MATLAB to Python Translation: Electron Microscope Tools

COSC 499: Software Engineering

Introduction

- Client: Misa Hayashida, a researcher for the National Research Council
- Project overview: Converting 3 tools from MATLAB to Python
  - qEELS
  - Nanomi Optics
  - Alignment software

NRC·CNRC Canada

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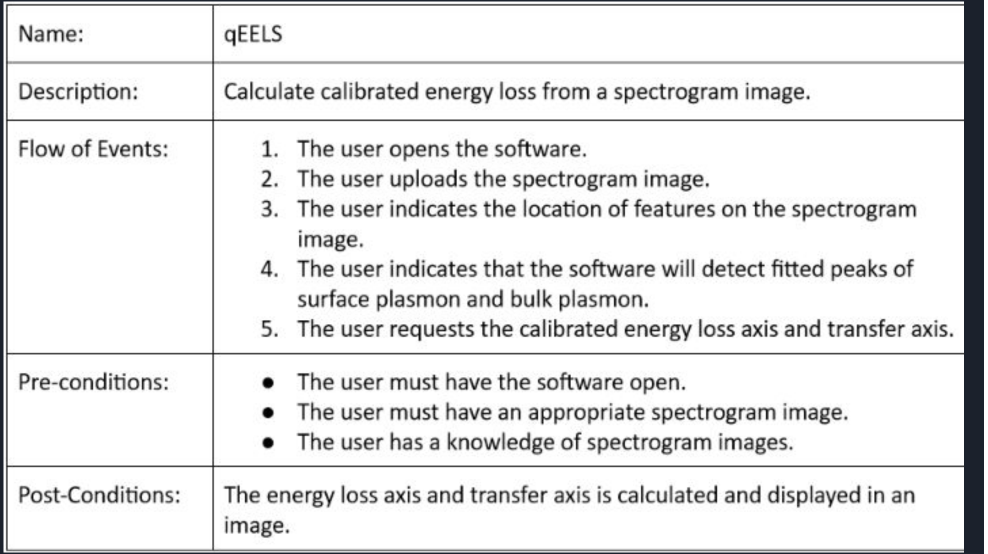
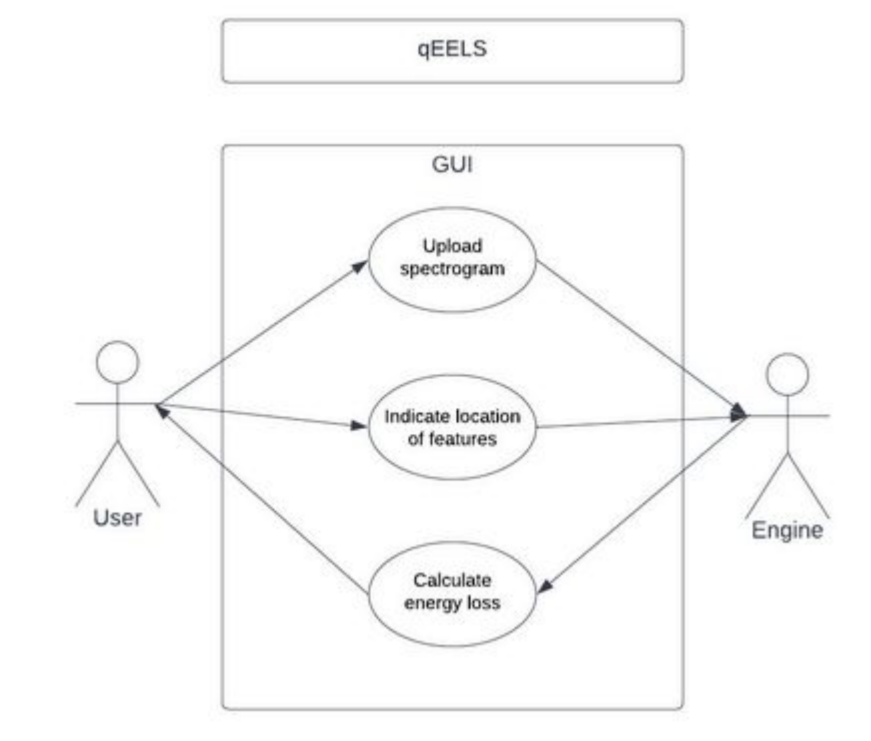
qEELS: Use Cases

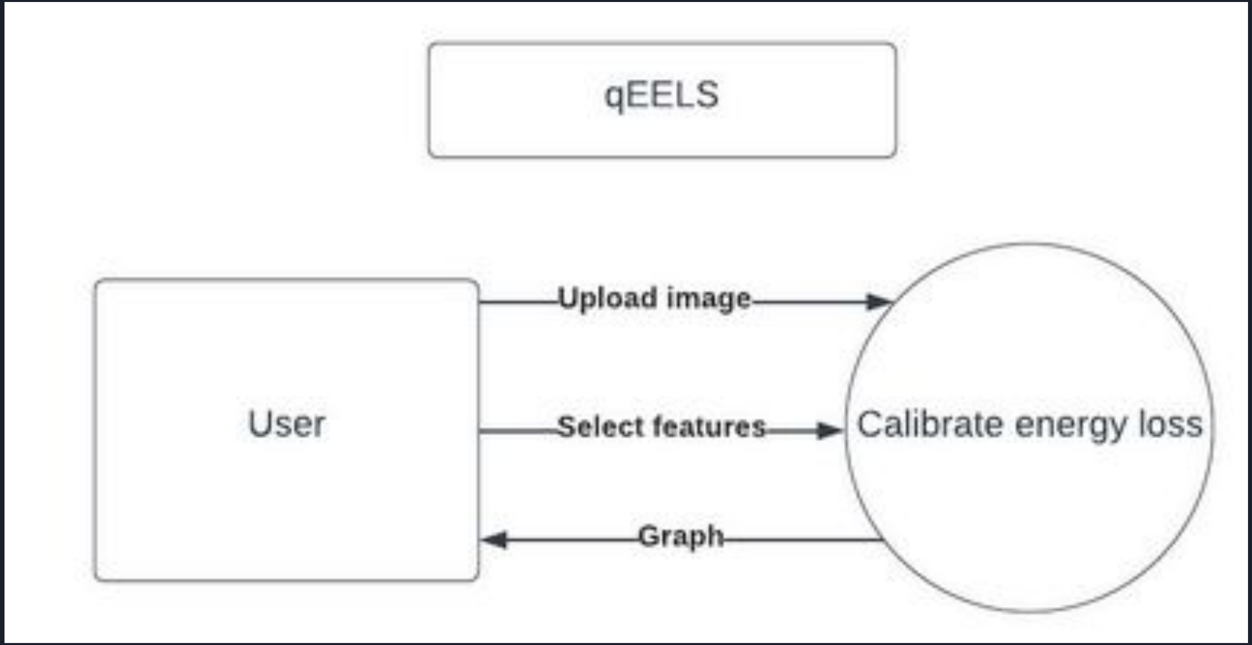


Name:	qEELS
Description:	Calculate calibrated energy loss from a spectrogram image.
Flow of Events:	1. The user opens the software. 2. The user uploads the spectrogram image. 3. The user indicates the location of features on the spectrogram image. 4. The user indicates that the software will detect fitted peaks of surface plasmon and bulk plasmon. 5. The user requests the calibrated energy loss axis and transfer axis.
Pre-conditions:	• The user must have the software open. • The user must have an appropriate spectrogram image. • The user has a knowledge of spectrogram images.
Post-Conditions:	The energy loss axis and transfer axis is calculated and displayed in an image.

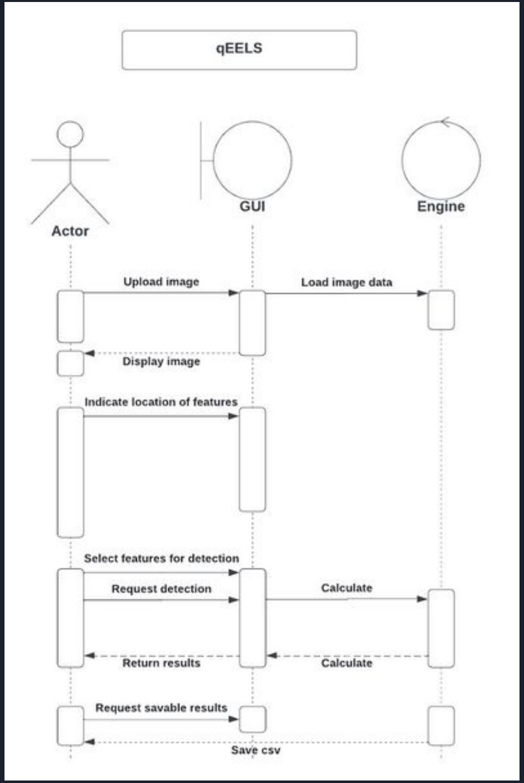


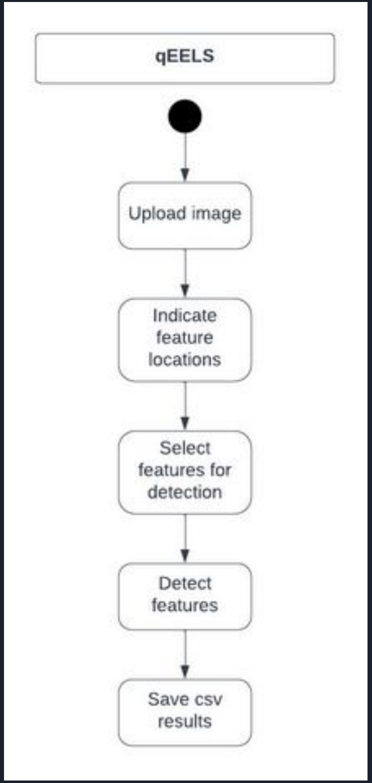
qEELS: Data Flow

Level 0 DFD

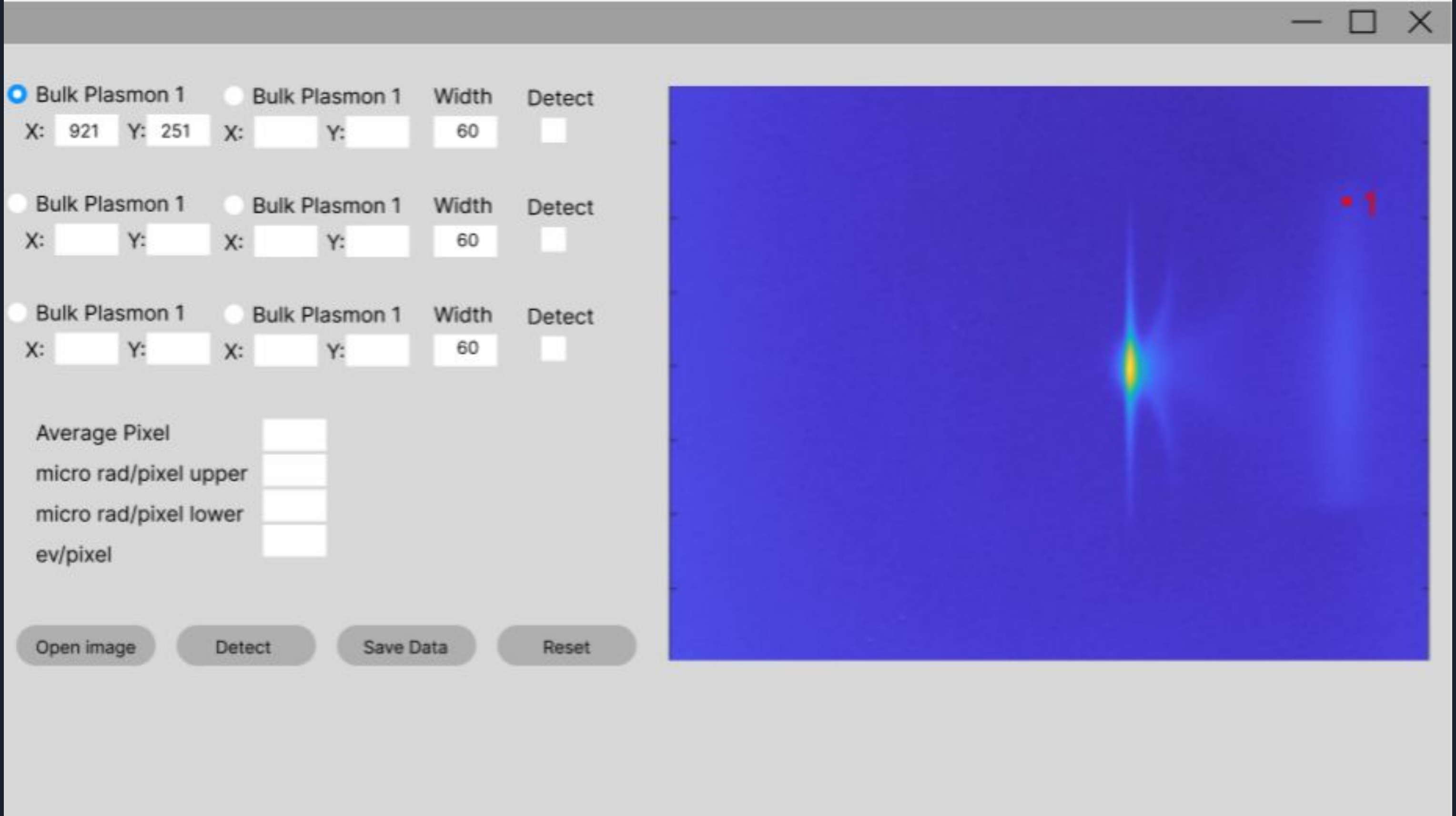


qEELS: Sequence diagram





qEELS: UI Mockup



● Bulk Plasmon 1		○ Bulk Plasmon 1		Width	Detect
X: 921	Y: 251	X:	Y:	60	□
○ Bulk Plasmon 1		○ Bulk Plasmon 1		Width	Detect
X:	Y:	X:	Y:	60	□
○ Bulk Plasmon 1		○ Bulk Plasmon 1		Width	Detect
X:	Y:	X:	Y:	60	□

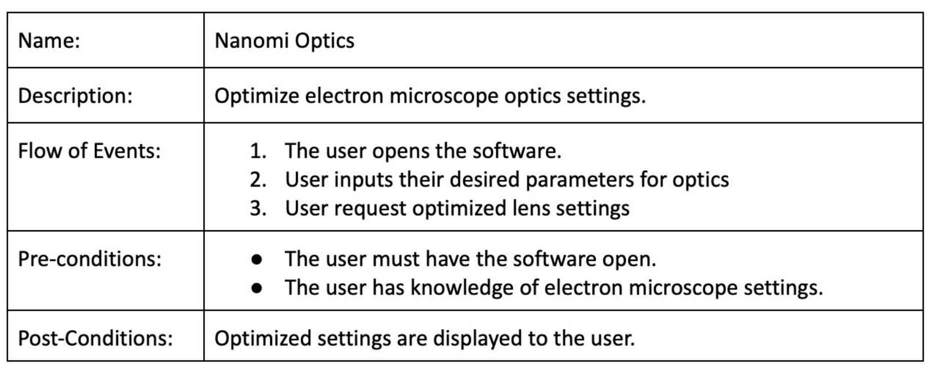
Average Pixel

micro rad/pixel upper

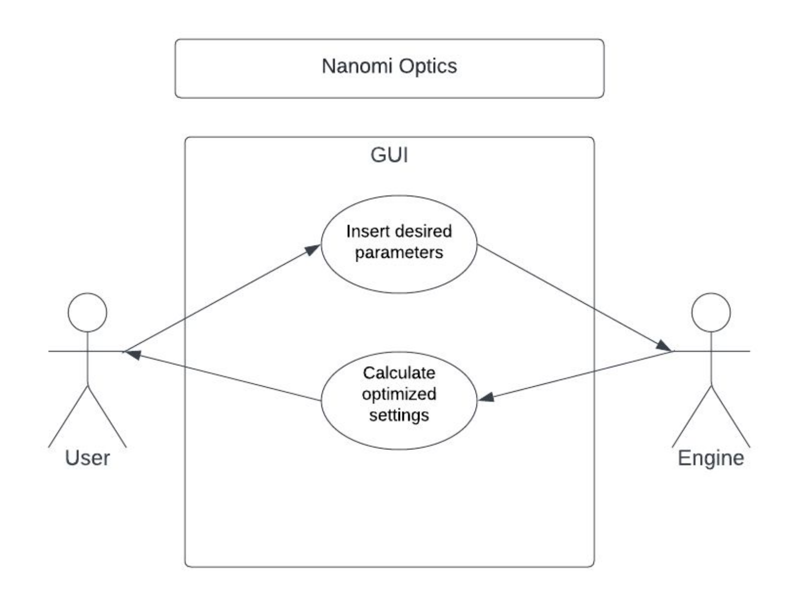
micro rad/pixel lower

ev/pixel

Nanomi Optics Use Cases

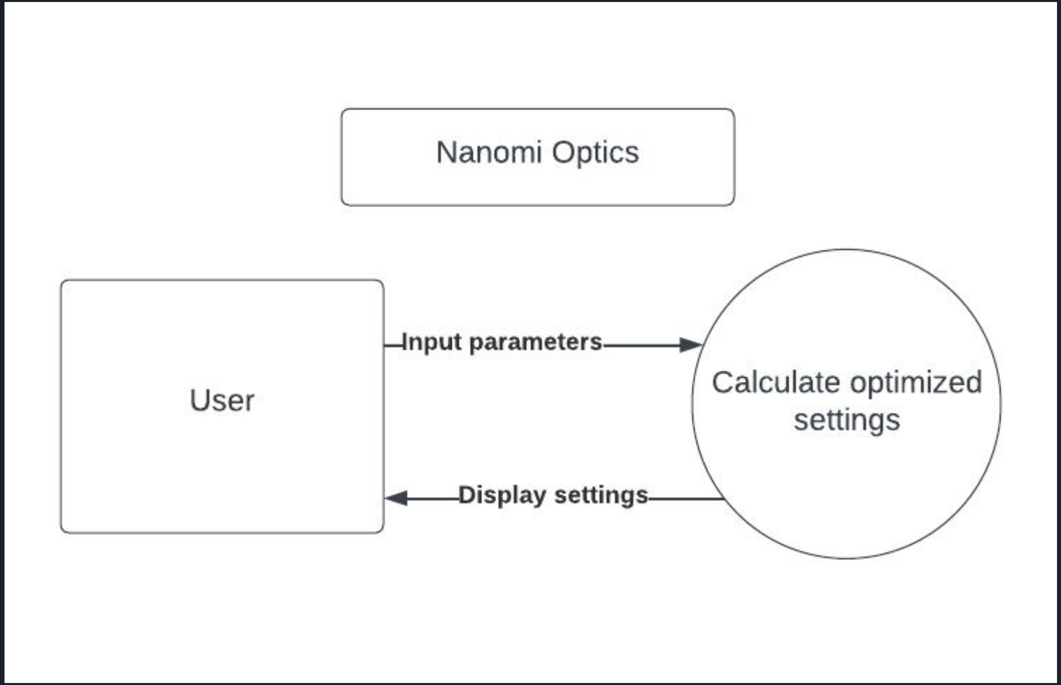


Name:	Nanomi Optics
Description:	Optimize electron microscope optics settings.
Flow of Events:	1. The user opens the software. 2. User inputs their desired parameters for optics 3. User request optimized lens settings
Pre-conditions:	● The user must have the software open. ● The user has knowledge of electron microscope settings.
Post-Conditions:	Optimized settings are displayed to the user.

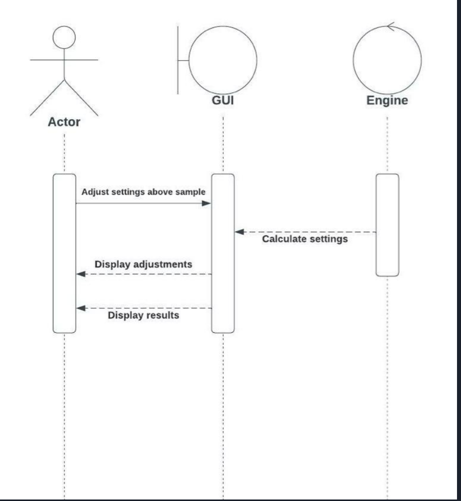


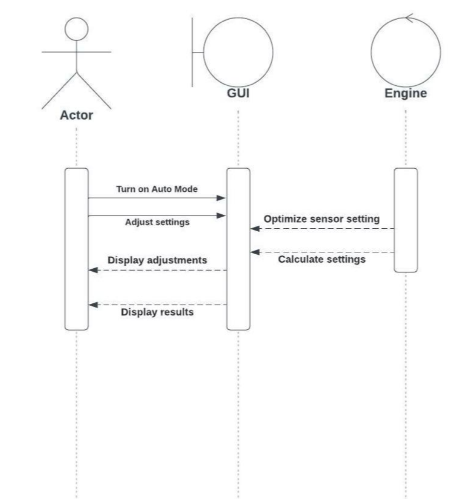
Nanomi Optics Data Flow

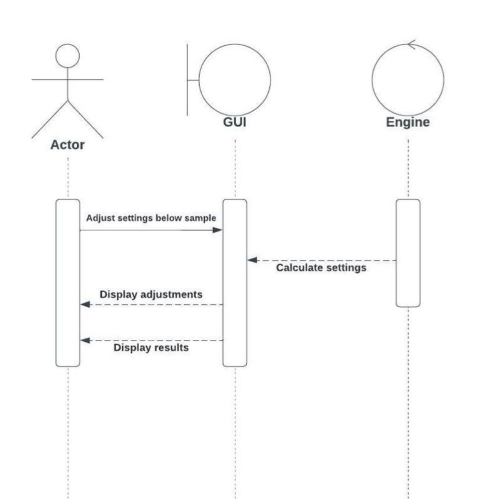
Level 0 DFD

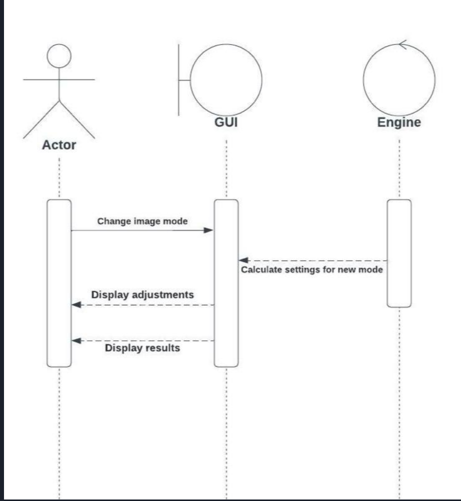


Nanomi Optics Sequence Diagrams

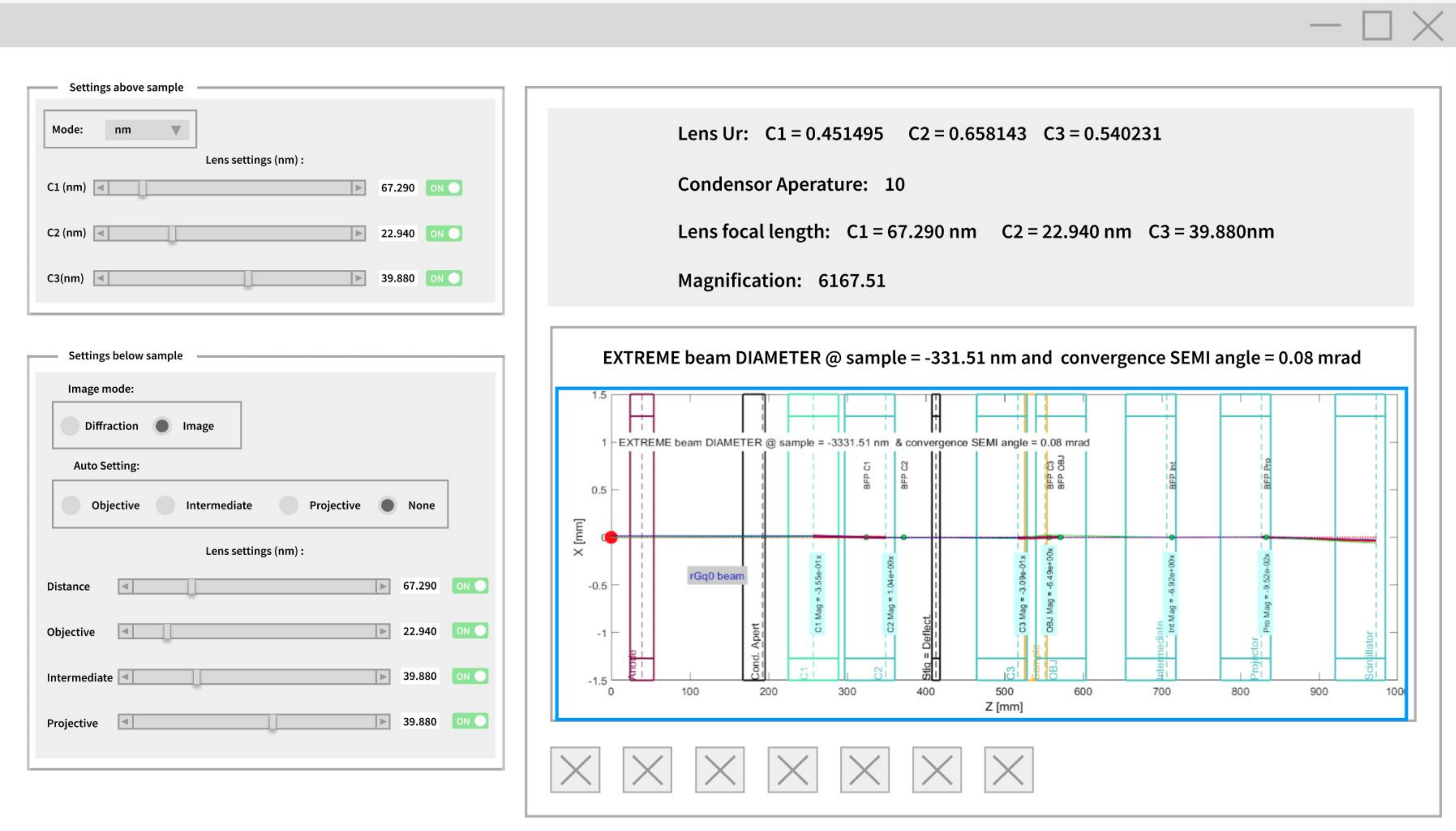








Nanomi Optics UI



Settings above sample

Mode: nm ▼

Lens settings (nm) :

C1 (nm) 67.290 ON

C2 (nm) 22.940 ON

C3(nm) 39.880 ON

Settings below sample

Image mode:

○ Diffraction ● Image

Auto Setting:

○ Objective ○ Intermediate ○ Projective ● None

Lens settings (nm) :

Distance 67.290 ON

Objective 22.940 ON

Intermediate 39.880 ON

Projective 39.880 ON

Lens Ur: C1 = 0.451495 C2 = 0.658143 C3 = 0.540231

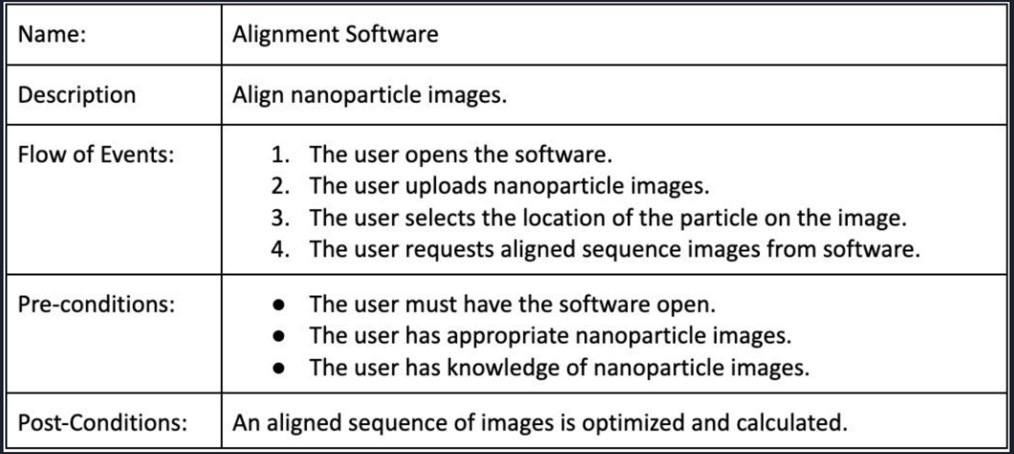
Condensor Aperature: 10

Lens focal length: C1 = 67.290 nm C2 = 22.940 nm C3 = 39.880nm

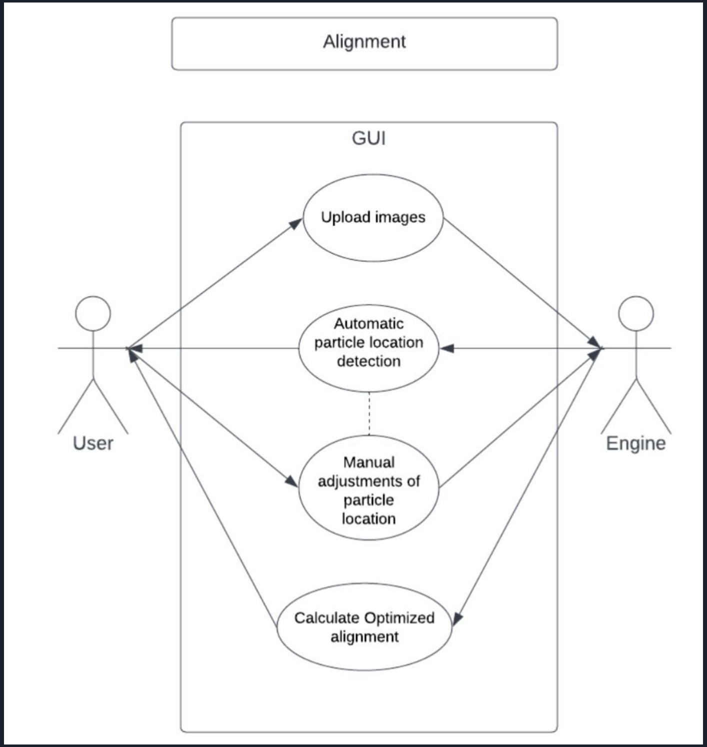
Magnification: 6167.51

EXTREME beam DIAMETER @ sample = -331.51 nm and convergence SEMI angle = 0.08 mrad

Alignment - Use Cases



Name:	Alignment Software
Description	Align nanoparticle images.
Flow of Events:	1. The user opens the software. 2. The user uploads nanoparticle images. 3. The user selects the location of the particle on the image. 4. The user requests aligned sequence images from software.
Pre-conditions:	● The user must have the software open. ● The user has appropriate nanoparticle images. ● The user has knowledge of nanoparticle images.
Post-Conditions:	An aligned sequence of images is optimized and calculated.


Alignment
GUI
Upload images
Automatic particle location detection
Manual adjustments of particle location
Calculate Optimized alignment
User
Engine

Alignment

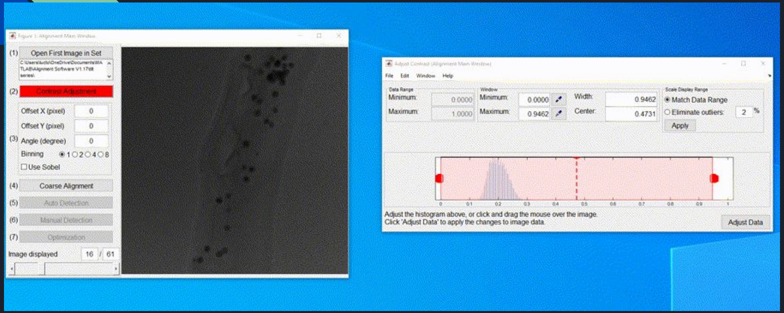


Figure 1: Alignment Main Window

(1) Open First Image in Set

C:\Users\ucto\OneDrive\Documents\MATLAB\Alignment Software V1.17\tilt series\

(2) Contrast Adjustment

(3) Offset X (pixel) 0

Offset Y (pixel) 0

Angle (degree) 0

Binning ● 1 ○ 2 ○ 4 ○ 8

□ Use Sobel

(4) Coarse Alignment

(5) Auto Detection

(6) Manual Detection

(7) Optimization

Image displayed 16 / 61

Adjust Contrast (Alignment Main Window)

File Edit Window Help

Data Range: Minimum: 0.0000 Maximum: 1.0000

Window: Minimum: 0.0000 Maximum: 0.9462 Width: 0.9462 Center: 0.4731

Scale Display Range: ● Match Data Range ○ Eliminate outliers: 2 %

Apply

Adjust the histogram above, or click and drag the mouse over the image.
Click 'Adjust Data' to apply the changes to image data.

Adjust Data

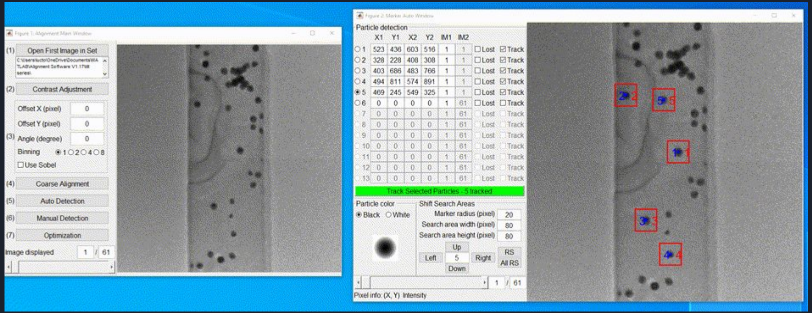


Figure 1: Alignment Main Window

(1) Open First Image in Set

C:\Users\ucto\OneDrive\Documents\MATLAB\Alignment Software V1.17\tilt series\

(2) Contrast Adjustment

(3) Offset X (pixel) 0

Offset Y (pixel) 0

Angle (degree) 0

Binning ● 1 ○ 2 ○ 4 ○ 8

□ Use Sobel

(4) Coarse Alignment

(5) Auto Detection

(6) Manual Detection

(7) Optimization

Image displayed 1 / 61

Figure 2: Marker Auto Window

Particle detection

	X1	Y1	X2	Y2	IM1	IM2		
○ 1	523	436	603	516	1	1	□ Lost	☑ Track
○ 2	328	228	408	308	1	1	□ Lost	☑ Track
○ 3	403	686	483	766	1	1	□ Lost	☑ Track
○ 4	494	811	574	891	1	1	□ Lost	☑ Track
● 5	469	245	549	325	1	1	□ Lost	☑ Track
○ 6	0	0	0	0	1	61	□ Lost	□ Track
○ 7	0	0	0	0	1	61	□ Lost	□ Track
○ 8	0	0	0	0	1	61	□ Lost	□ Track
○ 9	0	0	0	0	1	61	□ Lost	□ Track
○ 10	0	0	0	0	1	61	□ Lost	□ Track
○ 11	0	0	0	0	1	61	□ Lost	□ Track
○ 12	0	0	0	0	1	61	□ Lost	□ Track
○ 13	0	0	0	0	1	61	□ Lost	□ Track

Track Selected Particles - 5 tracked

Particle color: ● Black ○ White

Shift Search Areas

Marker radius (pixel) 20

Search area width (pixel) 80

Search area height (pixel) 80

Up Left 5 Right Down RS All RS

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Pixel info: (X, Y) Intensity

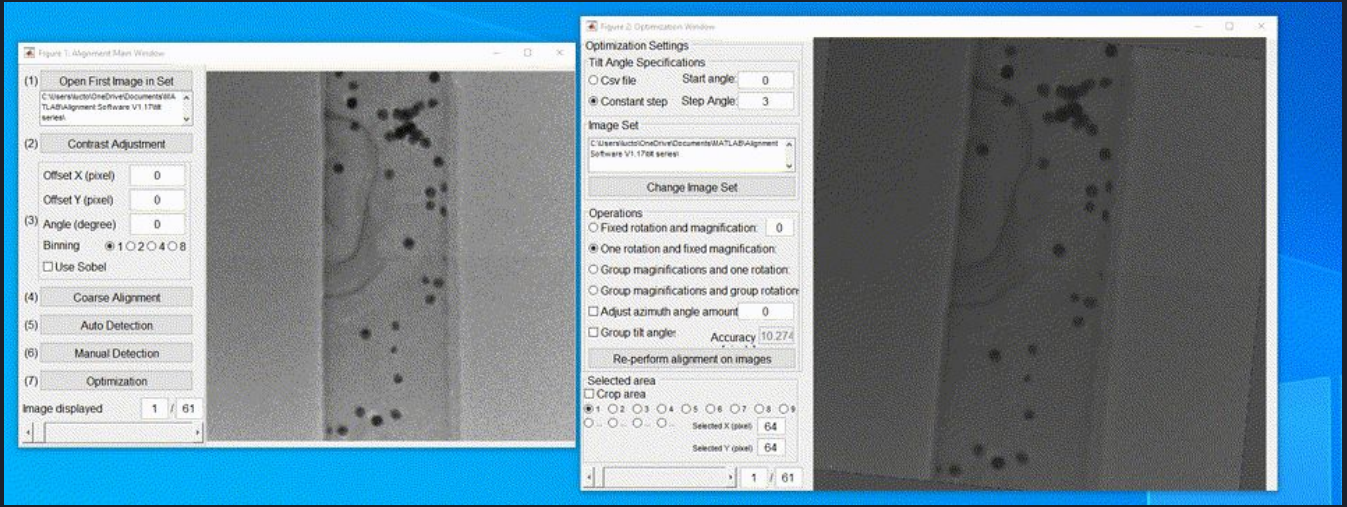

Figure 1: Alignment Main Window

(1) Open First Image in Set

C:\Users\ucto\OneDrive\Documents\MATLAB\Alignment Software V1.17\tilt series\

(2) Contrast Adjustment

(3) Offset X (pixel) 0

Offset Y (pixel) 0

Angle (degree) 0

Binning ● 1 ○ 2 ○ 4 ○ 8

□ Use Sobel

(4) Coarse Alignment

(5) Auto Detection

(6) Manual Detection

(7) Optimization

Image displayed 1 / 61

Figure 2: Optimization Window

Optimization Settings

Tilt Angle Specifications

○ Csv file Start angle 0

● Constant step Step Angle 3

Image Set

C:\Users\ucto\OneDrive\Documents\MATLAB\Alignment Software V1.17\tilt series\

Change Image Set

Operations

○ Fixed rotation and magnification 0

● One rotation and fixed magnification

○ Group maginifications and one rotation

○ Group maginifications and group rotation

□ Adjust azimuth angle amount 0

□ Group tilt angle Accuracy 10.274

Re-perform alignment on images

Selected area

□ Crop area

● 1 ○ 2 ○ 3 ○ 4 ○ 5 ○ 6 ○ 7 ○ 8 ○ 9 ○ ○ ○ ○

Selected X (pixel) 64

Selected Y (pixel) 64

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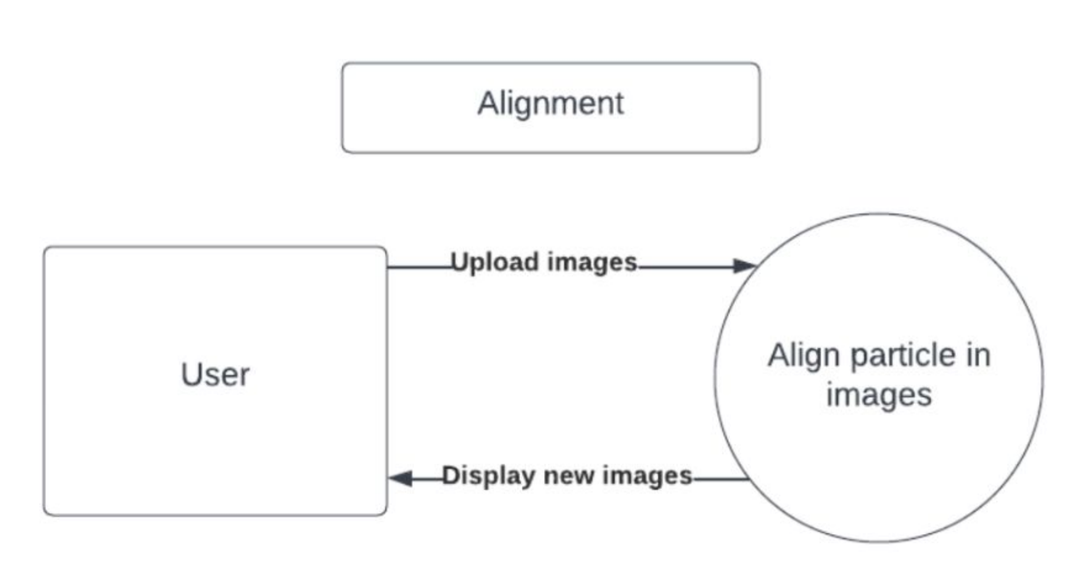
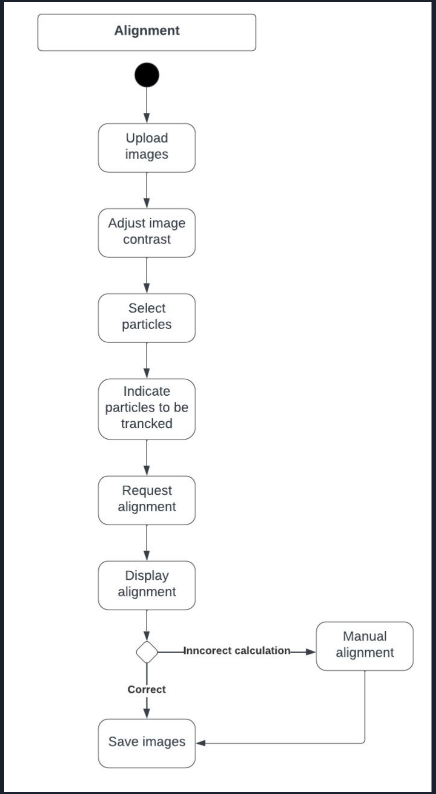
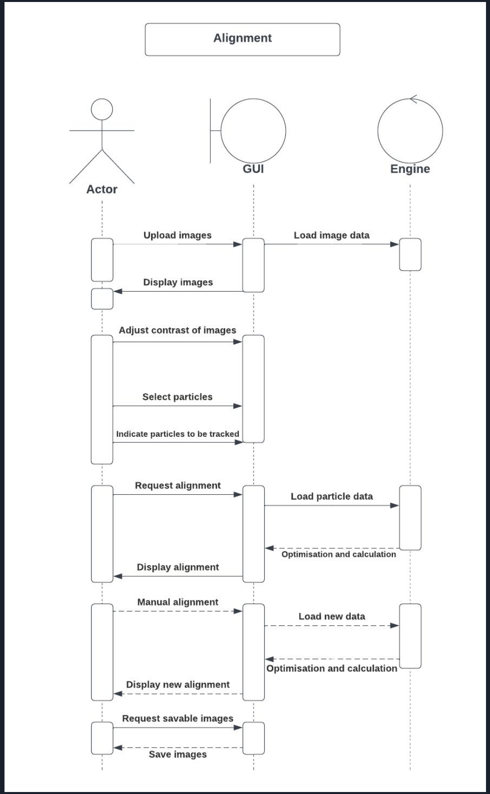
Alignment - Data Flow

Level 0 DFD

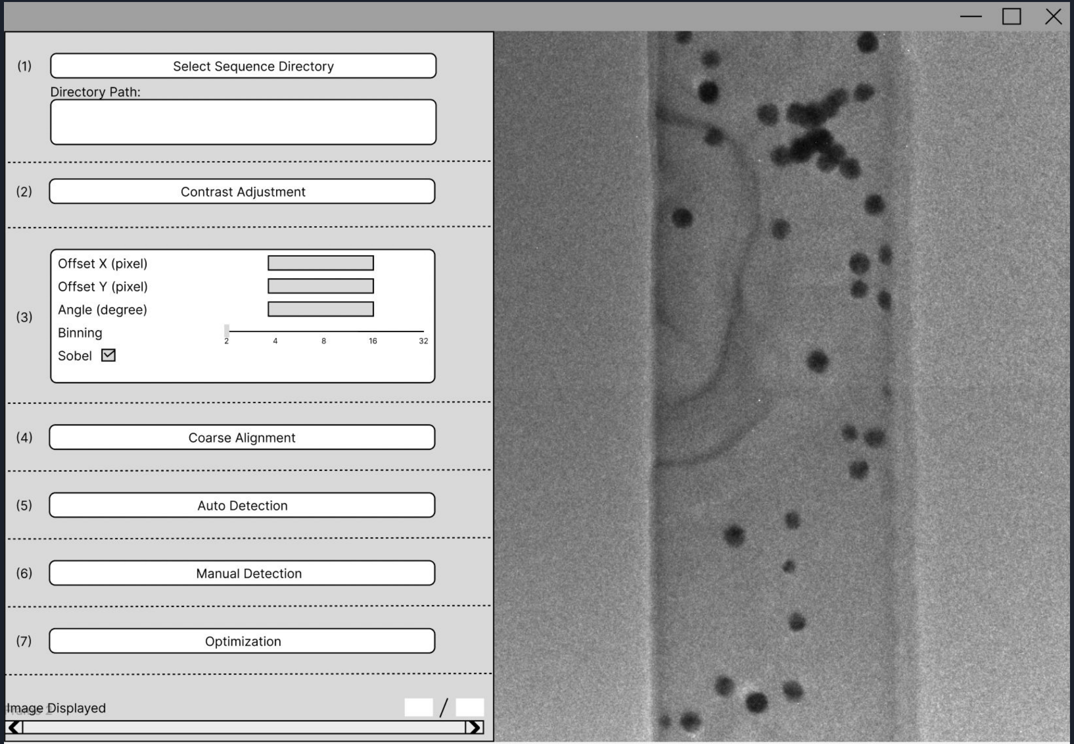


Alignment - Sequence Diagram





Alignment - Main Window UI



(1) Select Sequence Directory

Directory Path:

(2) Contrast Adjustment

(3)

Offset X (pixel)

Offset Y (pixel)

Angle (degree)

Binning

Sobel ☑

(4) Coarse Alignment

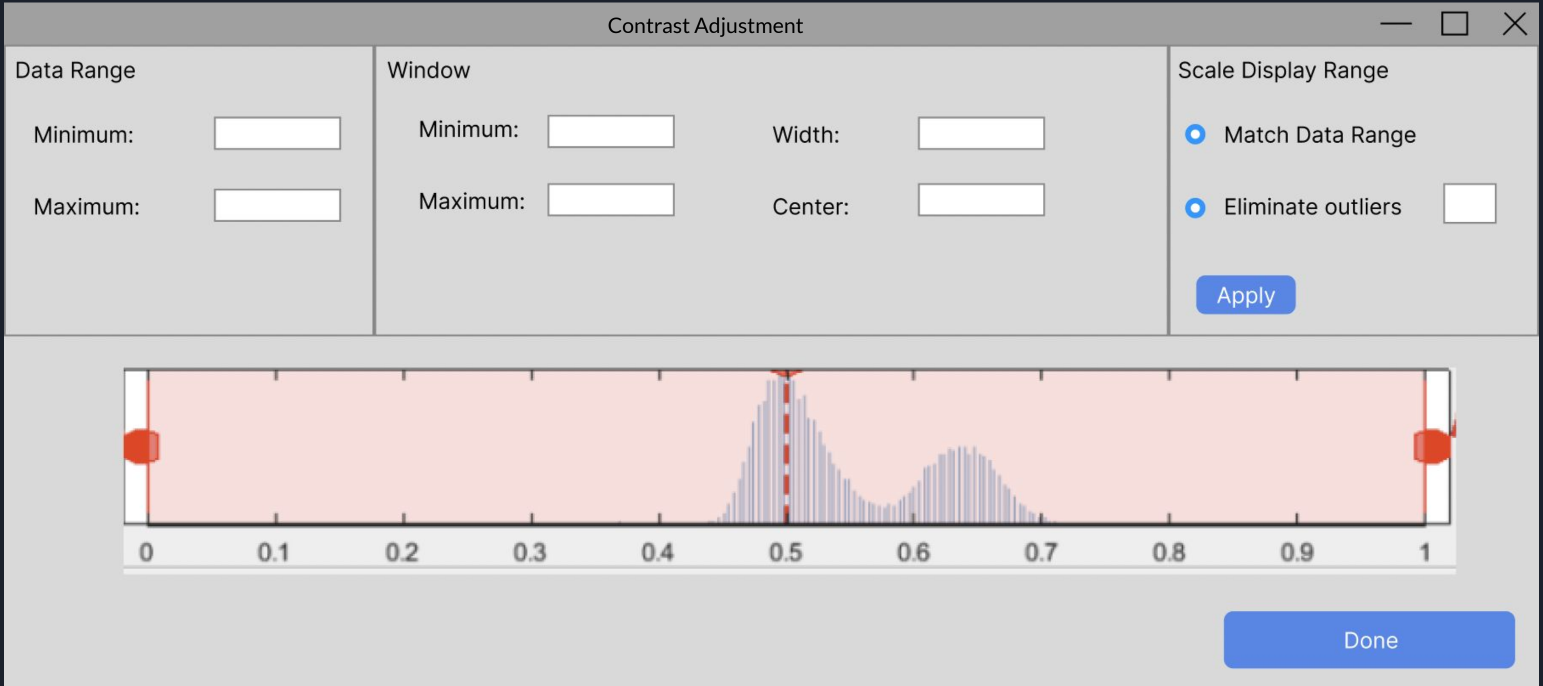
(5) Auto Detection

(6) Manual Detection

(7) Optimization

Image Displayed /

Alignment - Adjust Contrast UI



Contrast Adjustment

Data Range

Minimum:

Maximum:

Window

Minimum:

Maximum:

Width:

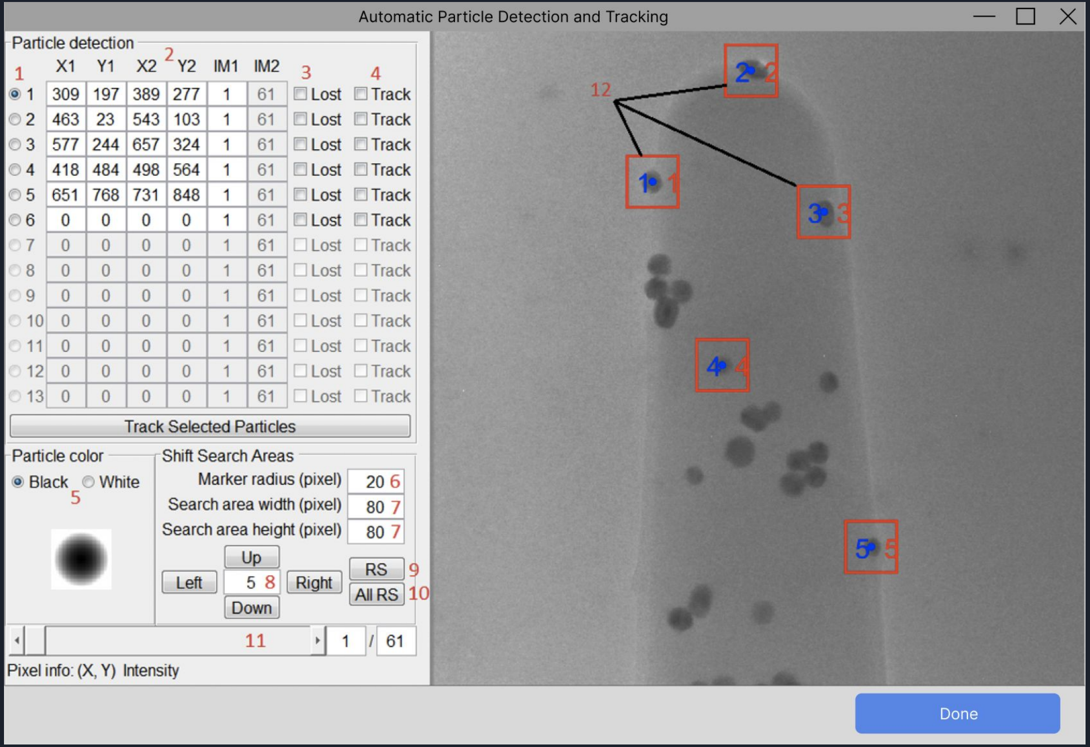
Center:

Scale Display Range

○ Match Data Range

○ Eliminate outliers

Alignment - Automatic Particle Detection and Tracking UI



Automatic Particle Detection and Tracking

Particle detection

	X1	Y1	X2	Y2	IM1	IM2		
● 1	309	197	389	277	1	61	□ Lost	□ Track
○ 2	463	23	543	103	1	61	□ Lost	□ Track
○ 3	577	244	657	324	1	61	□ Lost	□ Track
○ 4	418	484	498	564	1	61	□ Lost	□ Track
○ 5	651	768	731	848	1	61	□ Lost	□ Track
○ 6	0	0	0	0	1	61	□ Lost	□ Track
○ 7	0	0	0	0	1	61	□ Lost	□ Track
○ 8	0	0	0	0	1	61	□ Lost	□ Track
○ 9	0	0	0	0	1	61	□ Lost	□ Track
○ 10	0	0	0	0	1	61	□ Lost	□ Track
○ 11	0	0	0	0	1	61	□ Lost	□ Track
○ 12	0	0	0	0	1	61	□ Lost	□ Track
○ 13	0	0	0	0	1	61	□ Lost	□ Track

Track Selected Particles

Particle color

● Black ○ White

Shift Search Areas

Marker radius (pixel) 20

Search area width (pixel) 80

Search area height (pixel) 80

Up

Left 5 Right

Down

RS

All RS

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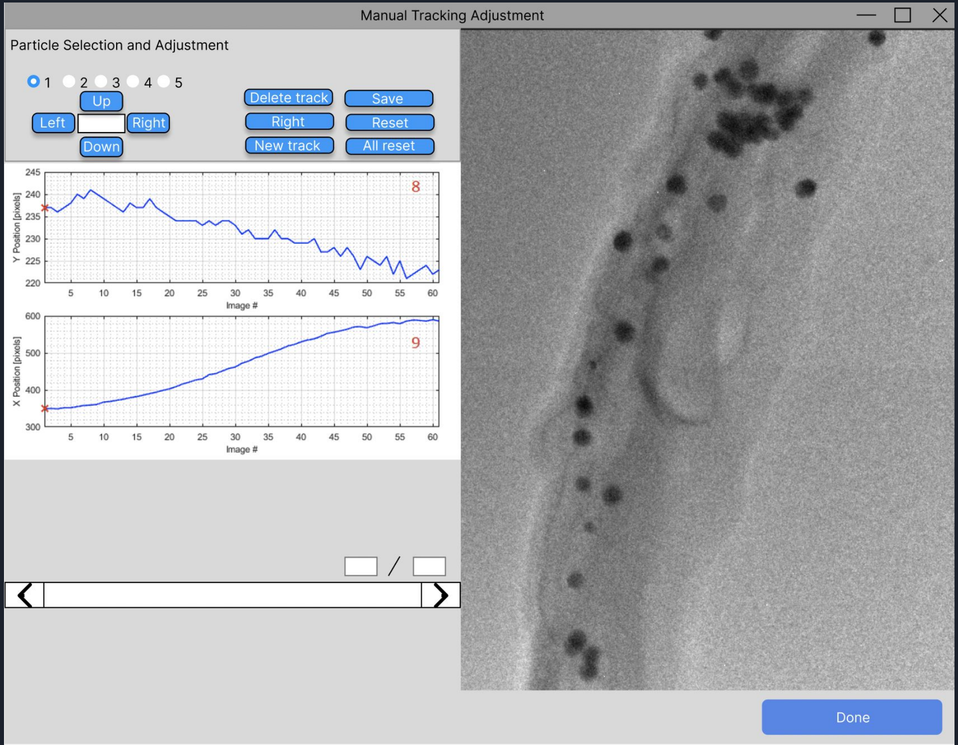
Pixel info: (X, Y) Intensity

Done

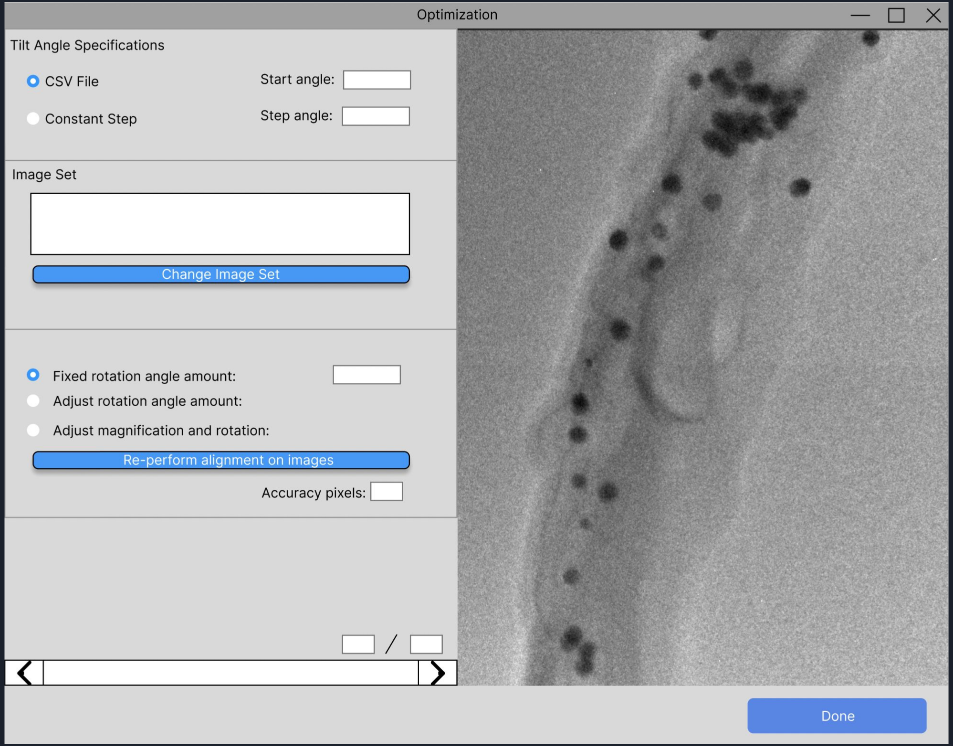
Alignment - Manual Tracking Adjustment UI



Manual Tracking Adjustment

Particle Selection and Adjustment

Alignment - Optimization UI



Optimization

Tilt Angle Specifications

- ● CSV File
- ○ Constant Step

Start angle: □

Step angle: □

Image Set

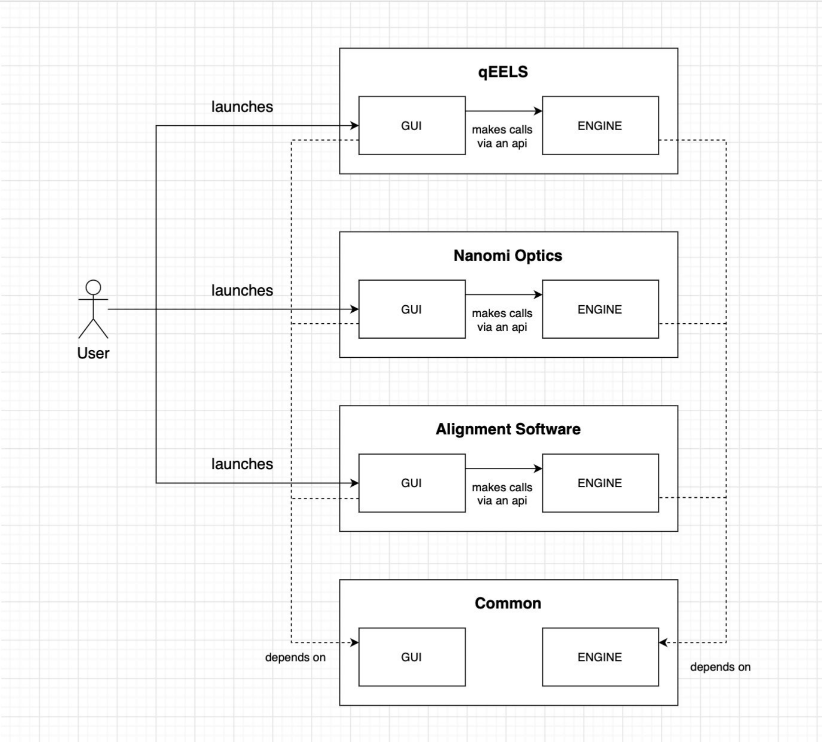
□

- ● Fixed rotation angle amount: □
- ○ Adjust rotation angle amount:
- ○ Adjust magnification and rotation:

Accuracy pixels: □

□ / □

Architecture



- Each project will be separate launcheable piece of software
- Each project will have a distinct GUI and ENGINE
- The GUI will make calls to the ENGINE
- The ENGINE will not make calls to the GUI
- Common functionality between the three softwares will be factored out into shared Common package

Tech Stack

Programming Languages:

- Python

Python Libraries:

- Tkinter (GUI)
- Matplotlib (Chart Rendering)
- Scipy (Optimization and other algorithms)
- Numpy (Efficient numeric arrays)
- Pillow (Image processing and transforms)
- Flake8 (Linting)
- Pytest (Unit Testing)

Tech Stack

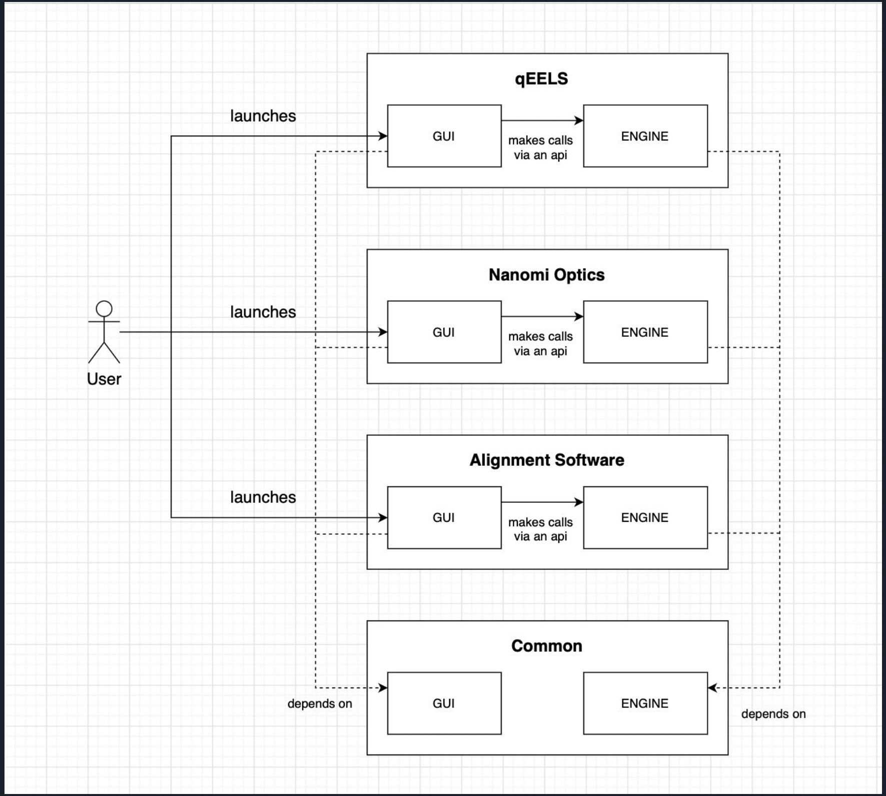
Supporting Technologies:

- Github
- Github Actions (CI/CD)
- Github Projects (Project Management)

Testing Plan

- Set up Github Actions workflows to run all tests automatically
- Pushing to the main branch directly will be blocked
- Merging pull requests without all tests passing first will be blocked
- All pull-requests will require an approving review
- Pull-requests should not be approved unless they include tests which demonstrate the functionality they implement
- All code will be linted with Flake8 automatically

Testing Plan: System Architecture



Testing Plan: Optimization Problems

- Nanomi Optics and the Alignment Software both use Optimization Algorithms
- Optimization output can vary from the original software
- Optimization output may vary run-to-run or machine-to-machine
- Instead of testing for an exact result, use some threshold tests to test the underlying conditions that the software is optimizing for

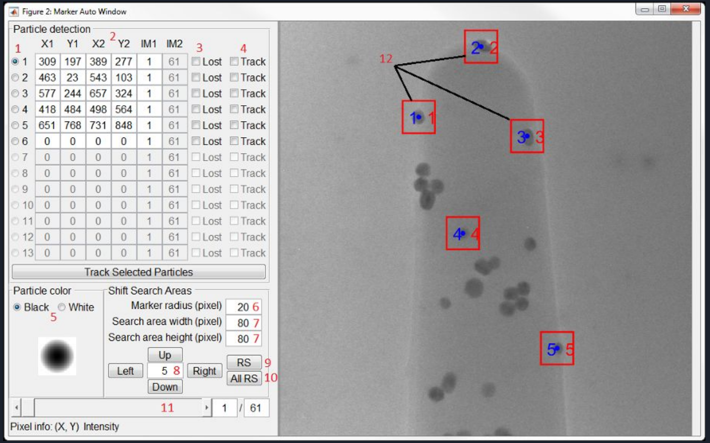


Figure 2: Marker Auto Window

Particle detection

	X1	Y1	X2	Y2	IM1	IM2		
● 1	309	197	389	277	1	61	□ Lost	□ Track
○ 2	463	23	543	103	1	61	□ Lost	□ Track
○ 3	577	244	657	324	1	61	□ Lost	□ Track
○ 4	418	484	498	564	1	61	□ Lost	□ Track
○ 5	651	768	731	848	1	61	□ Lost	□ Track
○ 6	0	0	0	0	1	61	□ Lost	□ Track
○ 7	0	0	0	0	1	61	□ Lost	□ Track
○ 8	0	0	0	0	1	61	□ Lost	□ Track
○ 9	0	0	0	0	1	61	□ Lost	□ Track
○ 10	0	0	0	0	1	61	□ Lost	□ Track
○ 11	0	0	0	0	1	61	□ Lost	□ Track
○ 12	0	0	0	0	1	61	□ Lost	□ Track
○ 13	0	0	0	0	1	61	□ Lost	□ Track

Particle color: ● Black ○ White

Shift Search Areas

Marker radius (pixel): 20

Search area width (pixel): 80

Search area height (pixel): 80

Shift: 5

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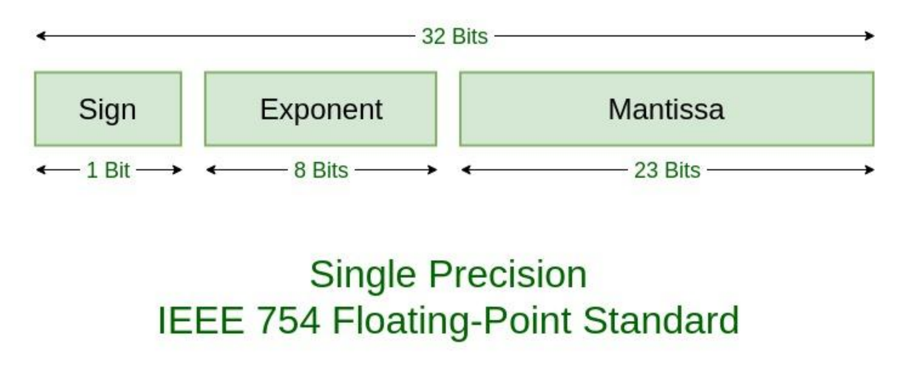
Pixel info: (X, Y) Intensity

Testing Plan: Floating-Point Problems

- All three of the softwares use floating-numbers extensively
- Not all numbers can be represented exactly by a floating-point number
- Some loss in precision when operations are performed
- Equality depends on order of operations
- Once again, use thresholds



Testing Plan: Large Output Problems

- Alignment Software performs many operations on large images which much be tested, such contrast adjustment and kernel convolution
- Could be to have an exact copy of the expected output, but that is difficult to hand-craft
- Use smaller sample images for test-cases which will make crafting test-cases easier