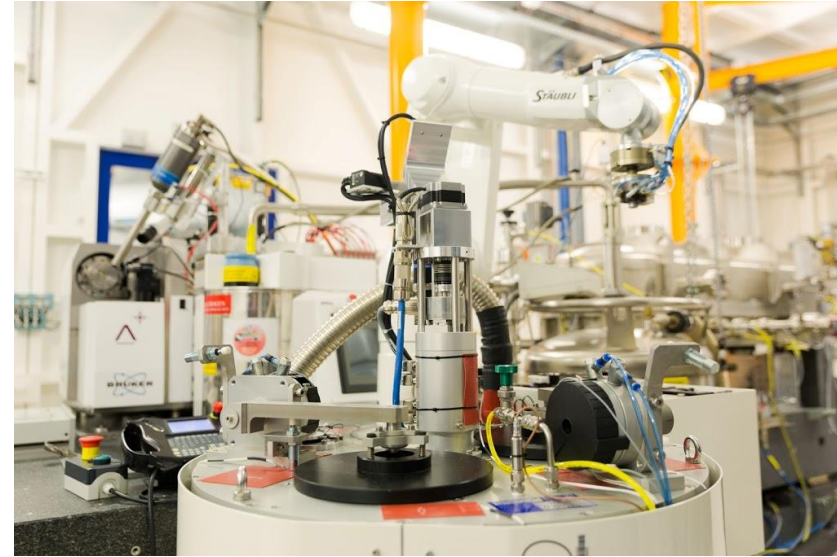


# CrystalDirect-to-Beam pipeline and FlexHCD sample changers at ESRF

Gergely PAPP

# Agenda

- FlexHCD sample changers:
  - Current status
  - Future perspectives
  - eCryoID sample tracking
- CrystalDirect-to-Beam
  - Proof of concept at ID30B
  - Massif1 fully automated beamline



# Agenda

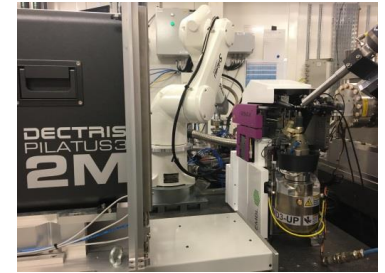
- FlexHCD sample changers:
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# FlexHCD sample changers @ ESRF

EMBL – ESRF  
collaboration

- All ESRF MX beamlines are equipped
  - ID30B
  - Massif 1, Massif 3
  - ID23\_1, ID23\_2
  - ID29 in the near future
- Same control software (since December 2020)
  - Low level StaubCom server on robot controller
  - High level Java software
  - Straightforward integration into MxCube3



StaubCom

Java

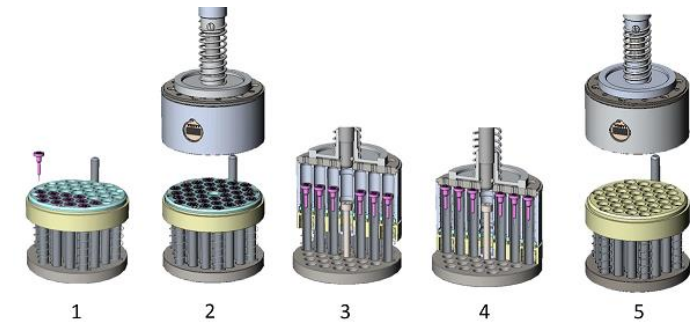
MxCube

# FlexHCD – Sample holder compatibility

	ID30B	Massif 1	Massif 3	ID23_1	ID23_2
SPINE – SC3 pucks	Fade out				
SPINE - Unipuck	Yes (single & double gripper)	Yes (single & double gripper)	Yes	Yes	Yes (single & double gripper)
miniSPINE	Yes (single & double gripper)				

# FlexHCD – miniSPINE compatibility

- New harvesting & storing tool for miniSPINE
  - Easier handling
- Same footprint than Unipucks
  - Immediate compatibility with FlexHCD dewars
- To make a beamline compatible:
  - Update of smart magnet for a parallel pole model
- Storage capacity:
  - With Unipucks  $24 \times 16 = 384$
  - miniSPINE  $24 \times 36 = 864$
  - 24 hour turnover  $2 \text{ min/pin} = 720$

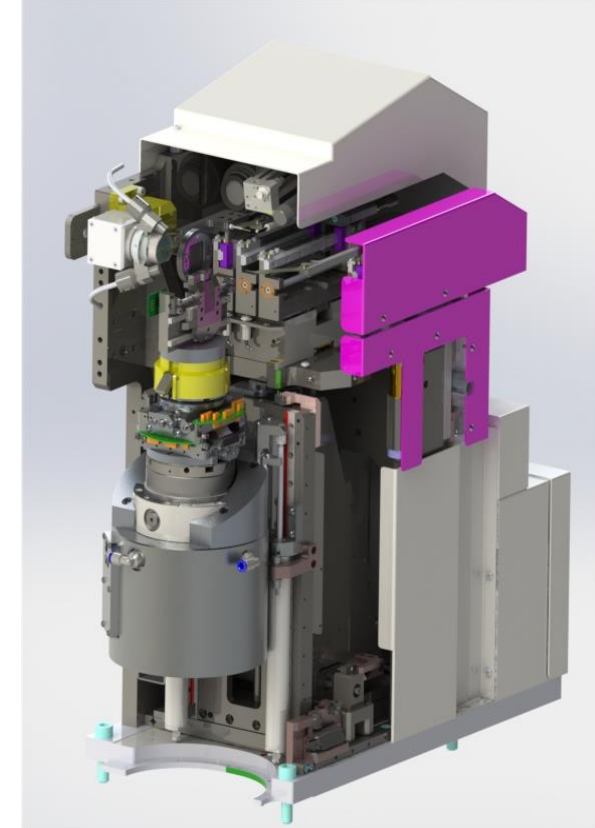
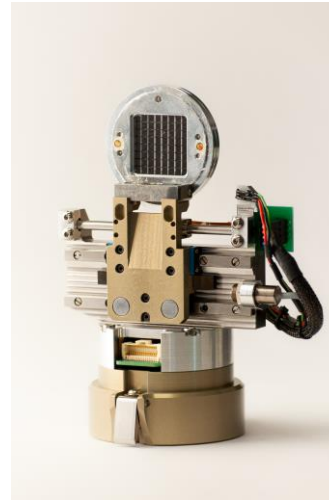


# FlexHCD – Sample holder compatibility perspectives

	ID30B	Massif 1	Massif 3	ID23_1	ID23_2
SPINE – SC3 pucks	Yes		Yes	Yes	
SPINE - Unipuck	Yes (single & double gripper)	Yes (single & double gripper)	Yes	Yes	Yes (single & double gripper)
miniSPINE	Yes (single & double gripper)	(Yes)	(Yes)	(Yes)	(Yes)

# FlexHCD – transfer of SSX samples

- Development of a fast scan head for MD3up goniometers
- First integration on ID29 in April 2021
  - Chopper synchronization 1kHz
  - Speed 30mm/sec
  - Precision  $\pm 1\mu\text{m}$
- Automated sample transfer with Flex sample changer



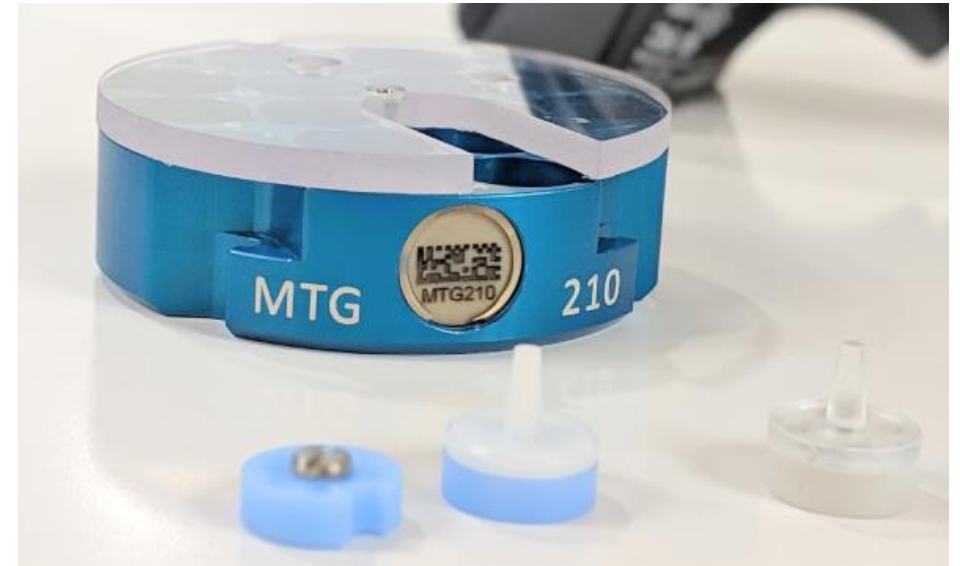


# FlexHCD – Sample holder compatibility perspectives

	ID30B	Massif 1	Massif 3	ID23_1	ID23_2	ID29
SPINE – SC3 pucks	Yes		Yes	Yes		
SPINE - Unipuck	Yes (single & double gripper)	Yes (single & double gripper)	Yes	Yes	Yes (single & double gripper)	
miniSPINE	Yes (single & double gripper)	(Yes)	(Yes)	(Yes)	(Yes)	
SSX samples						Yes

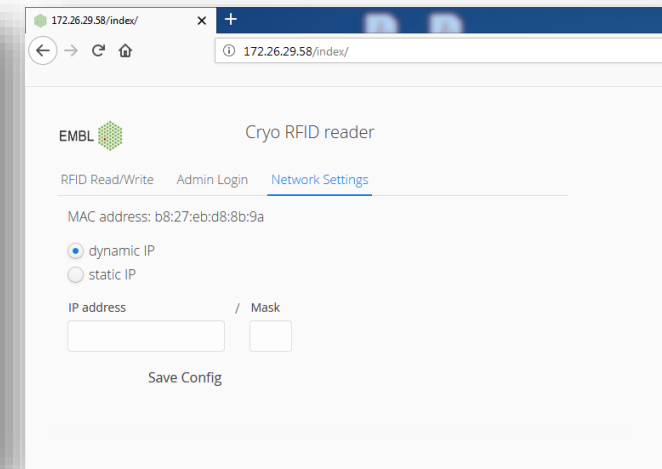
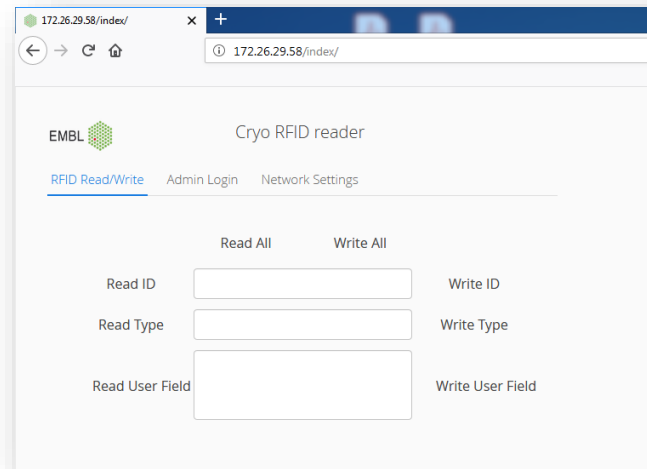
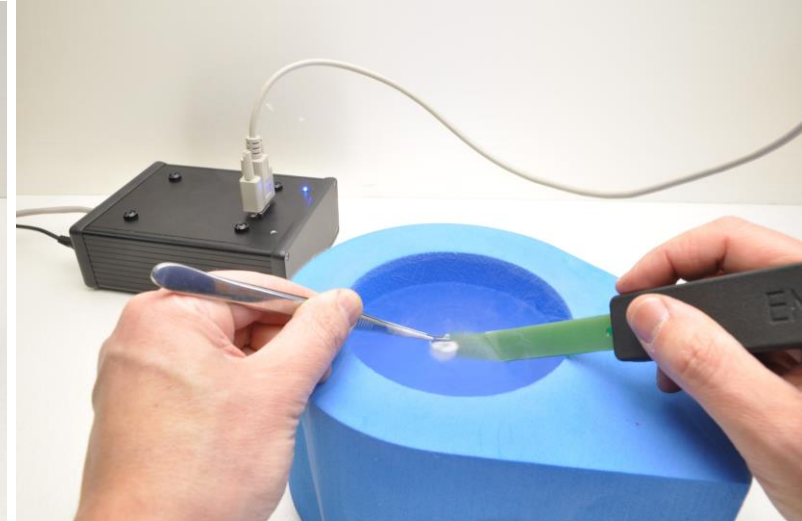
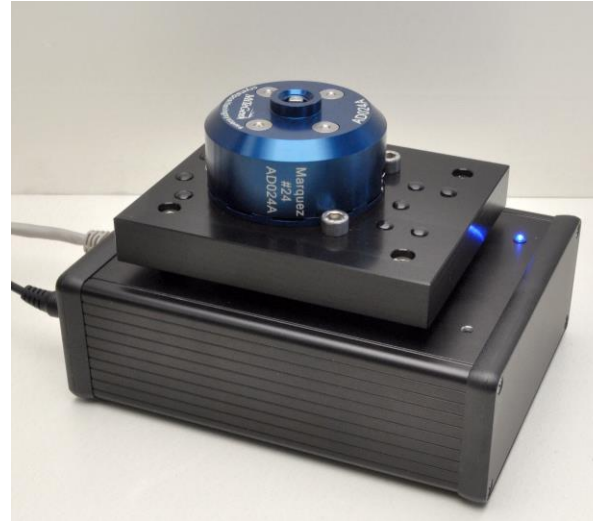
# FlexHCD – eCryoID tracking

- **RFID** : **R**adio **F**requency **I**Dentification
- First tests started in 2012 in the frame of NewPin project to track MX pucks and pins
- Technology transposed to CryoEM pucks and boxes



# eCryoID – Reader/Writer

- Compatible Room & Cryo Temperatures
- M2M communication
  - All Flex sample changers are ready to accept the reader
- GUI over standard web browser
  - For use in prep labs eg: clipping station
- Fields stored in each chip:
  - Unique ID (eg: AD024A)
  - Device Type (eg: MX1 for Unipuck)
  - User Field:
    - Free user field space 196 characters
    - Read/write possible at any time
    - Ideal to describe which sample is where in a puck/box etc...



# FlexHCD – Sample holder compatibility perspectives

	ID30B	Massif 1	Massif 3	ID23_1	ID23_2	ID29
SPINE – SC3 pucks	Fade out					
SPINE - Unipuck	Yes (single & double gripper)	Yes (single & double gripper)	Yes	Yes	Yes (single & double gripper)	
miniSPINE	Yes (single & double gripper)	(Yes)	(Yes)	(Yes)	(Yes)	
SSX samples						Yes
eCryoID tracking	Yes	Yes	(Yes)	(Yes)	(Yes)	(Yes)

# Agenda

- FlexHCD sample changers:
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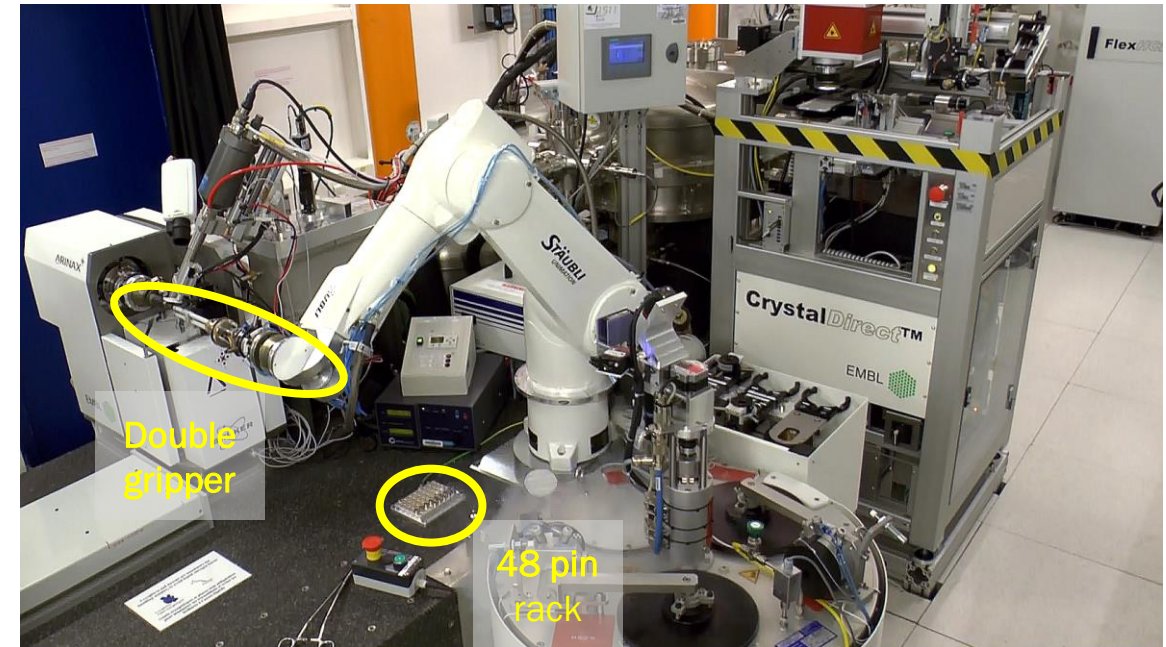
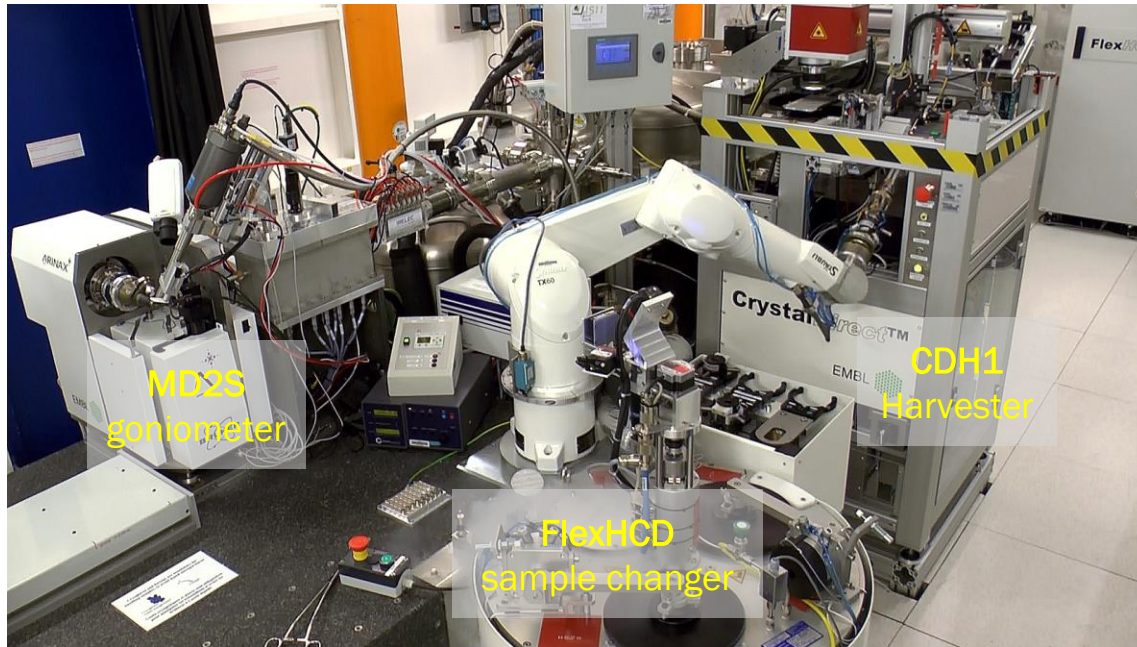
# Agenda

- FlexHCD sample changers:
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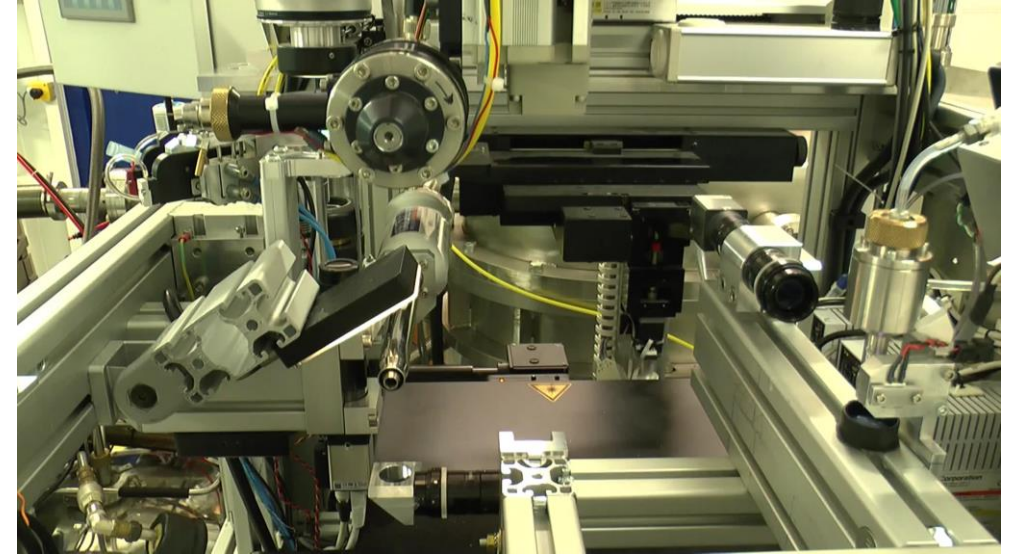
# CrystalDirect-to-Beam @ ID30B

- Ephemeral setup in 2017
  - Proof of concept
  - Fully automated harvest & collect pipeline up to 48 pins



# CrystalDirect-to-Beam @ ID30B - Process

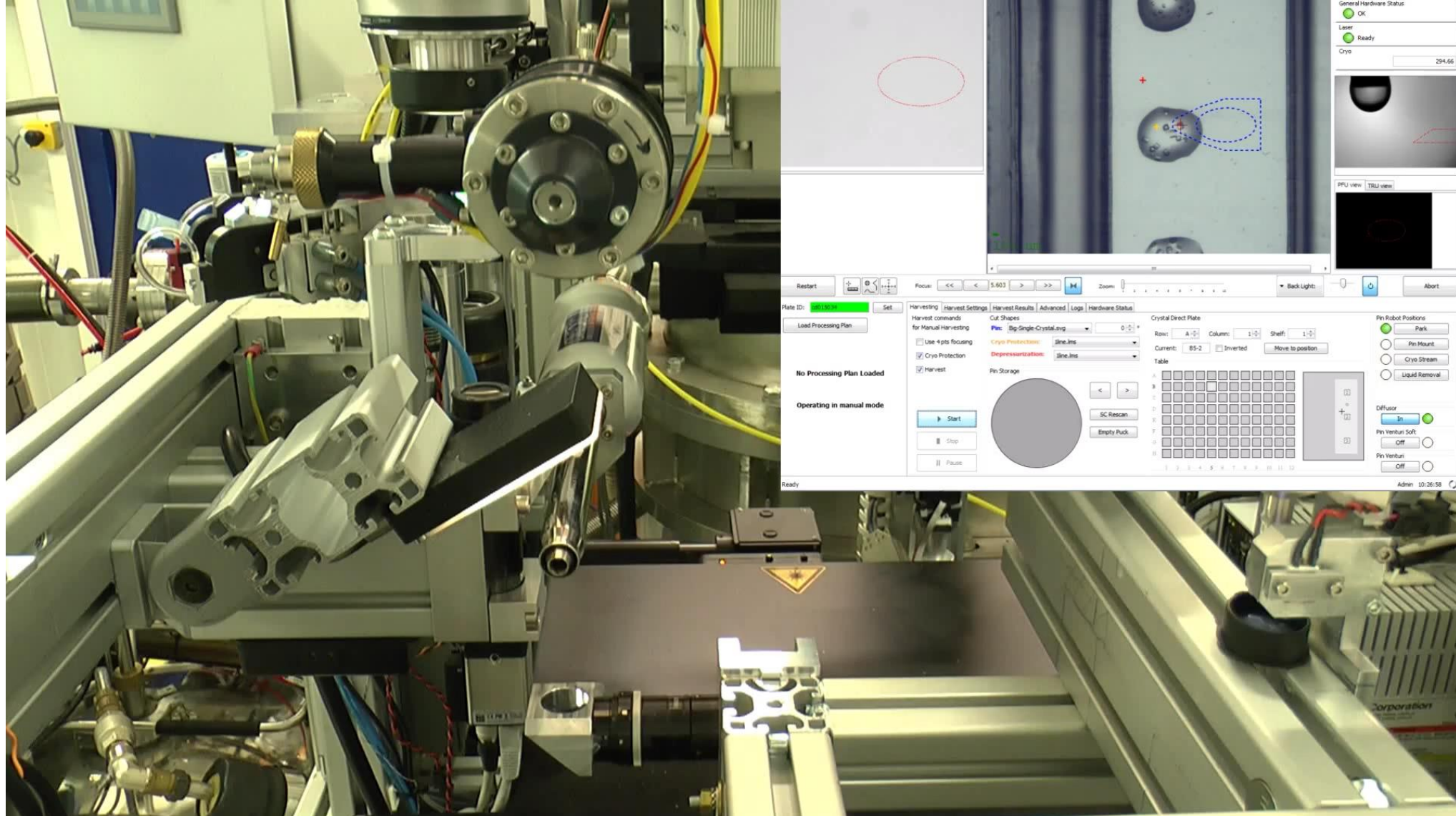
- Install CD plate on the harvester
- Feed the empty pin rack
- Load processing plan defined in CRIMS web interface (user pointings, cut shapes ...)
- Click on "Harvest all"



- The harvesting process is started
  - ➔ A crystal is harvested and frozen in the harvester, available to the **Flex robot**
  - ➔ A new harvesting occurs as soon as the frozen sample is picked up by the **Flex robot**
- Data collection pipeline like MXpress (MASSIF 1)
  - ➔ But **Flex** loads the sample from the harvester instead of the HCD



# CrystalDirect-to-Beam @ ID30B - Video

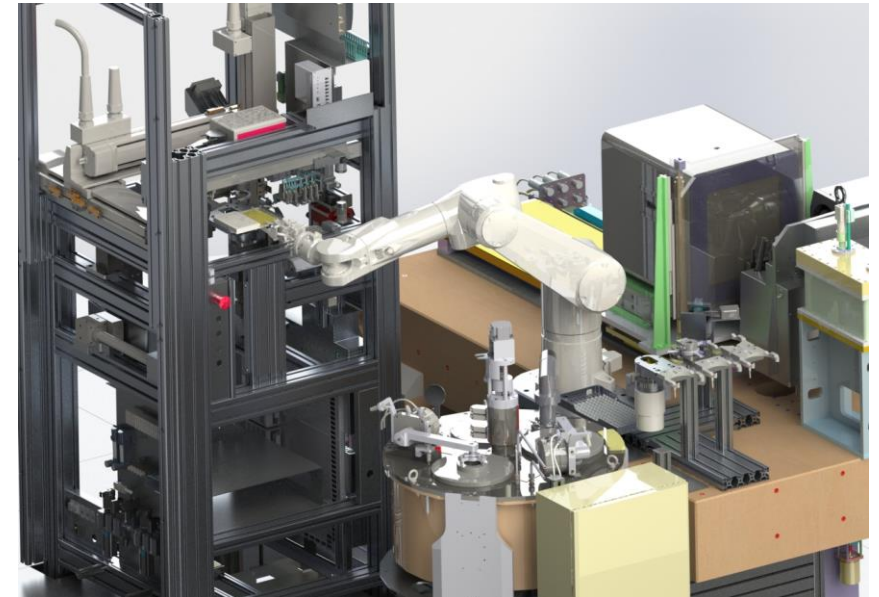
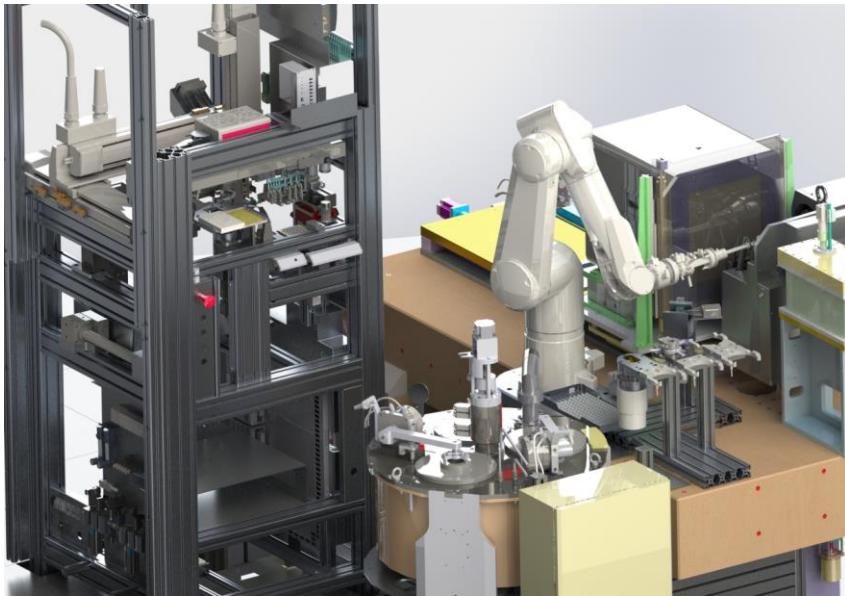


# CrystalDirect-to-Beam @ ID30B – Preliminary results

- Crystal harvesting time (CDH1) ~1'30'' < average data collection time
- Apparent crystal exchange time using double gripper ~10''
- Pre-centering precision using CDH1 coordinates:  $\pm 150 \mu\text{m}$  (with constant film orientation)

# Massif1 – Harvest to collect pipeline

- Installation of refurbished CDH2 directly to the beamline
  - Starting in May shutdown (2021)
  - First users after summer shutdown (August-September 2021)
- Fully automated harvest to collect pipeline
- Automated plate transfer from storing rack
- Use of NewPin sample holders (small, cheap, precise positioning)



# FlexHCD – Sample holder compatibility perspectives

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SPINE - Unipuck	Yes (single & double gripper)	Yes (single & double gripper)	Yes	Yes	Yes (single & double gripper)	
miniSPINE	Yes (single & double gripper)	(Yes)	(Yes)	(Yes)	(Yes)	
SSX chips						Yes
CrystalDirect Plates		Yes				
NewPin		Yes				
eCryoID tracking	Yes	Yes	(Yes)	(Yes)	(Yes)	(Yes)

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