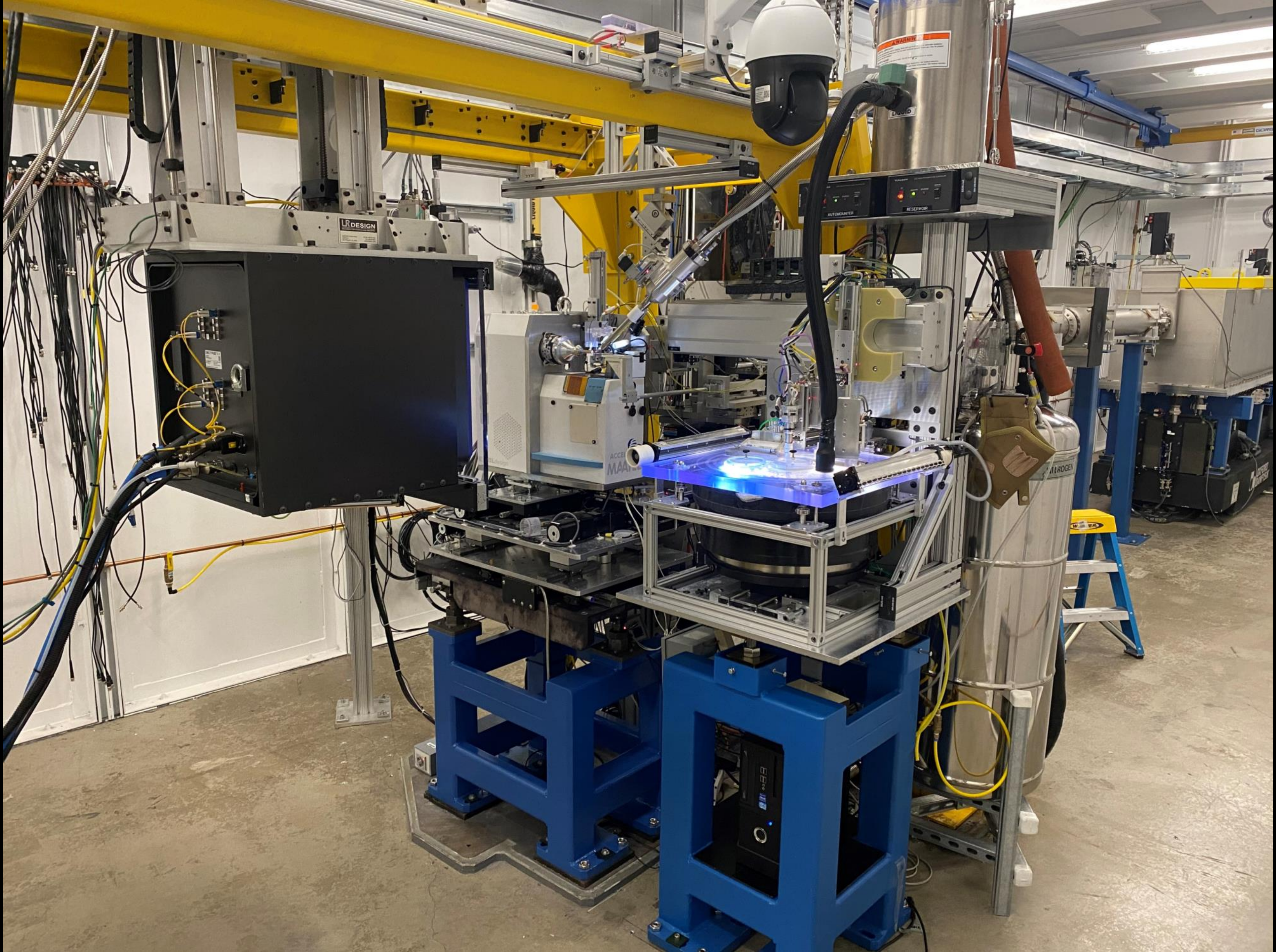
March 16, 2021

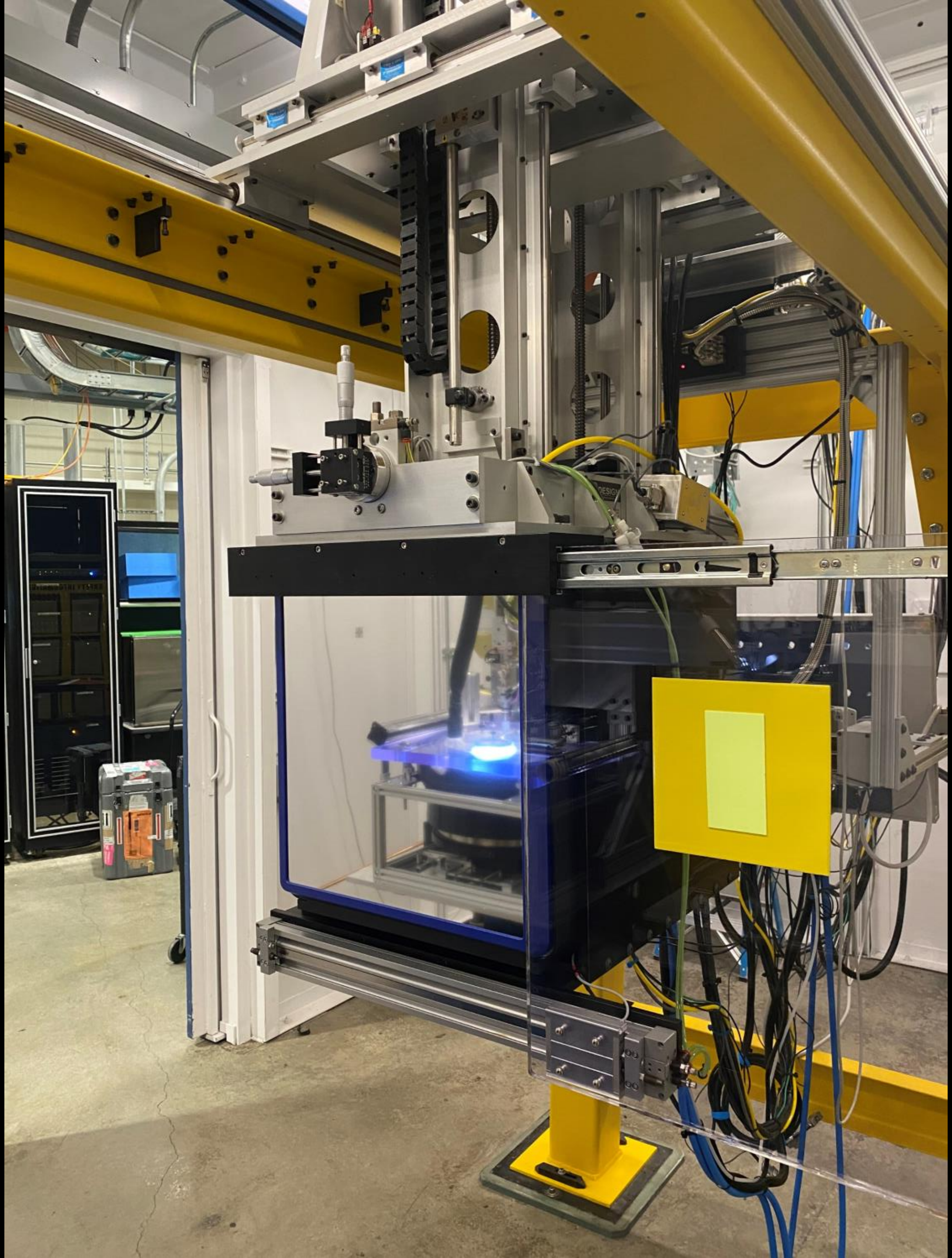
Sector 24 Optical Schematics

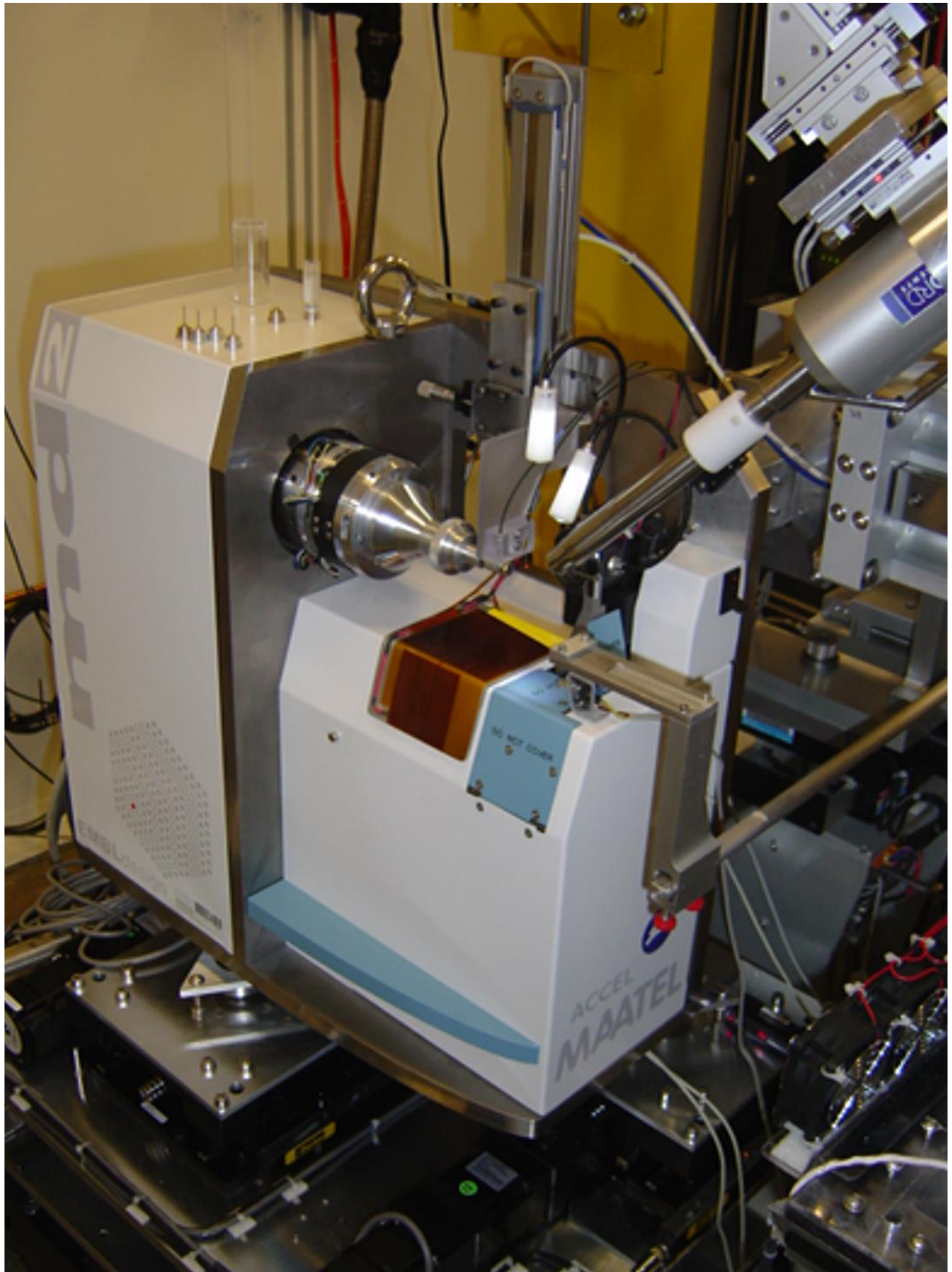


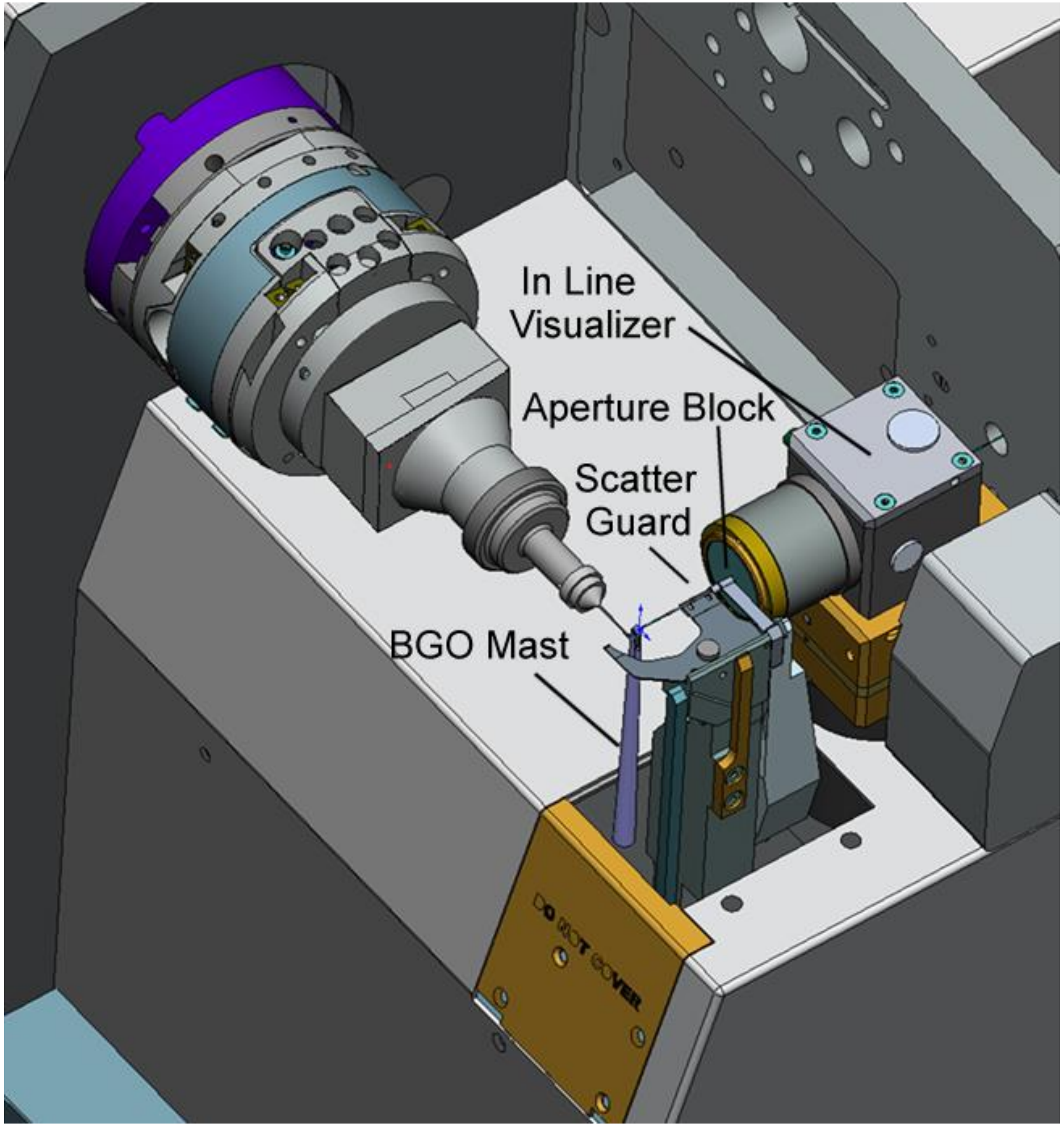
Beam Line Optical Parameters

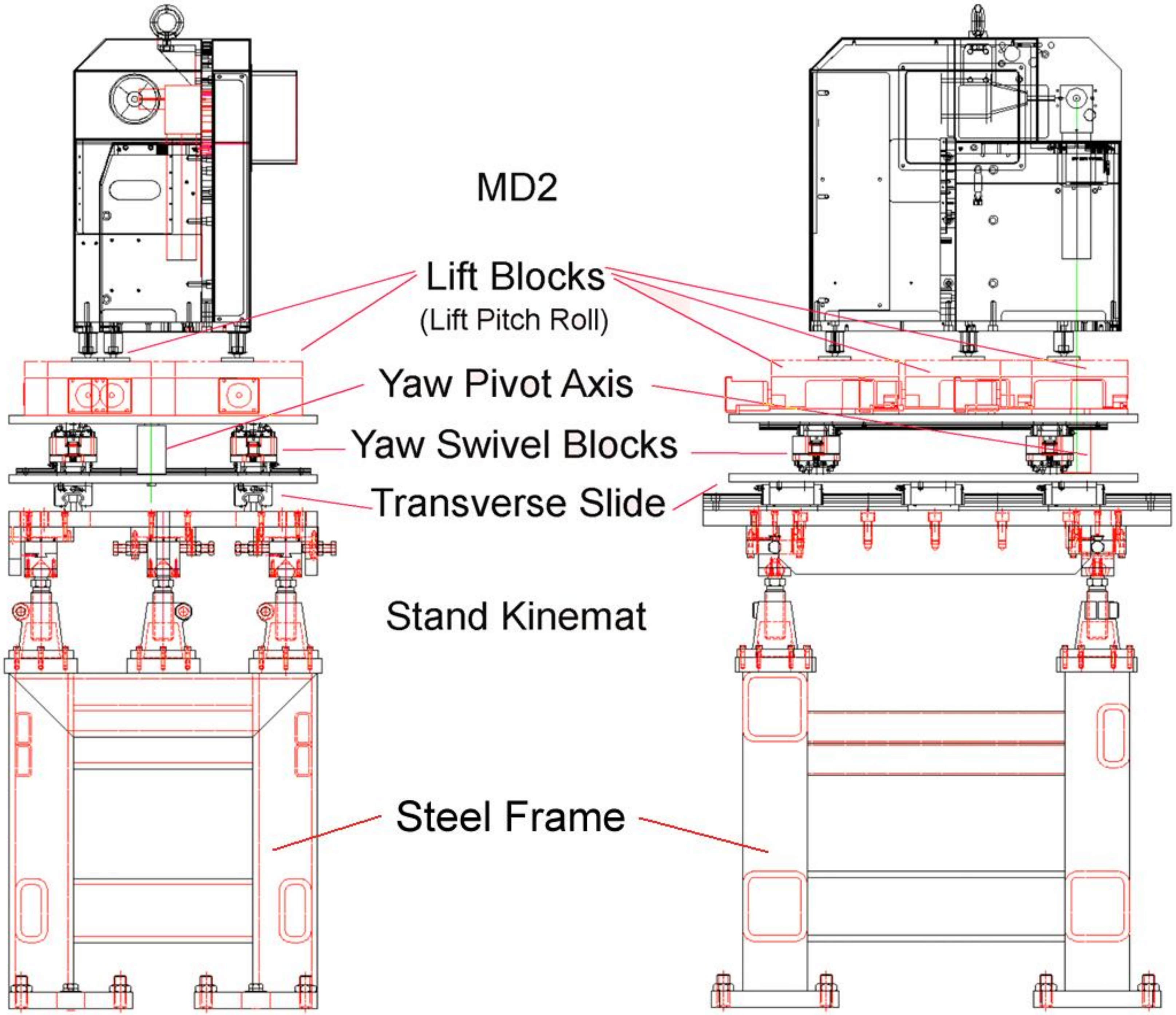
Optical Property	24_ID_C	24_ID_E
Spectral Range	6 – 20 KeV	12.66 KeV
Spectral Bandwidth	1×10^{-4} Δλ / λ	2×10^{-4} Δλ / λ
Total Flux 12.66 KeV	2×10^{13} phot / sec	1×10^{13} phot / sec
Best Focus	3 x 20 μ (1 σ, V x H)	4 x 38 μ (1 σ, V x H)
Positional Stability	1.5 x 2.5 μ (RMS, V x H)	0.75 x 1.0 μ (RMS, V x H)
Apertured Beam Diameter	5x70, 5x30, 5x10 μ (V x H)	5x50, 5x20, 5x5 μ (V x H)
Refocused Beam Diameter (in development)	na	5x5 μ (without aperture)


AUTOMOUNTER
RESERVOIR

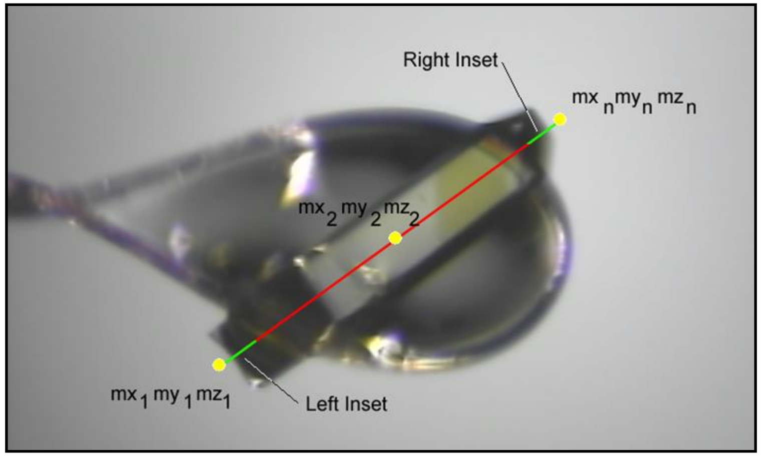





In Line Visualizer
Aperture Block
Scatter Guard
BGO Mast
DO NOT COVER

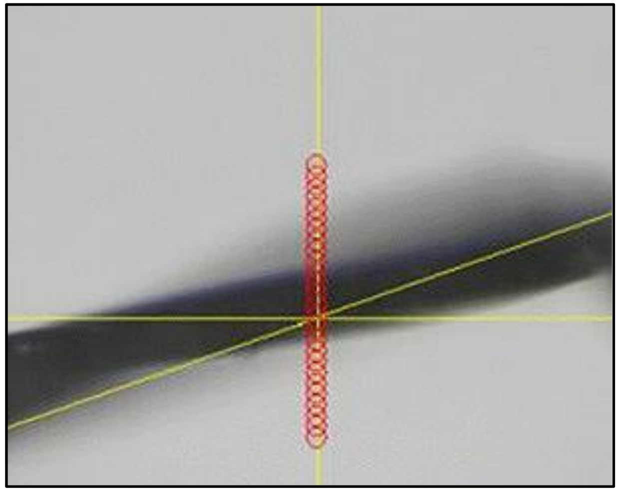

MD2
Lift Blocks
(Lift Pitch Roll)
Yaw Pivot Axis
Yaw Swivel Blocks
Transverse Slide
Stand Kinemat
Steel Frame

Scanned Data Collection Modes



Definition of Spanning Vector

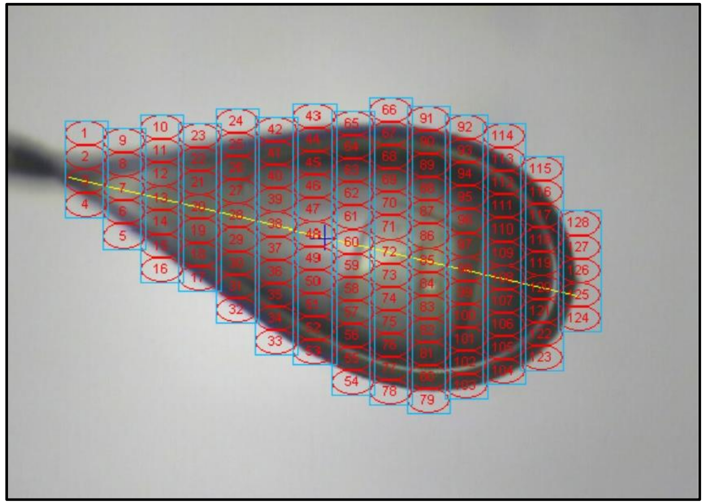
Arbitrary Vector Scan (quality, location)



Vertical Linear Scan (location)

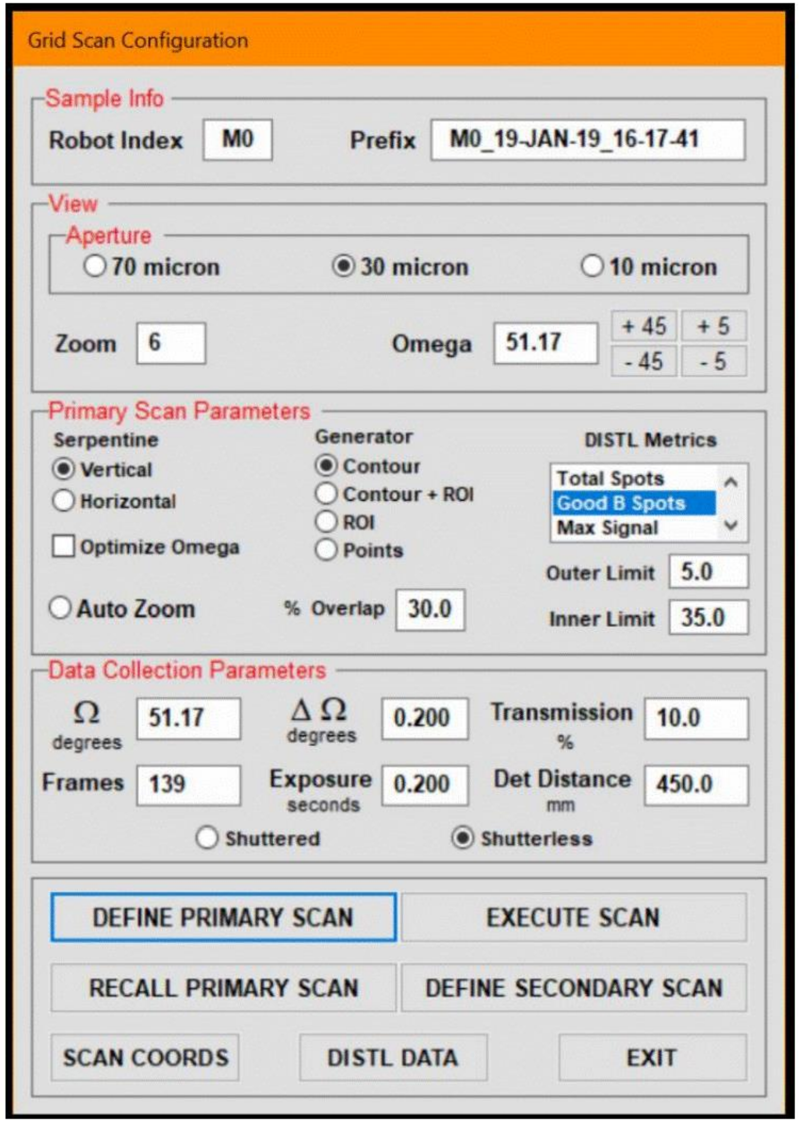
Continuous Vector Run
(dose spreading)

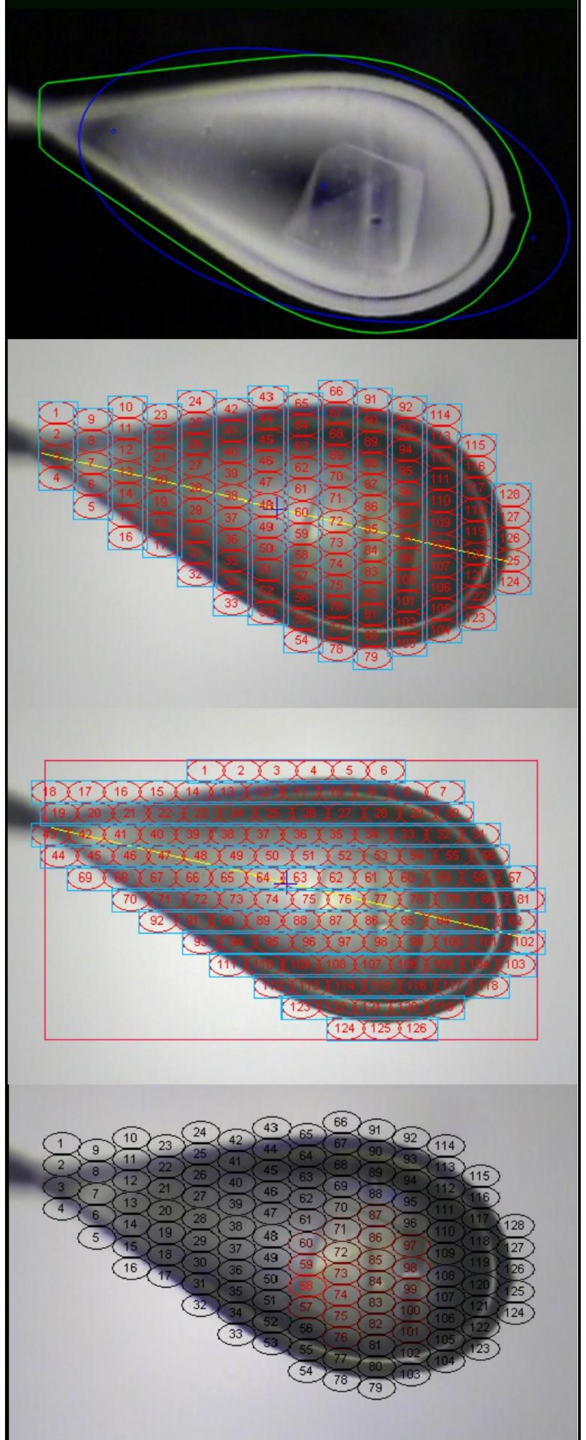
Discrete vector Run
(quality, dose spreading)

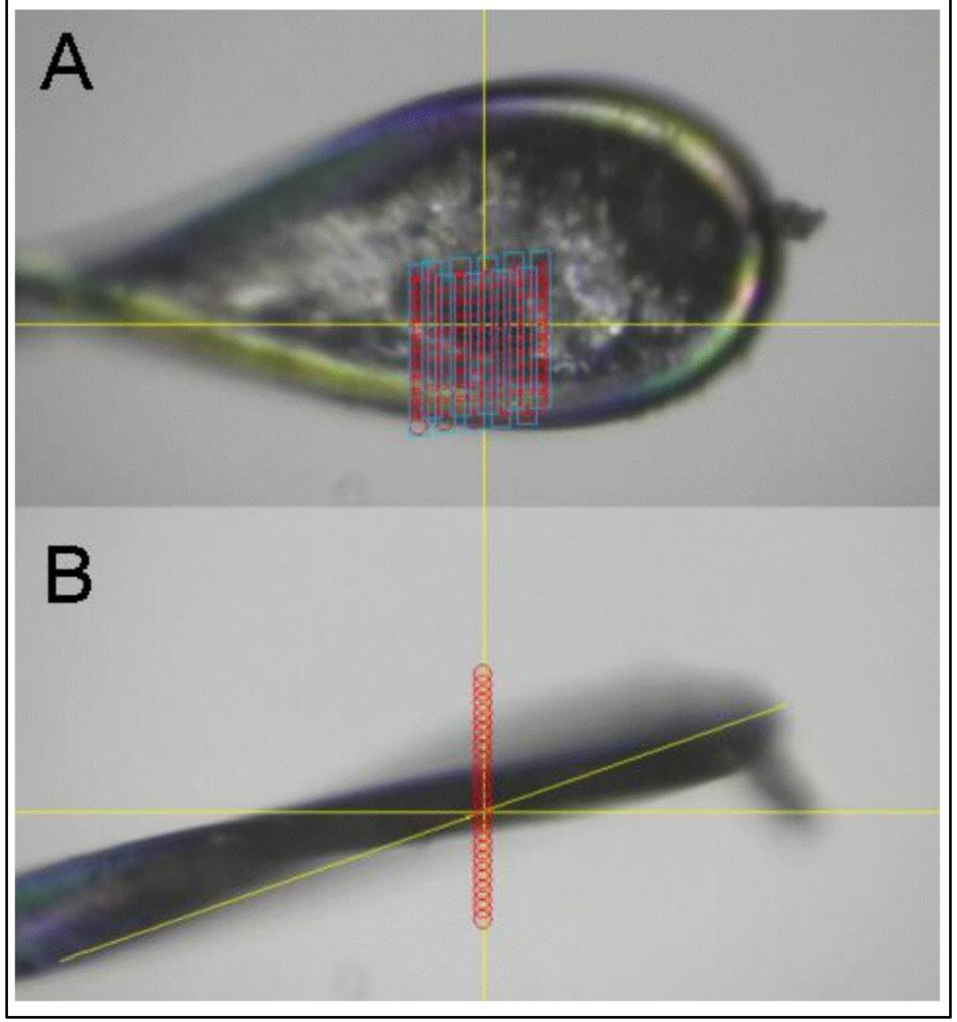


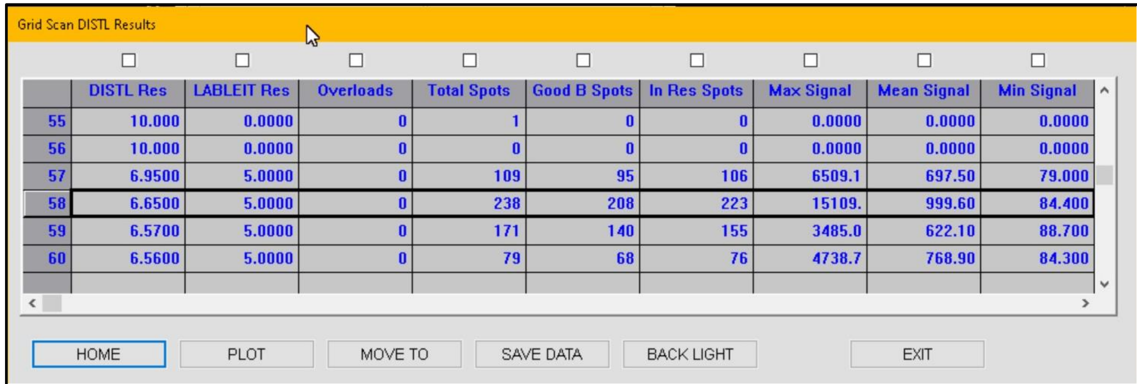
Grid Scan (location, quality)

Grid Scan Dlg









	DISTL Res	LABLEIT Res	Overloads	Total Spots	Good B Spots	In Res Spots	Max Signal	Mean Signal	Min Signal
55	10.000	0.0000	0	1	0	0	0.0000	0.0000	0.0000
56	10.000	0.0000	0	0	0	0	0.0000	0.0000	0.0000
57	6.9500	5.0000	0	109	95	106	6509.1	697.50	79.000
58	6.6500	5.0000	0	238	208	223	15109.	999.60	84.400
59	6.5700	5.0000	0	171	140	155	3485.0	622.10	88.700
60	6.5600	5.0000	0	79	68	76	4738.7	768.90	84.300

Automated Grid Scanning for Serial MX or Unattended Survey Operations

1) Auto-center sample.

2) Determine most oblate presentation (Ω angle) of sample:
   a) compute convex hull and fit ellipse to hull over an Ω samplings, subtending omega with max oblateness
   b) move to Ω angle with max fitted vertical ellipse semi major axis.
   c) auto-center loop at this Ω and re-compute convex hull.

3) Compute raster scan lines bounded by convex hull and user supplied constraints.

4) Configure and execute shutterless Eiger run over entire raster scan line set
   a) gate Eiger frame ready signal off during raster line transitions
   b) involves single Eiger arming event (Eiger arming operation is time costly)

5) Binary stream converted to CBFs on fly and submitted to multithreaded DISTL server.

6) Translate loop to coincide likely target position (determined from DISTL metrics).

7) Rotate omega 90º and execute single vertical line scan (VLS) spanning vertical hull limits above and below selected target point.

8) Move vertical alignment pseudo axis to coincide with location with best VLS DISTL metric.

9) Acquire partial rotation data set at selection loop position.

Repeat steps 2b,c and 6 through 9 to process entire loop.

For serial MX generate composite data set (cladistic merging).

For unattended survey acquire full data set at centered DISTL target locations.

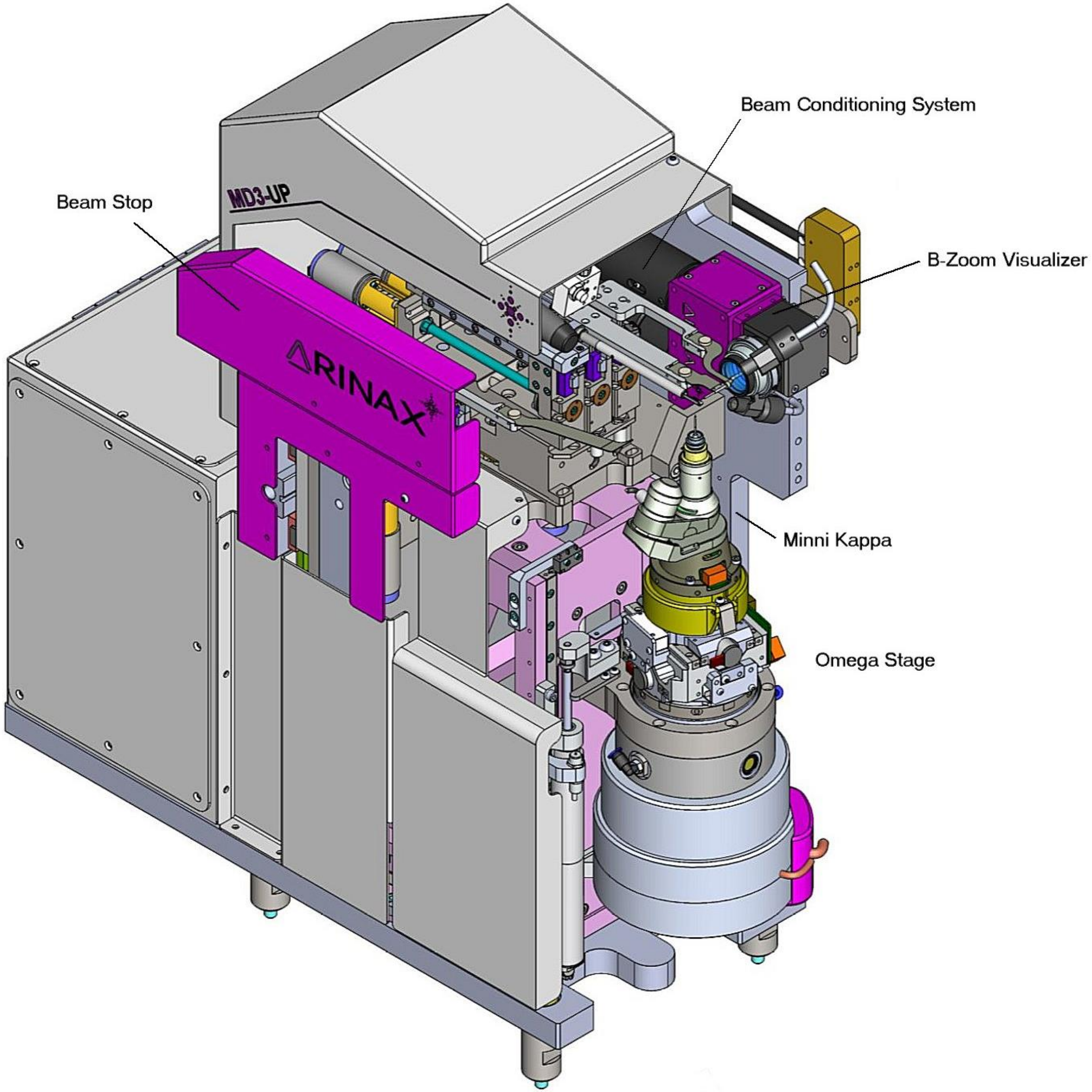
Converting from Arinax MD2 to the MD3UP Microdiffractometer

Motivation:

1) NE-CAT's MD2 microdiffractometers are 15 years old
   Spares/replacements are difficult or impossible to obtain
      Delta Tau PMAC2 components   Visualizer zoom tubes
      Arinax driver/interface boards

2) Working with progressively smaller sample crystals
   Scanning and data collection requires a spindle with reduced sphere of confusion

3) Improved sample / beam visualization



Arinax MD3UP

Vertically oriented omega axis avoids gravitational deflections of centering/ Kappa head…improved sphere of confusion.

Dual high speed digital sample and beam imager
  Eliminates fault prone Zoom tube.
  Provides higher video resolution.
  Image server software.

High speed data shutter (< 5 msec opening time)

Variable distance beam stop assembly.

Better cryostream aerodynamics in relation to cleaning capillary and aperture block manipulators

Plans for MD3UP Installation and Commissioning

Reuse most of existing MD2 support system components:

1) Precision elevation, pitch roll and yaw adjustments of the MD3, with a coordinate system centered on the MD3 aperture.

2) Existing MD2 image analysis based auto-alignment scripting will work with MD3UP with minor revisions.

3) Replace steel support frame with granite plinth.

MD3UP uses a Delta Tau Power PMAC controller with a C-like command language (no similarity to MD2's PMAC2 syntax or lexical structure).

1) Arinax provides low level drivers: Python, Epics and Tango.

2) Redis-based command interface to their low-level drivers under development.

3) NE-CAT will develop a shim driver to Redis interface to avoid reworking of existing Console scripting for MD2.

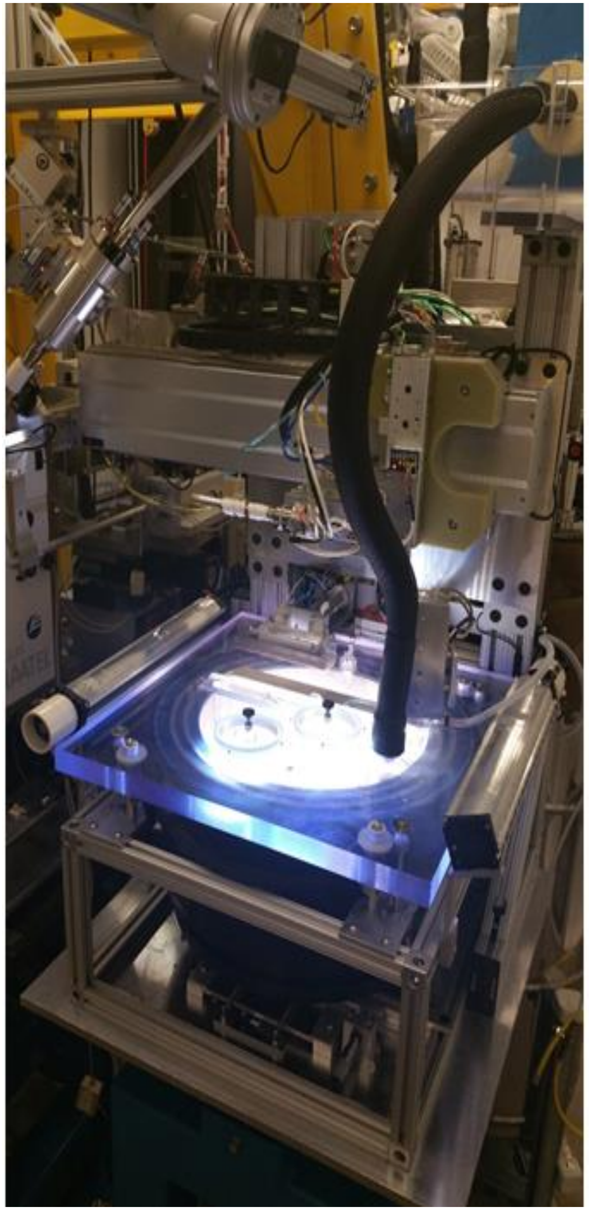
Large Magazine ALS-Style Automounter with MD3UP Compatibility

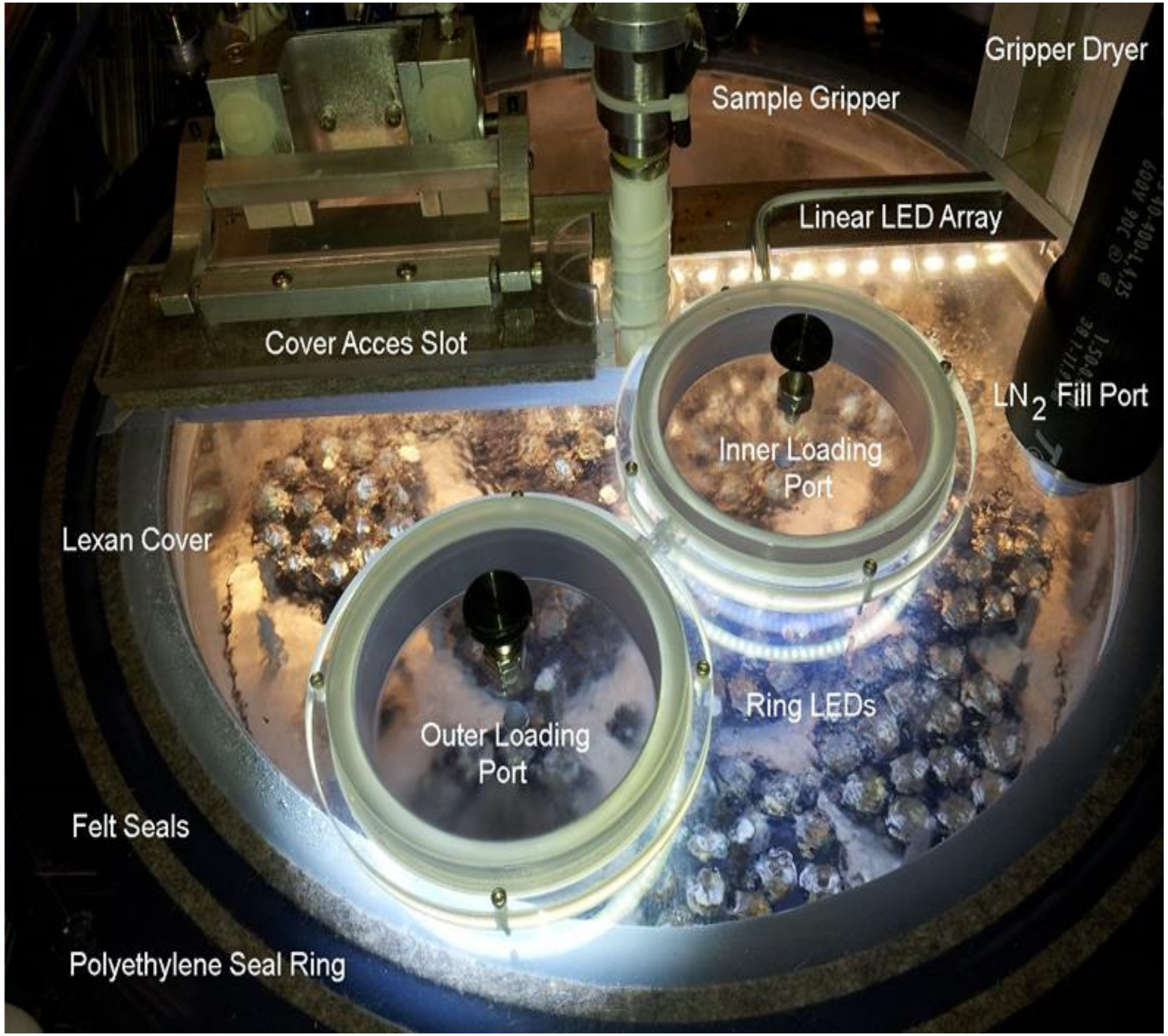
Motivation:

1) Accommodate vertical orientation of MD3UP spindle.

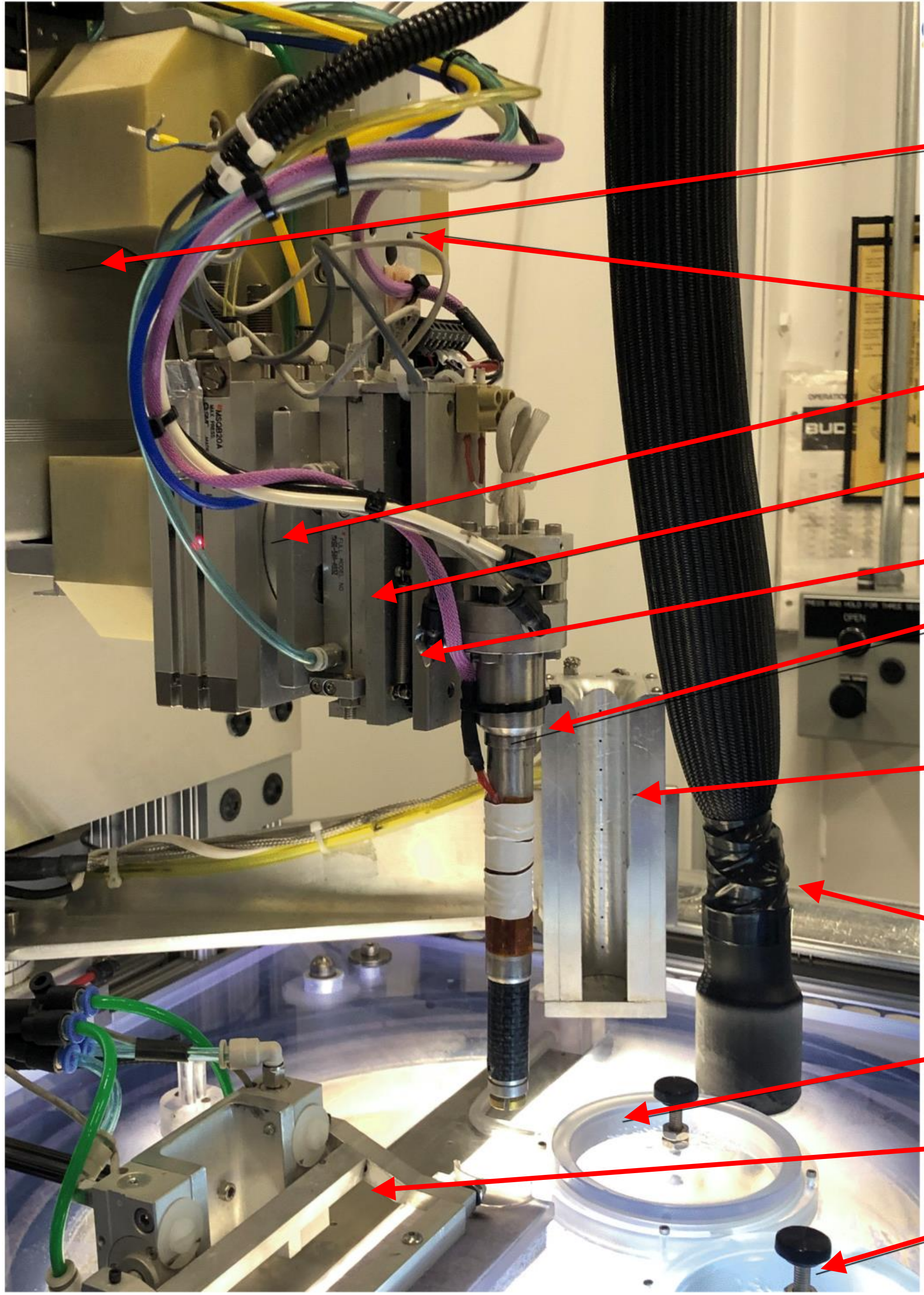
2) Increased sample capacity:
    a) Reduce frequency of staff trips to facility.
    b) Increased granularity of remote user scheduling.
    c) Facilitate unattended/fully automated sample survey and data collection.

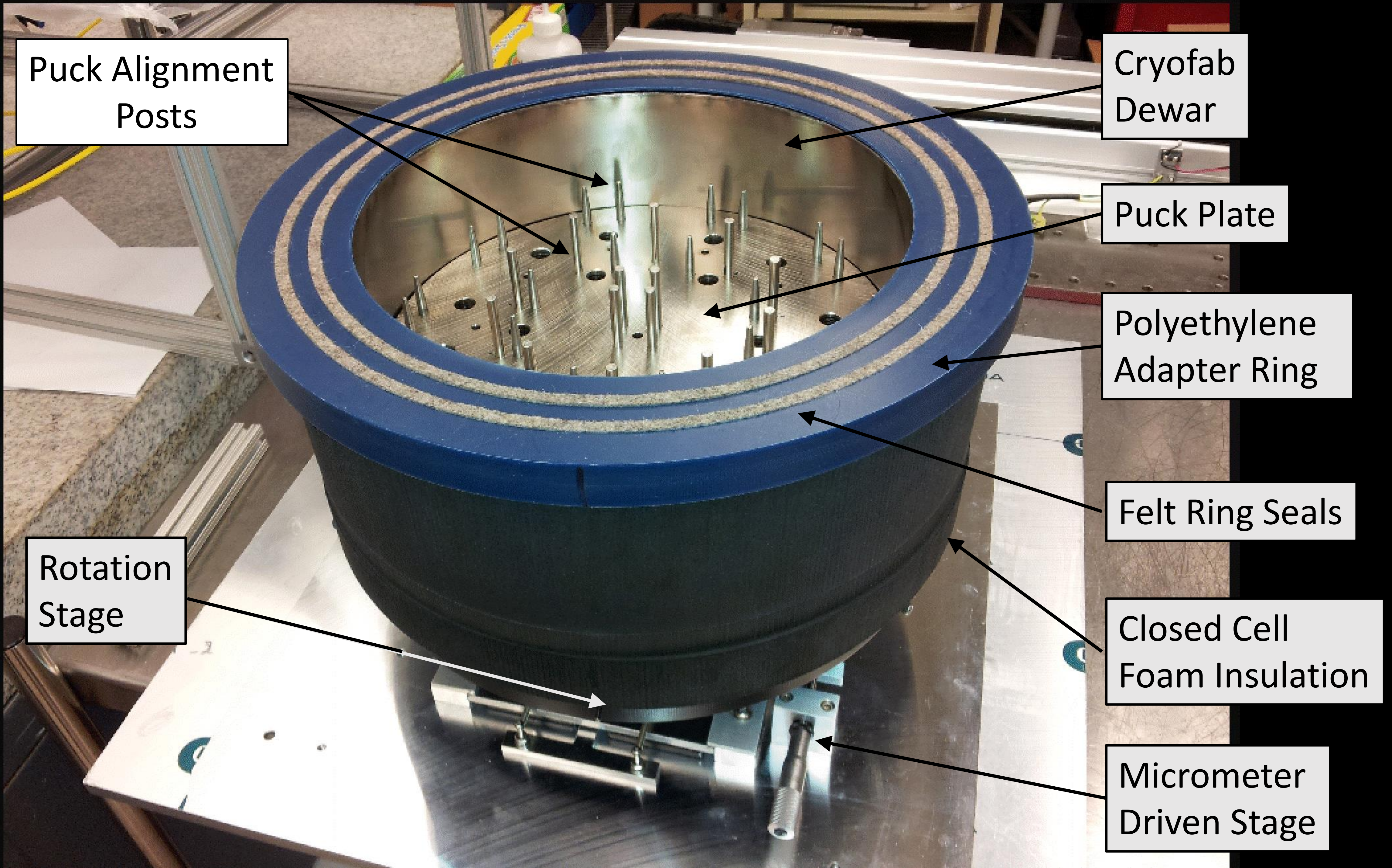
Current 14 Puck Autoloader

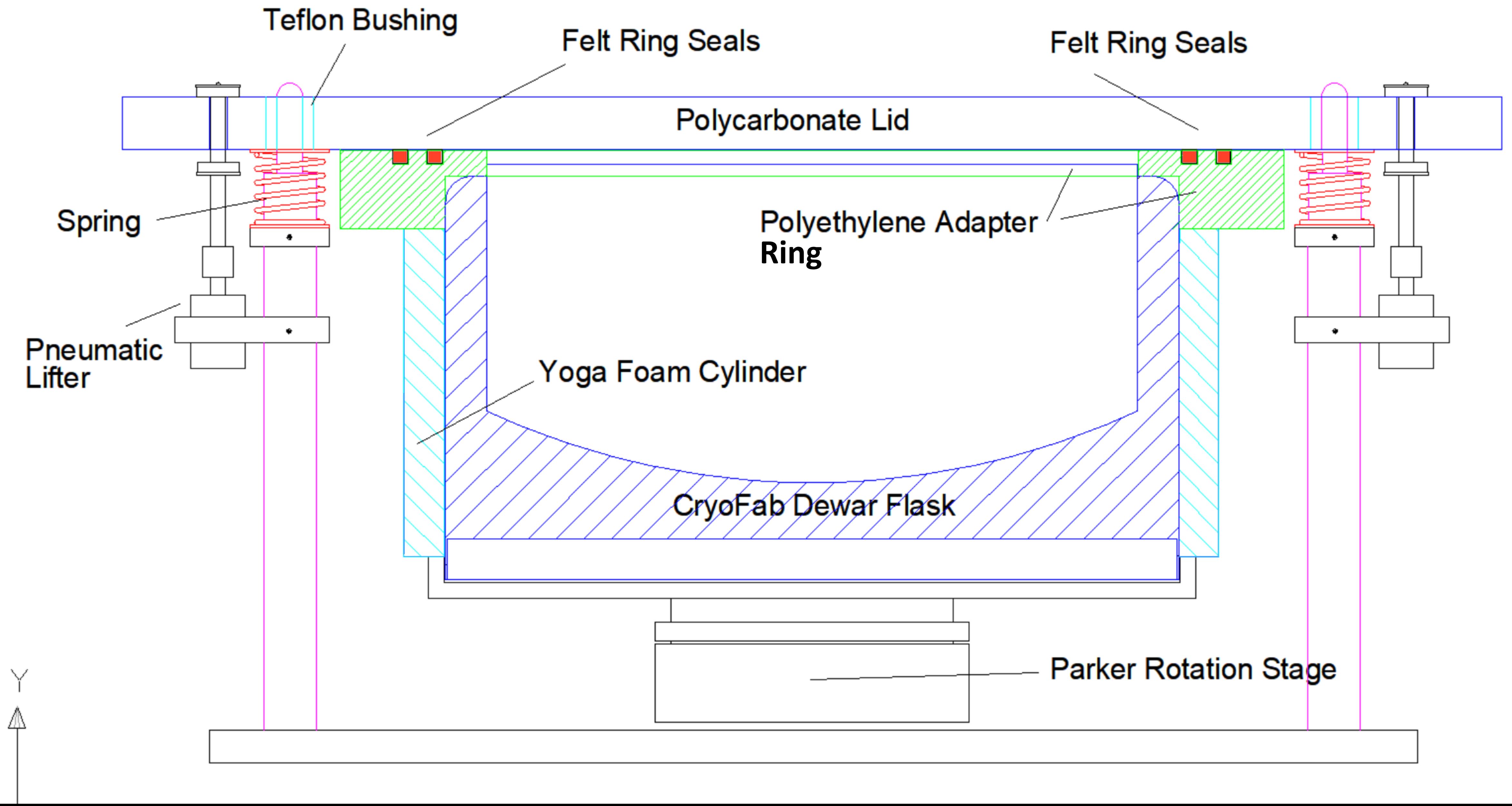


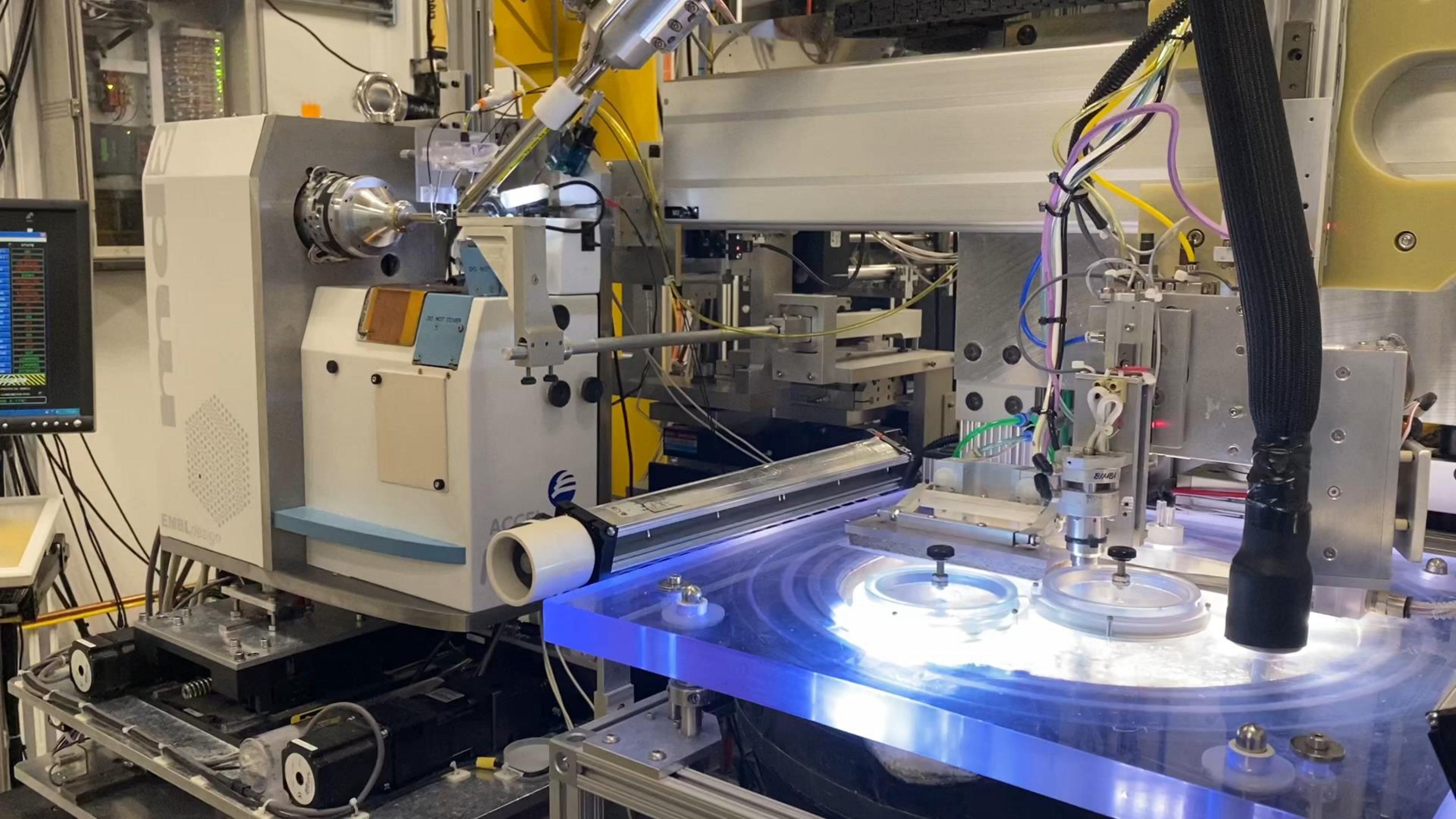


Gripper Stack




Puck Alignment Posts
Cryofab Dewar
Puck Plate
Polyethylene Adapter Ring
Felt Ring Seals
Closed Cell Foam Insulation
Rotation Stage
Micrometer Driven Stage


Teflon Bushing
Felt Ring Seals
Felt Ring Seals
Polycarbonate Lid
Spring
Polyethylene Adapter Ring
Pneumatic Lifter
Yoga Foam Cylinder
CryoFab Dewar Flask
Parker Rotation Stage
Y


DO NOT COVER
EMBL design

Redesign of NE-CAT Autoloader for Increased Capacity & Compatibility with the MD3UP

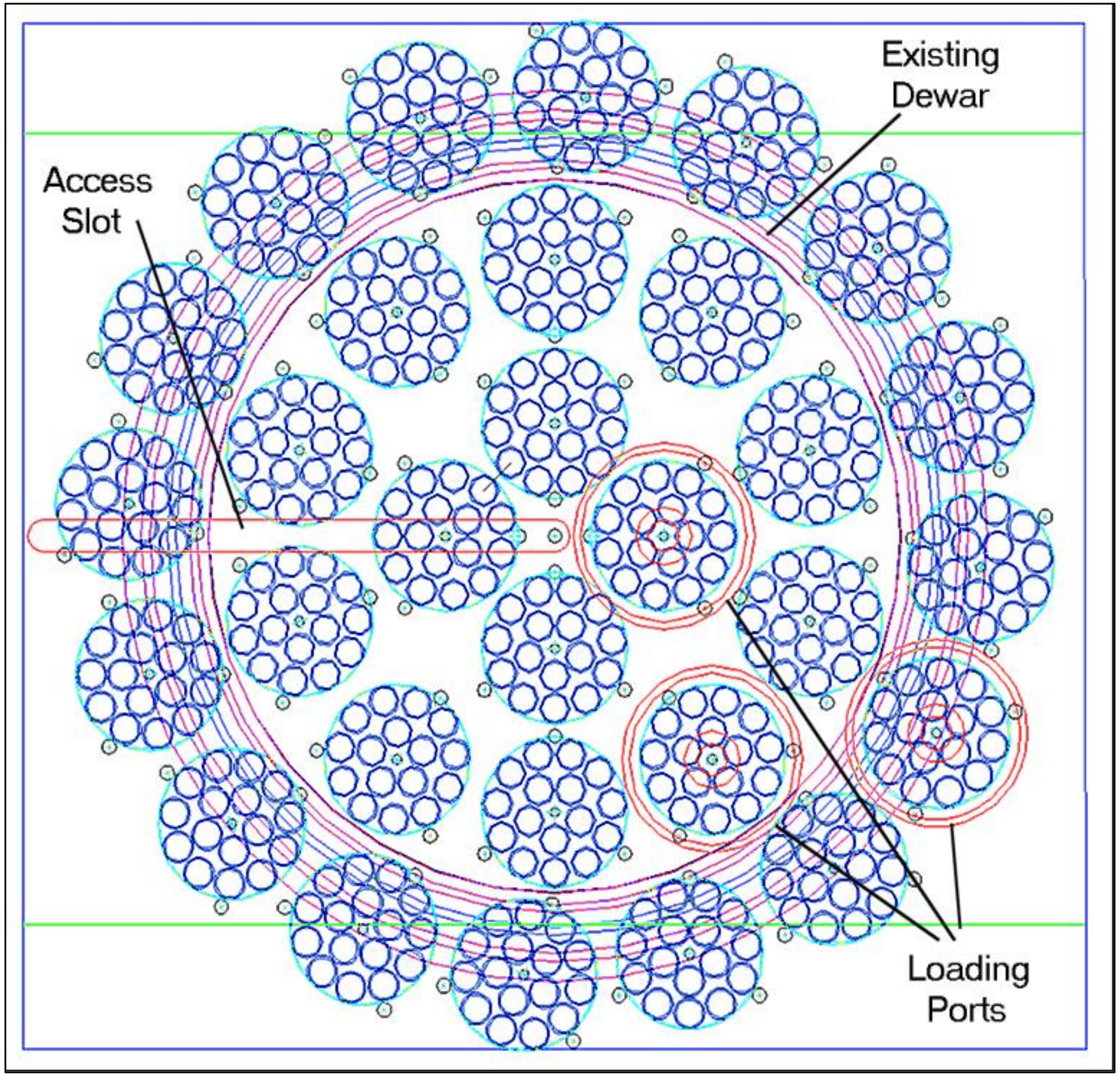
1) Modify diameter of dewar and base plates to accommodate additional outer ring of 16 pucks (total of 30) yielding a maximum sample load of 480….more than doubling current sample capacity.

2) Eliminate gripper assembly pneumatic rotation stage, increase throw of gripper assembly “vertical” pneumatic slide. Gripper remains in vertical position throughout load/unload cycle, additional clearance for MD3UP spindle.

3) Add additional small horizontal pneumatic slide to gripper assembly stack (increased separation between dewar and spindle due to size of new dewar).

4) Situate cryostream head below magnetic pulse motor rail, to project upwards towards spindle (avoids aerodynamic interactions with MD3UP’s BGO mast and beam shaper.

Puck Plate Plan View



Remaining Effort on Project

1) Design and fabricate dewar components:
   - Dewar seal assemblies
   - Puck support plates
   - Dewar rotary stage
   - Lexan dewar cover.
   - Support structure

2) Software revision
   - optimization of duty cycle (current mount-next cycle time 40 sec).

Acknowledgements

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NIGMS P30, GM124165

Mechanical Systems Detailed Design & Fabrication:
Anthony Lynch, Cornell, NE-CAT

Electronics, Driver Software:
Jim Withrow, Cornell, NE-CAT

MD2 Driver Software (PGPMAC):
Keith Brister, Northwestern, LS-CAT

Eiger Binary Stream->CBF Converter, High Performance DISTL Server:
John Schuermann, Cornell, NE-CAT

Remote Interface Software:
Frank Murphy, Cornell, NE-CAT

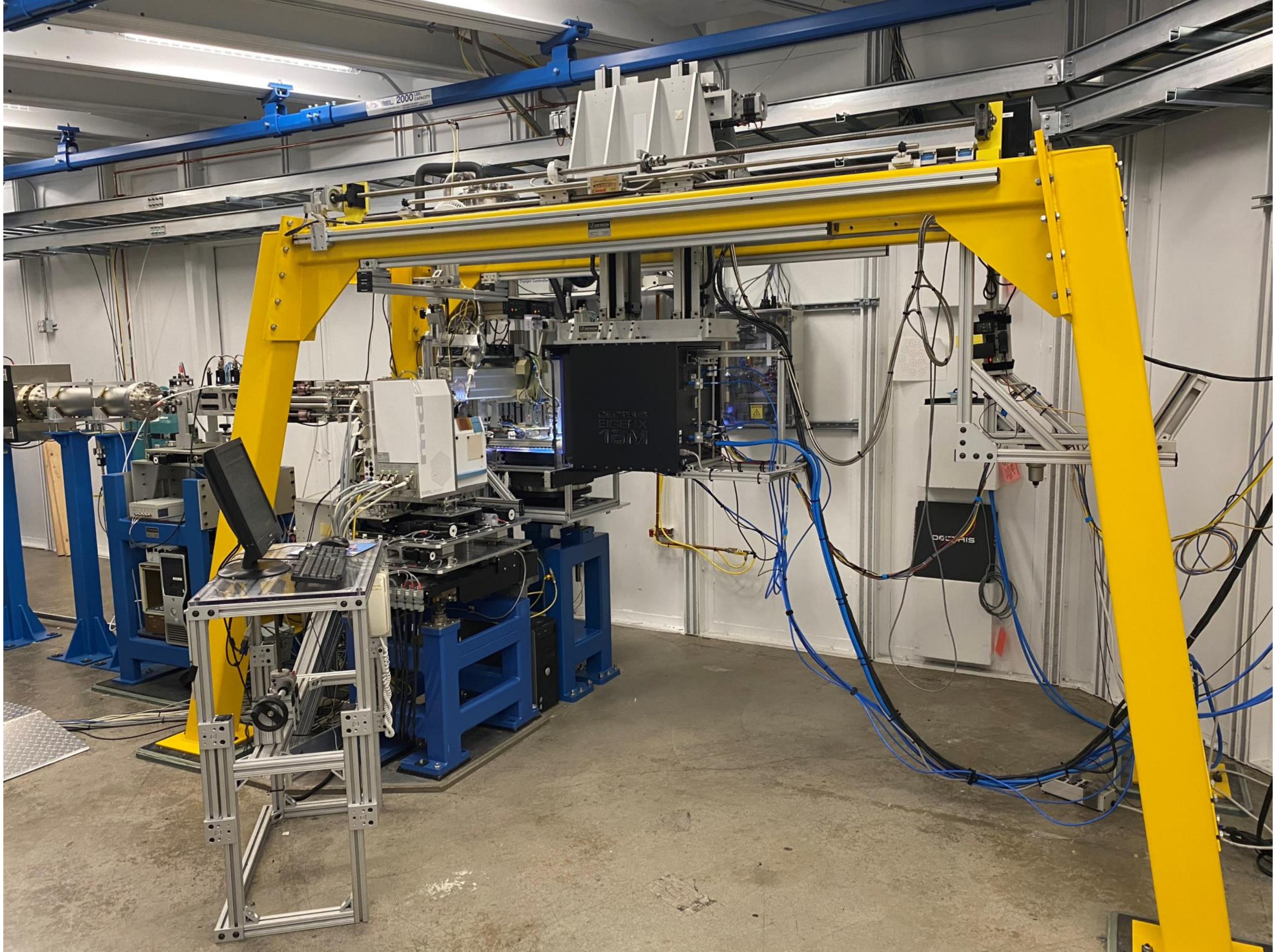
Design, High Level Controls & Scripting:
Malcolm Capel, Cornell, NE-CAT

Auxiliary Slides

Comparison: MD2 MD2-S MD3

Device / Specification	MD2	MD2-S	MD3
Control System **CPU** **CPU Clock** **Ethernet**	Delta Tau PMAC CPCI 80/230 MHz 1 GHz	Omron/Delta Tau Power Brick 1 GHz 1 GHz	Omron/Delta Tau Power Brick 1 GHz 1GHz
Visualizer System **Resolution Pixels** **Scale Range µm / pixel**	OAV Navitar Zoom Tube Analogue Camera 659 x 493 0.27 – 27.0	B Zoom Fixed Achromats Dual Digtial Cameras 2560 x 2048 0.16 – 1.9	B Zoom Fixed Achromats Dual Digital Cameras 2560 x 2048 0.16 - 1.9
Omega Stage **Sphere of Confusion** **Angular Resolution** **Max Angular Speed** **Dynamic Accuracy**	2 µm 0.1 mdeg 120 deg/sec +/- 1 mdeg	2 µm 0.1 mdeg 720 deg/sec +/- 1 mdeg	100 nm 0.1 µdeg 720 deg/sec +/- 0.5 µdeg
CX,CY Centering Table **Range** **Resolution** **Repeatability**	Open Loop Steppers 6 mm 5 nm +/- 2 µm	Open Loop Steppers 6mm 5 nm +/- 2 µm	Encoded Steppers 5mm 10 nm +/- 100 nm
Beam Conditioning Axes **Aperture Horizontal** **Max Speed** **Resolution** **Repeatability** **Aperture Vertical** **Max Speed** **Resolution** **Repeatability**	2 mm/sec 16 nm 1 µm 2 mm/sec 16 nm 1 µm	2 mm/sec 16 nm 1 µm 10 mm/sec 45 nm 1 µm	2 mm/sec 16 nm 1 µm 10 mm/sec 45 nm 1 µm

Device / Specification	MD2	MD2-S	MD3
Cleaning Capillary Horizontal **Max Speed** **Resolution** **Repeatability** **Cleaning Capillary Vertical** **Max Speed** **Resolution** **Repeatability** **BGO Mast Vertical** **Max Speed** **Resolution** **Repeatability**	2 mm/sec 16 nm 2 µm 20 mm/sec 90 nm 2 µm 8 mm/sec 97 nm 2µm	2 mm/sec 16 nm 2 µm 20 mm/sec 90 nm 2 µm 20 mm/sec 97 nm 2 µm	2 mm/sec 16 nm 2 µm 3.8 mm/sec 50 nm 2µm 20 mm/sec 97 nm 2 µm
Beam Stop Motions **Parallel to Beam Axis** **Range** **Resolution** **Repeatability** **Perpendicular to Beam Axis** **X,Y** **Range** **Resolution** **Repeatability**	NA NA	NA NA	89 mm 1.5 µm 2 µm 4 mm, 4 mm 3 nm, 3 nm 2 µm, 2µm
Rough Pricing **Base** **+MK3** **+Beam Stop**	NA	$418K	$605


DECTRIS


CRYOFAB
WARNING
LIQUID
RESERVOIR

Puck Plate Sub Base Plate

Material $\frac{3}{8}$" Low Carbon Steel ground top and bottom 16" x 16" all holes .251" (45 total)

Puck Plate