Smart Automated STEM

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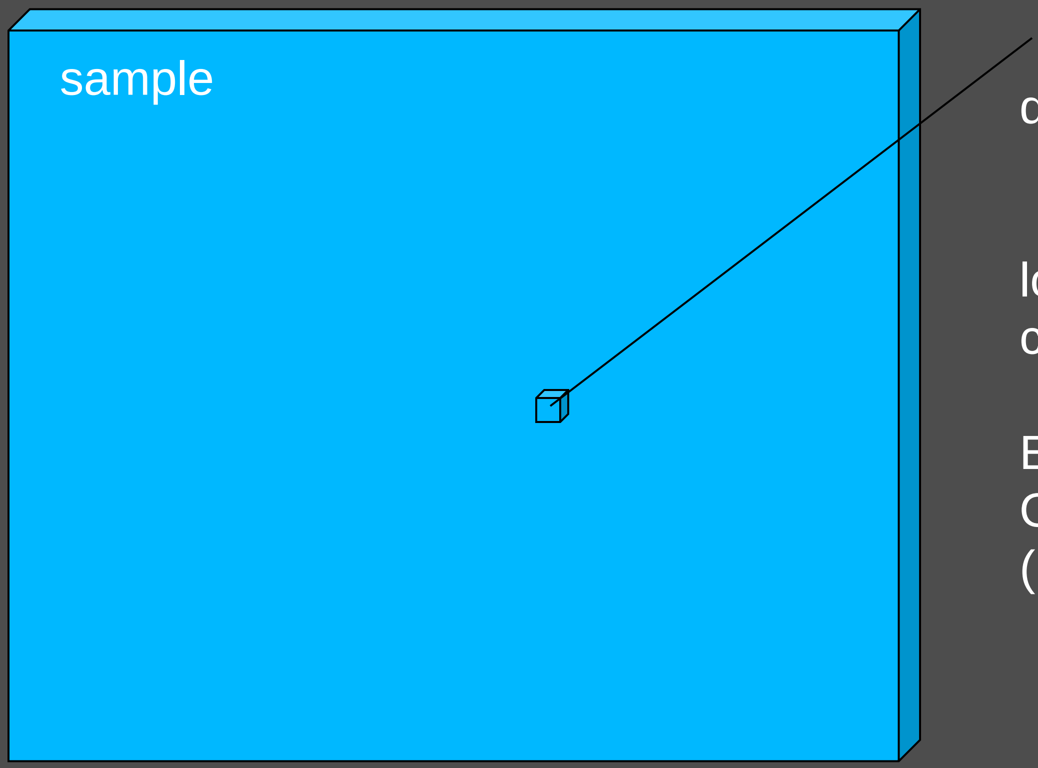
For MLSTEM 2024 workshop

Main developer of technique:

Austin Houston, Utkarsh Pratiush

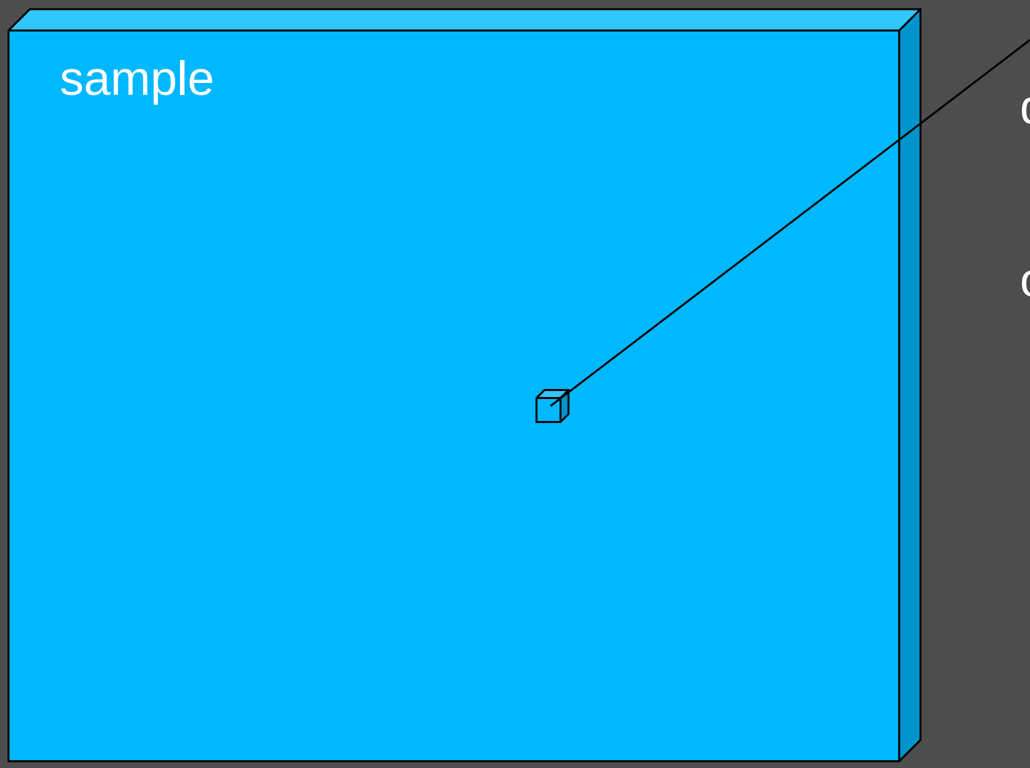
Maximal Possible Information in STEM



diffraction pattern
(different convergence angles
or only parts),
low-loss EELS,
core-loss EELS
(several energy-windows),
EDS,
Others
(like Cathodoluminescence
or secondary electrons)

For
Different volume sizes
Different angles
Ideally with knowledge of number
of incoming electrons

Current State of the Art



diffraction pattern
(only part of pattern
- HAADF:large angles),
one STEM condition
- EDS spectrum
- EELS (high- and low-loss)
- diffraction pattern

For
one volume size
one tilt angle
small area

Current Data Collection Strategies

- Spectrum Imaging, 4D-STEM:
  - Grid Scan:
  - Fully filled matrix
  - Usually: 90% of data points are unimportant
- **Compressed sensing** (also known as **compressive sensing**, **compressive sampling**, or **sparse sampling**)
  - (more or less) random selection of points used to interpolate whole dataset.
  - Sparse matrix
  - Important parts may be missed

$$\begin{bmatrix} X & X & X & \cdot & \cdot & \cdot & \cdot \\ X & X & \cdot & X & X & \cdot & \cdot \\ X & \cdot & X & \cdot & X & \cdot & \cdot \\ \cdot & X & \cdot & X & \cdot & X & \cdot \\ \cdot & X & X & \cdot & X & X & X \\ \cdot & \cdot & \cdot & X & X & X & \cdot \\ \cdot & \cdot & \cdot & \cdot & X & \cdot & X \end{bmatrix}$$

Alternative Data Collection Strategies

- Select data points smartly
  - Use all possibilities of machine learning discussed in this workshop

  And select the points of interest.
- Collect data remotely
- Select various of all available signals of a STEM

- Avoid investment in infrastructure and instrument time to collect a lot of data that are never used.

Minimum Requirement for Smart Acquisition

- Overview image
- Drift Correction
- Algorithm to select points
  - Complexity depends only on computing power
- Ability to collect data at selected points

Minimum Requirement for Smart Acquisition for EELS

- Get image
- Shift beam
- Get spectrum

Nice to have but not immediately necessary:

- Drift
- Set dispersion and energy offset
- Get dispersion and energy offset once

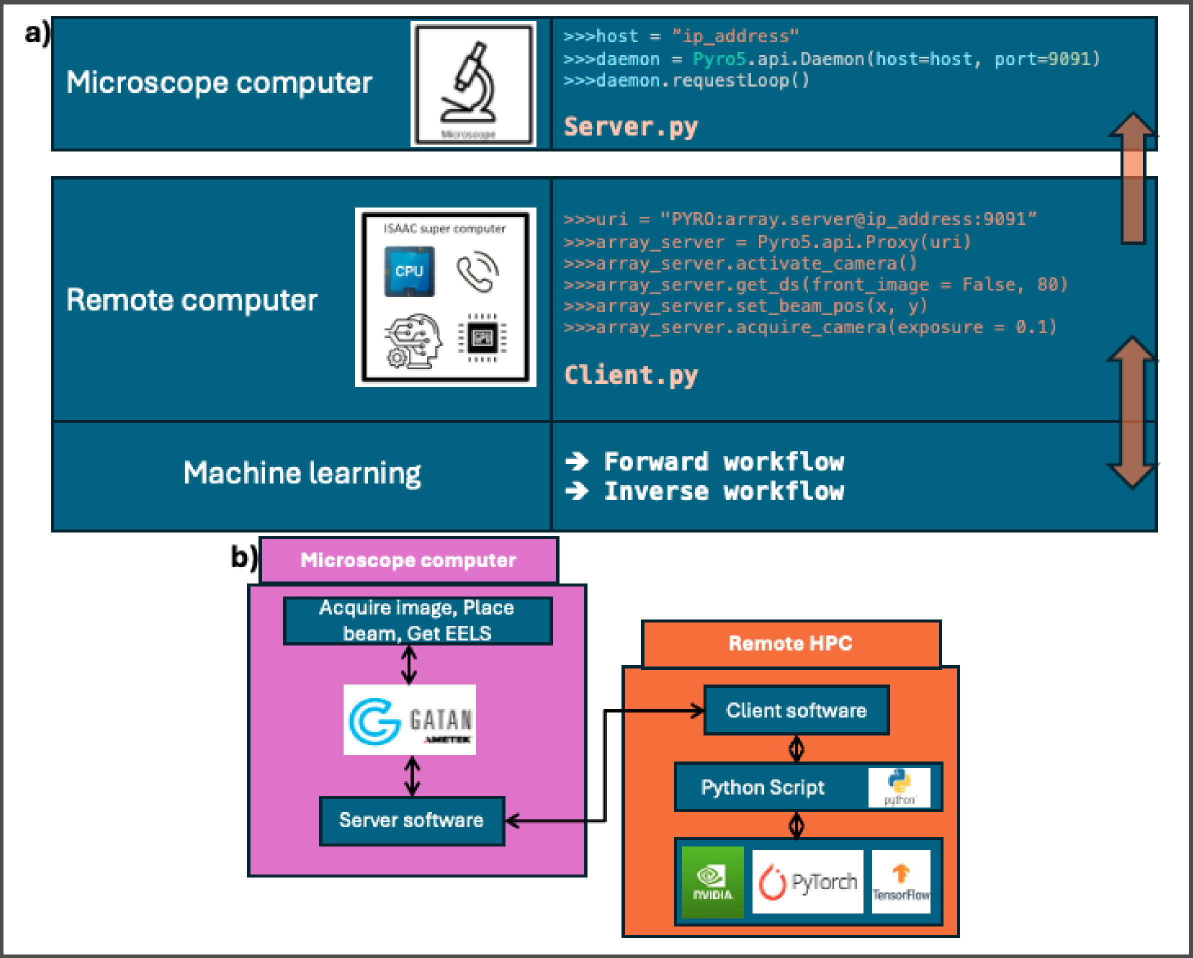
Implementation in Digital Micrograph

- Make a server software in python
  - Acquire digiscan image
  - Set beam position
  - Get (part) of ccd camera

This functionality is readily available in DM

Several server software packages available in python

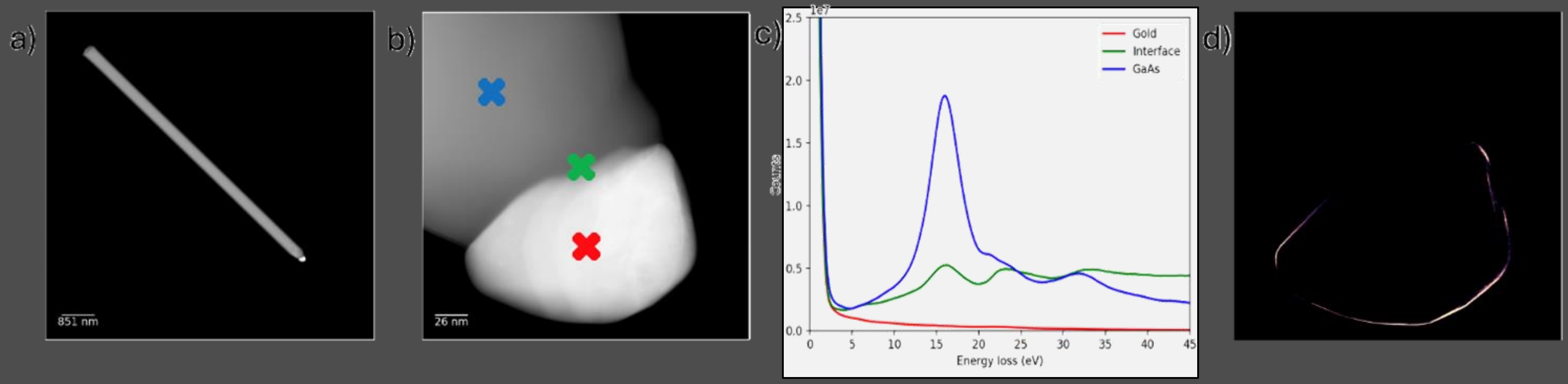
Implementation of Smart Collection



The client

- Can be any remote computer
- Can be a supercomputer to provide enough computing power for on-the-fly machine learning algorithms.
- Jupyter notebook: so data are directly accessible to all python packages

Example



Acquisition of single spectrum is 2 times slower for low loss than in spectrum image.

Acquisition of 1/10000 data points in grid scan.

Advantages

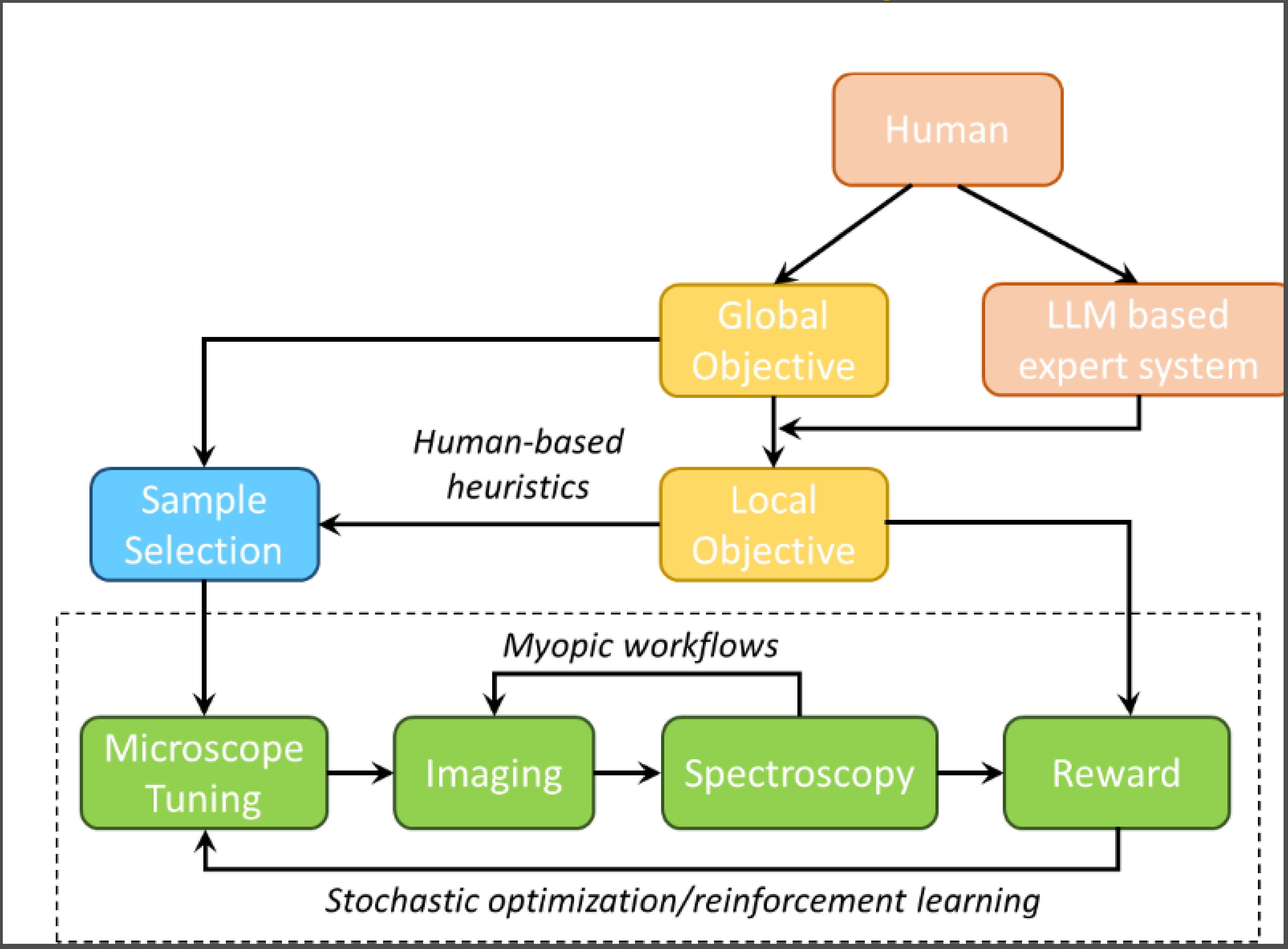
- Truly large areas can be investigated
- Mostly relevant data points chosen for acquisition
- Variation of method to determine data points
  - Active Learning
  - Clustering
  - Edge detection
  - DCNN
  - …
- Learning algorithms can be applied to increasing data volume

Further Development

- Keep STEM at optimum condition
- Change STEM optics and detectors
  - Get diffraction and EELS spectra from same sub pixel areas
- Smart drift correction
- Get metadata

- Develop methods for correlated data

Human in the Loop Workflow



Human in the Loop Workflow