Automated sample scanning and positioning for high repetition rate X-ray free-electron lasers

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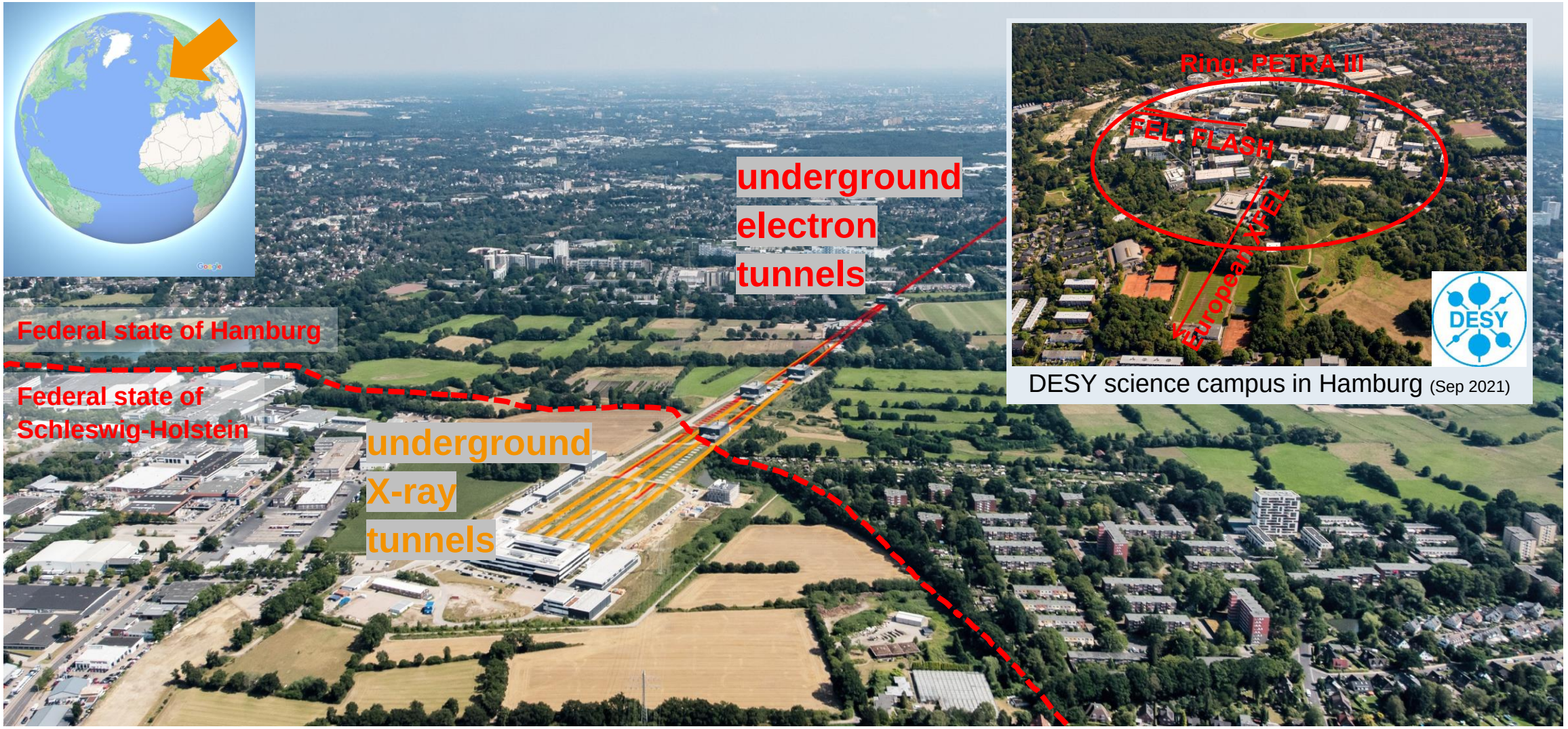
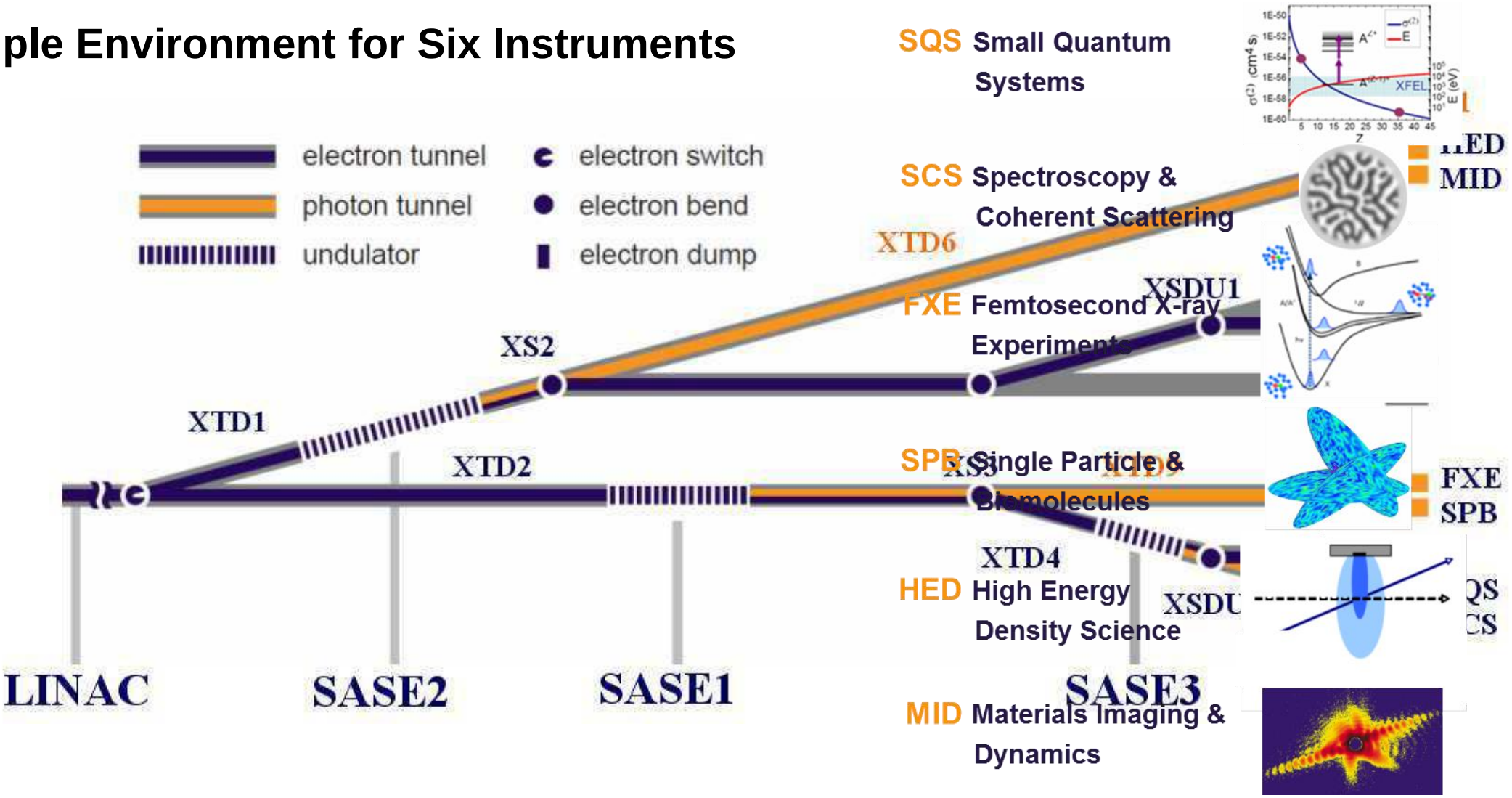
Granada, 6th October 2022



DESY science campus in Hamburg (Sep 2021)

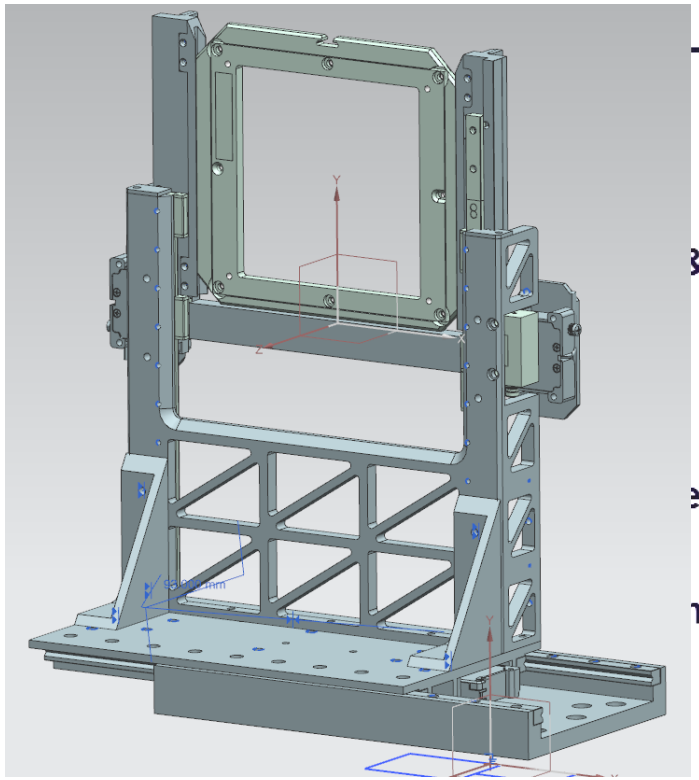
Underground tunnels drawn on an aerial picture (August 2020)

Sample Environment for Six Instruments

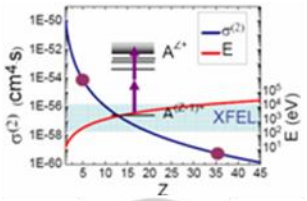


Fixed target sample delivery

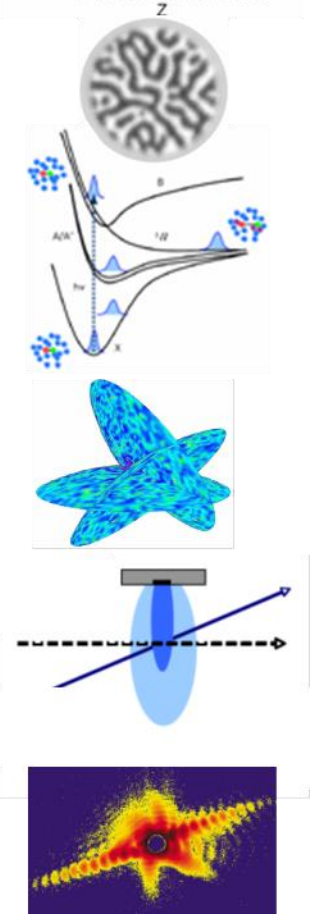
- Seven instruments deliver X-rays to user experiments
  - Samples provided by users
  - Large variety
  - Sizes typically in µm scale
  - Repetition rate 10 Hz
- Specification for 2D sample holders
  - Target area: 50x50 or 100x100 mm
  - Travel range: 50 to 120 mm in X and Y
    some millimetres in focal plane
  - Accuracy: 1 to 10 µm
  - Speed: 1 to 5 mm with 10 Hz start/stop



SQS Small Quantum Systems

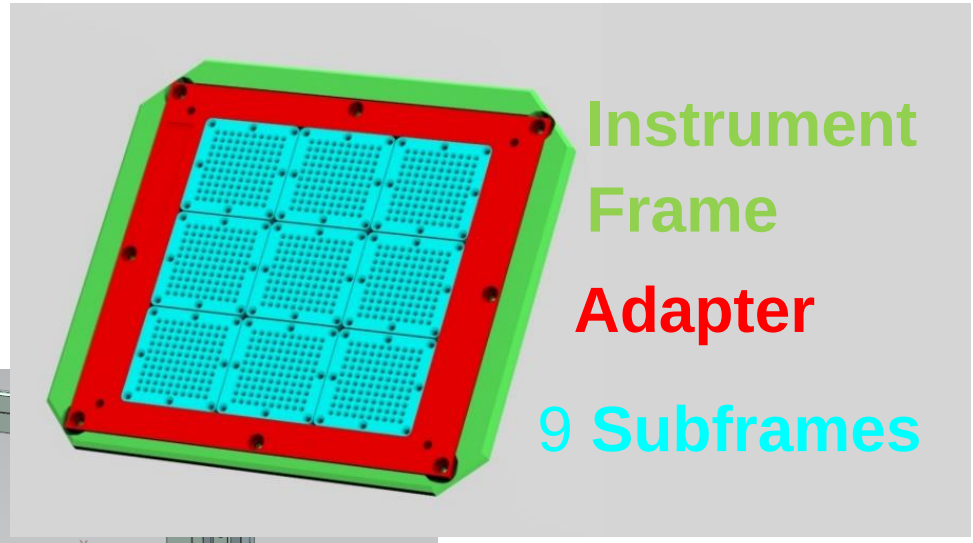


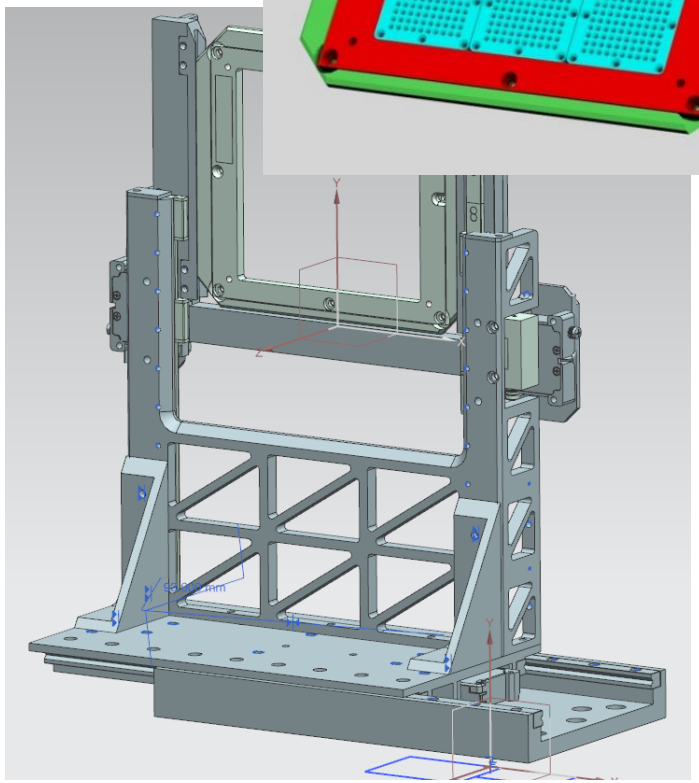
SCS Spectroscopy & Coherent Scattering

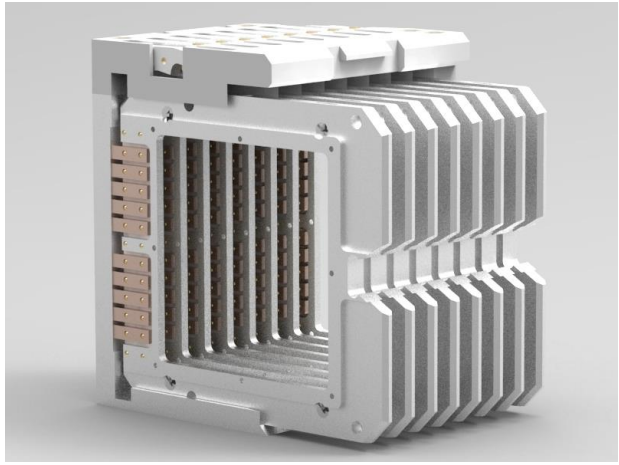


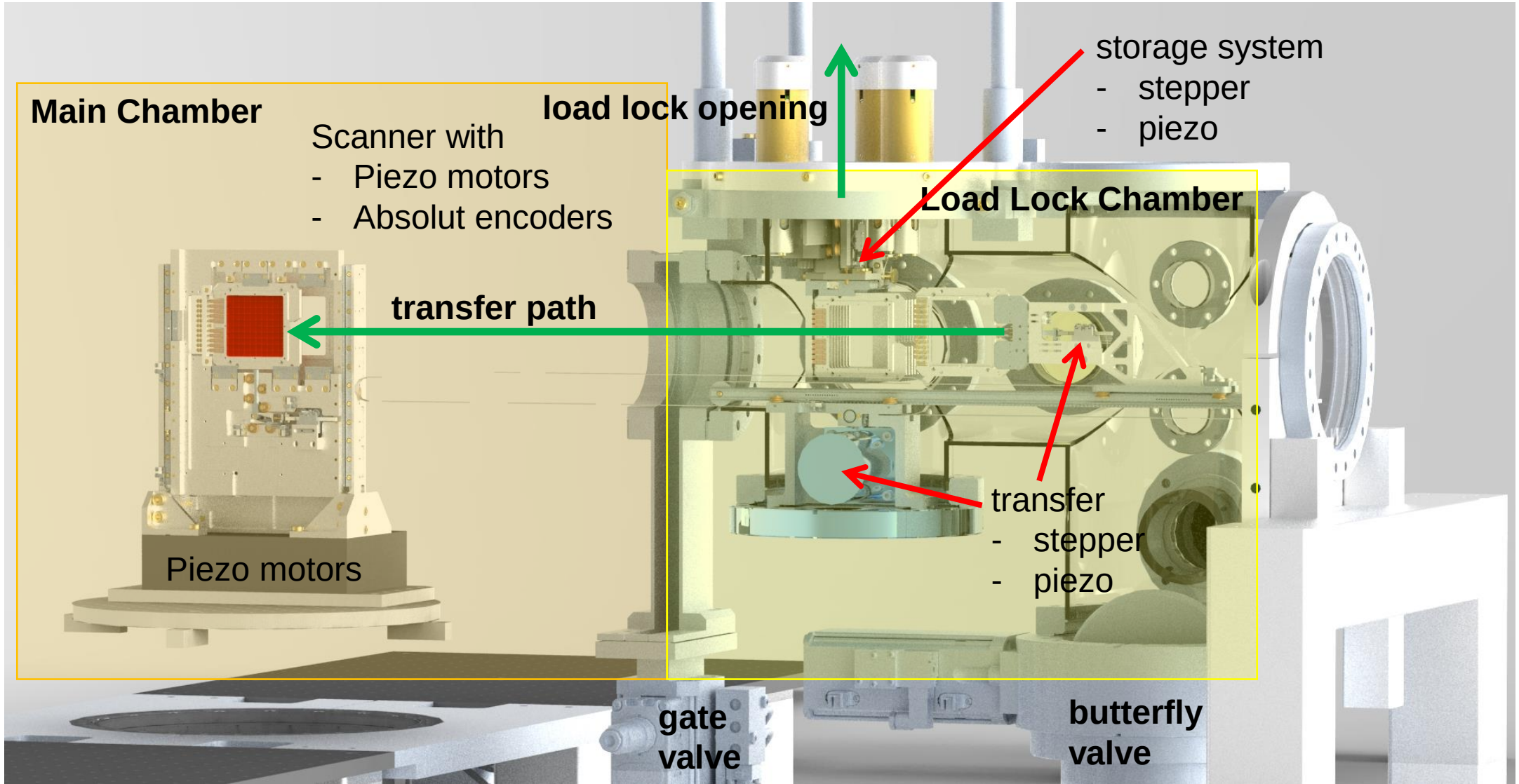
Challenges for high-intensity experiments

- Sample damage and debris
  - 1 sample per mm²
  - 100x100 mm -> 10.000 samples
  - Sample for 1000 seconds at 10 Hz
    - ► A bit more than ¼ hour
- Automated sample changer required
  - Load lock for vacuum operation
    - ► Insert sample without venting main chamber
    - ► Store new sample in a safe place
  - Cartridge system
    - ► Here for eight 50x50 mm frames





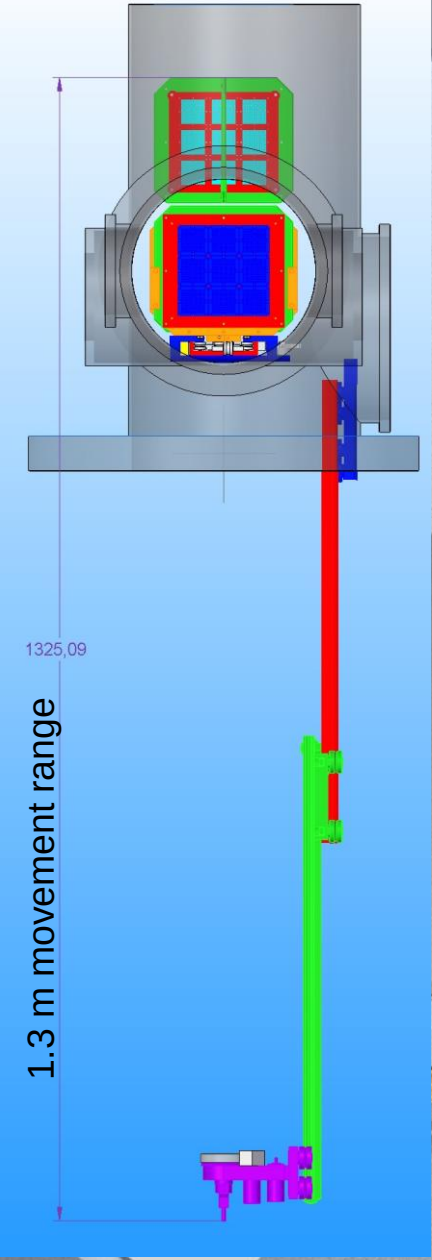



Main Chamber
Scanner with
- Piezo motors
- Absolut encoders
load lock opening
storage system
- stepper
- piezo
Load Lock Chamber
transfer path
Piezo motors
transfer
- stepper
- piezo
gate valve
butterfly valve

Need for:

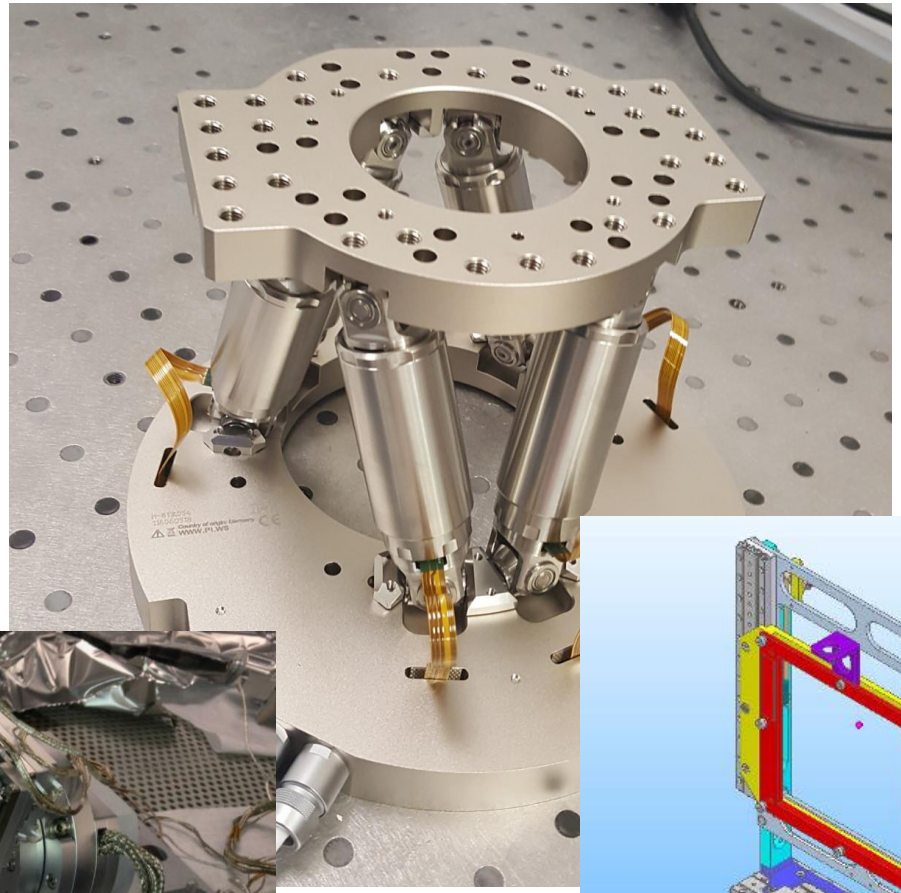
- Better fast stages and encoders
  - Movement in **vacuum**
  - Reliable and accurate positioning in **µm scale**
  - Fast acceleration and stopping within **100 ms**
  - Capable of repeated **small movements**
  - **Absolute encoders**
  - Concepts for the **control system** software

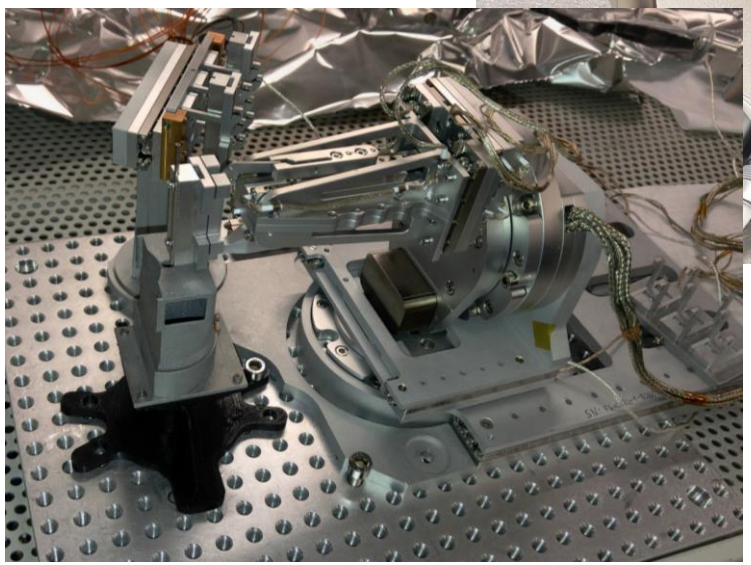
Alternative: Top Loader

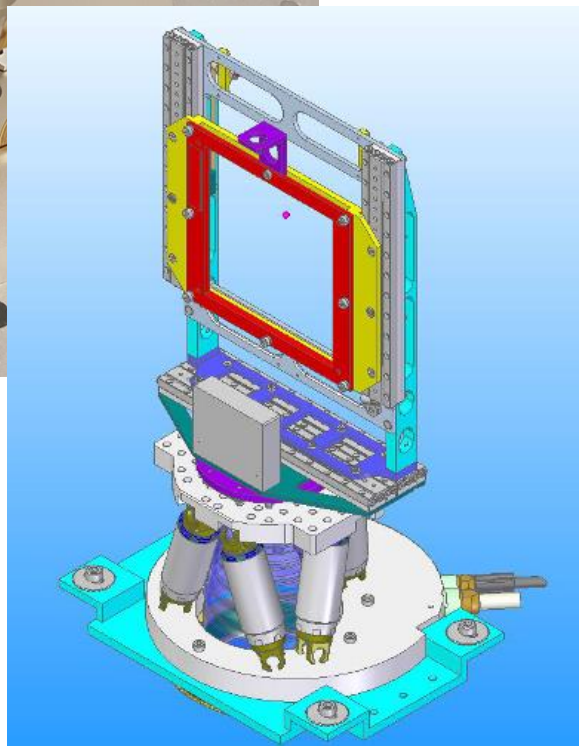


Other Systems

- Hexapod systems
  - Most compact system for 6 degrees of freedom
  - But:
    - ► Limited movement range
    - ► Complex dependences
- Robotic arms
  - Issues with
    - ► Vacuum compatibility
    - ► Space restrictions



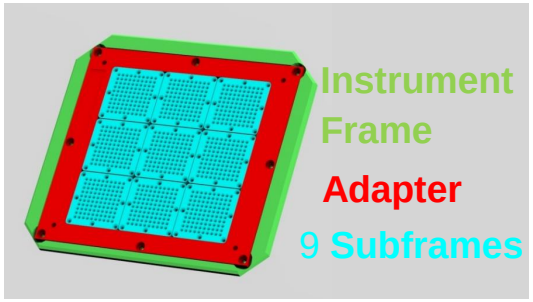




Standard Sample Frame System

- **Instrument frame** optimized to fit to the instrument
  - Integrational part of the scanner stage
  - or transferable frame for vacuum systems
  - Interface to the inside is standardized
  - Used at three Instruments (SPB/SFX, HED, FXE)
    ► Modified version at SCS and MID

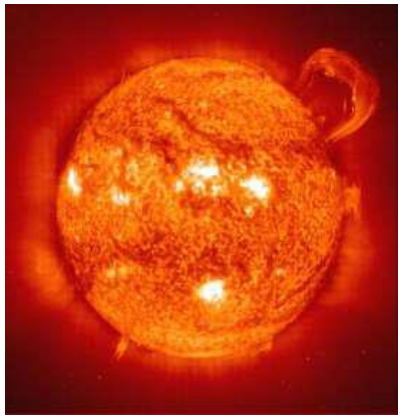
- **Subframe** optimized for a specific type of sample
  - Directly in the instrument frame
    or many of them in an adapter
  - Fiducials for target localization
  - Unique identifier



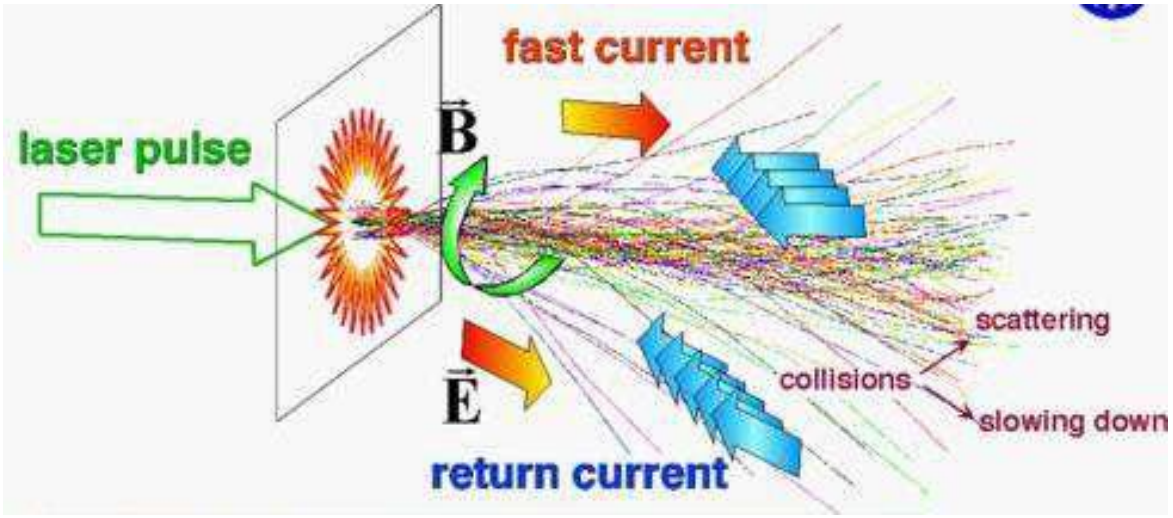
Need for:

- Standardized frames
  - **Cheap and easy** purchase for external users
    ► Catalogue ware
  - **Variations** to user specs
  - **Unique ID** engraved on frame
  - Included **fiducials**

EMP hardness



- We’re combining high energy and high power lasers with femtosecond X-ray pulses
- Electromagnetic pulses (EMP)
  - Cause high induction currents
  - Can damage stages, motors and electronics
- **Need for EMP hard solutions!**



Using Machine Learning for Sample Characterization

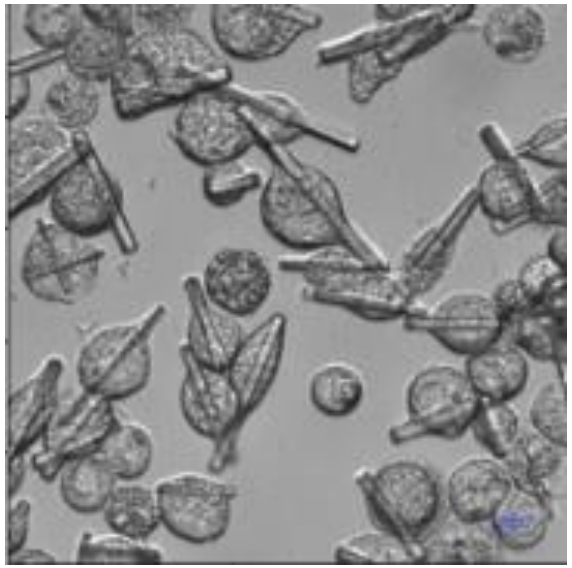
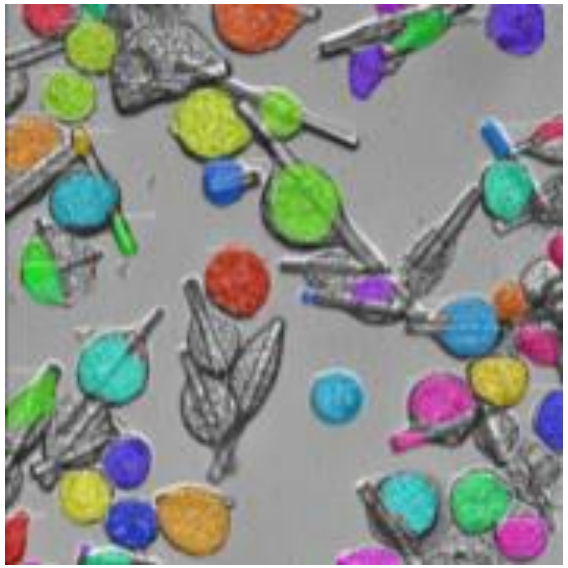
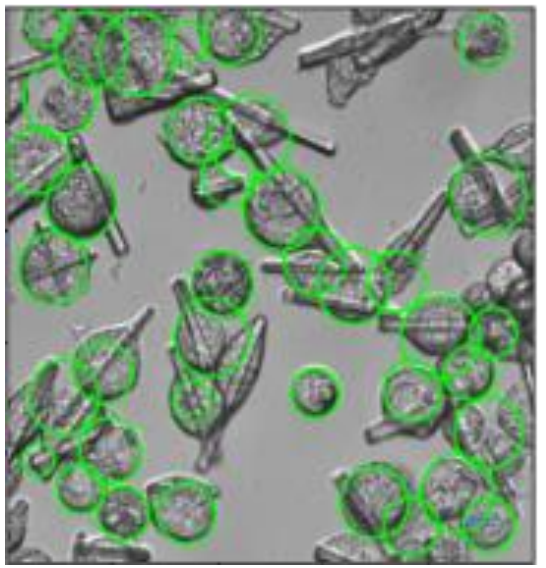


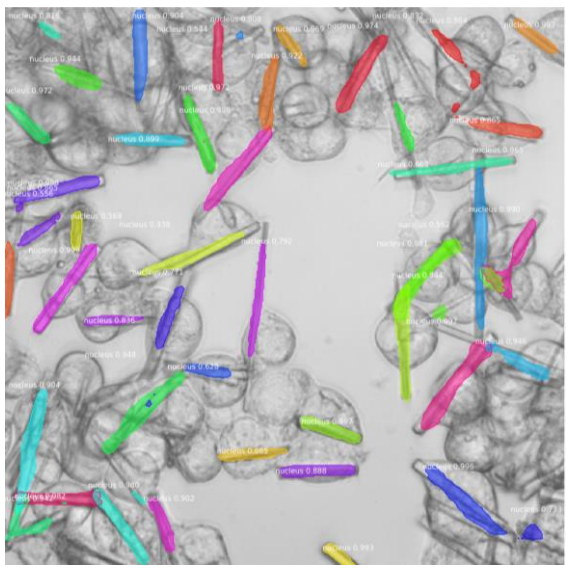
Image:
In-vivo crystallization



Segmentation prediction:
using Mask R-CNN



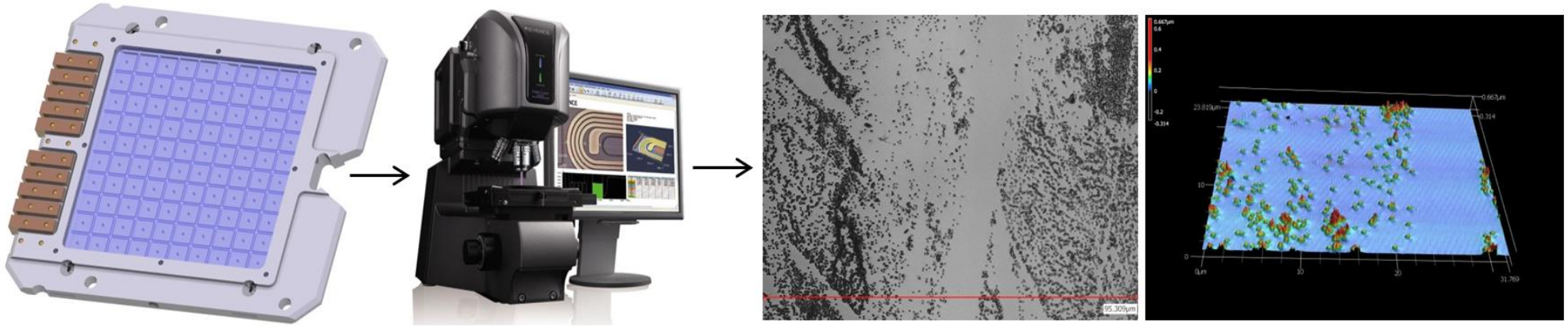
Searching for circles:
Hough Transform

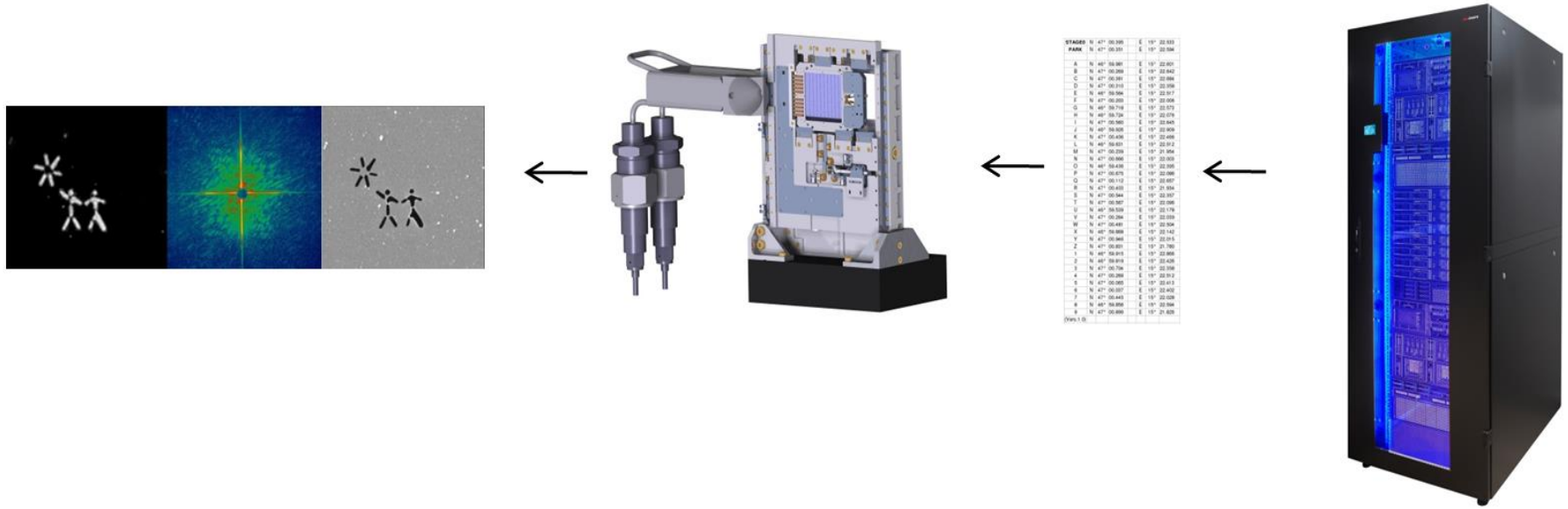


Crystal detection:
Mask R_CNN
trained on 30 images only!

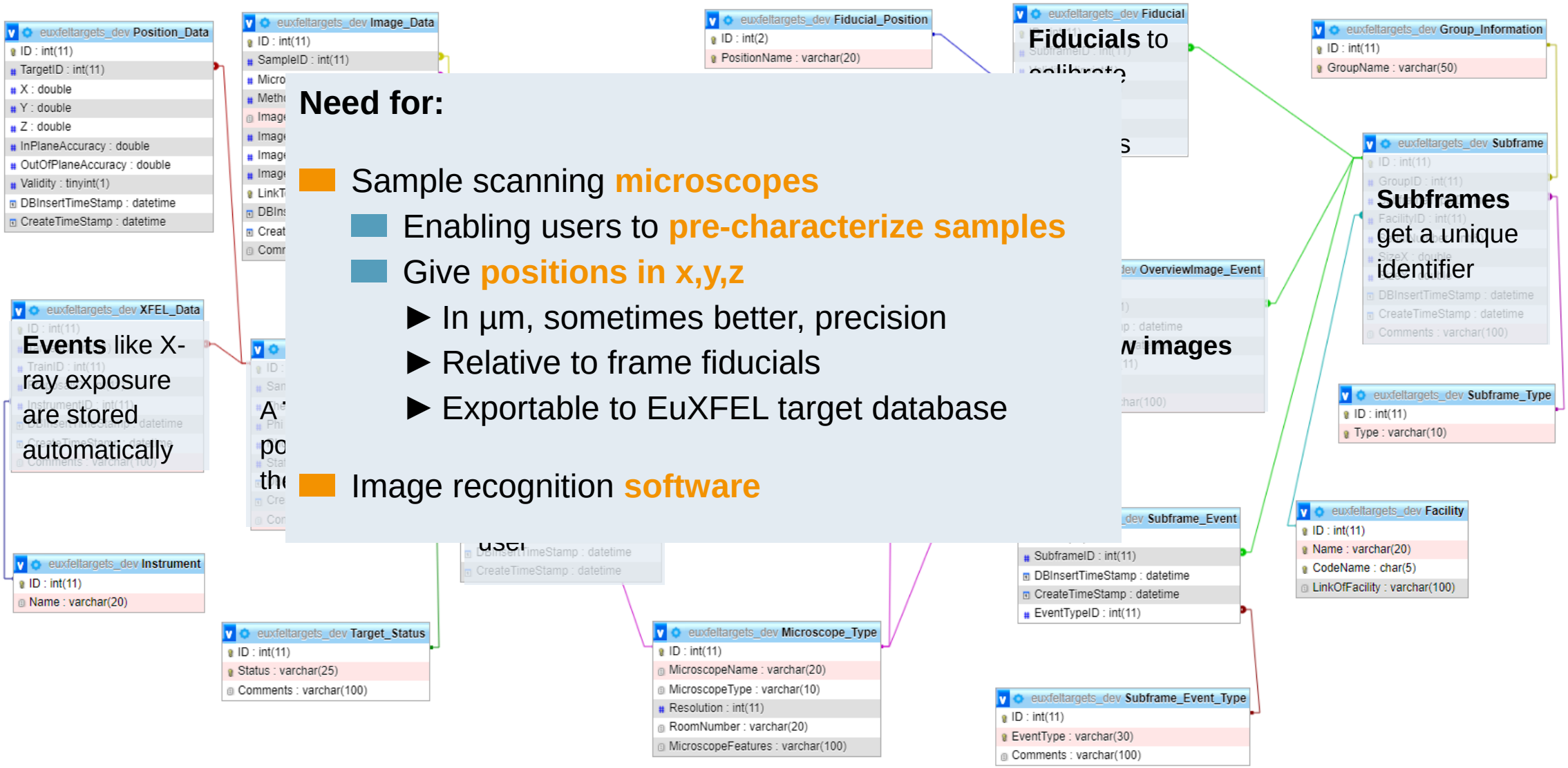
- Sample: Iñaki de Diego Martinez
- Algorithm development: Amirhossein Kardoost

Towards a Workflow from Sample Pre-Characterization to Automatic 10Hz Measurements





Target database in preparation



Our industrial needs

- We develop compact, fast positioning systems
  - we are interested in new motor concepts for doing this
    - ► Accuracy in the order of µm
    - ► Movements 100 mm
    - ► 1 mm start-stop in 0.1 second
  - EMP hardness is an issue
- Enable users to pre-characterize samples at home
  - Microscopes with absolute, global positioning
    - ► Light microscopes
    - ► Confocal microscopes
    - ► Electron microscopes
    - ► Production devices and facilities
  - Software frontends to transfer data points
    - ► To a database
    - ► Using web protocols or XML files