NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

CHRNS CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING NIST

Development of an Interface for Analyzing Neutron Dark Field Imaging Data

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*Certain commercial software programs are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

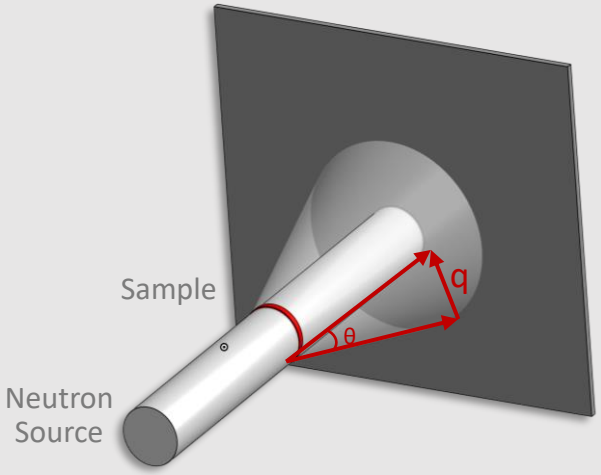
SANS

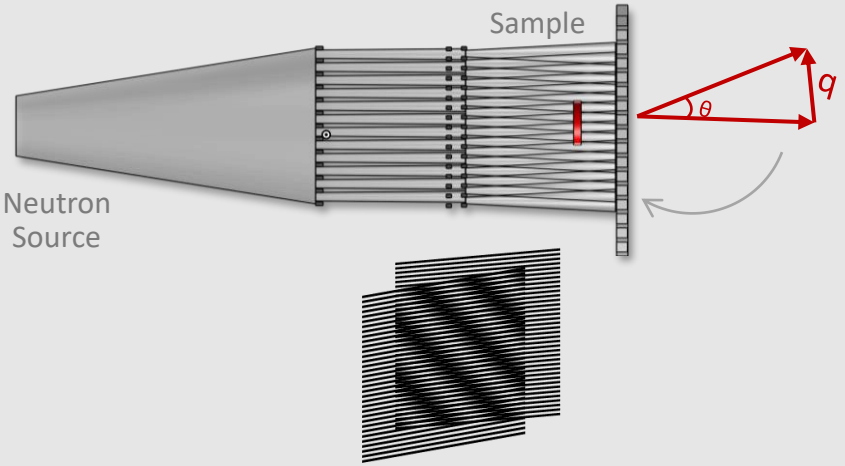
(Small Angle Neutron Scattering)

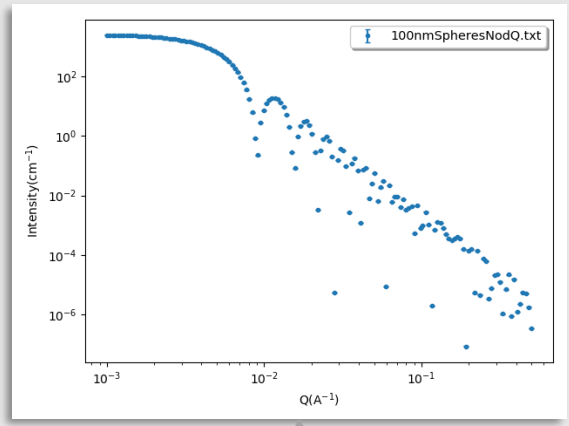
VS

NEUTRON INTERFEROMETER

(Neutron Far Field Interferometry and Dark Field Imaging)







Equations For Graph

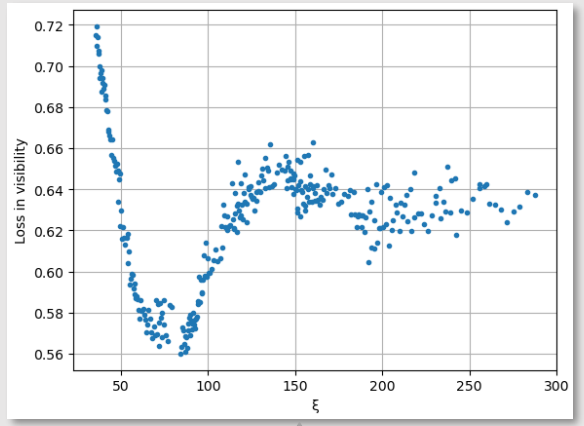
$$|q| = \frac{4\pi}{\lambda}\sin\left(\frac{\theta}{2}\right) = \frac{2\pi n}{d}$$

$$I(q) = n\Delta p^2 V^2 P(q) S(q) + \text{background}$$

Equations For Graph

$$\text{Loss in Visibility} = \frac{V_S}{V_O}$$

$$\xi = \frac{z\lambda}{P_D}$$

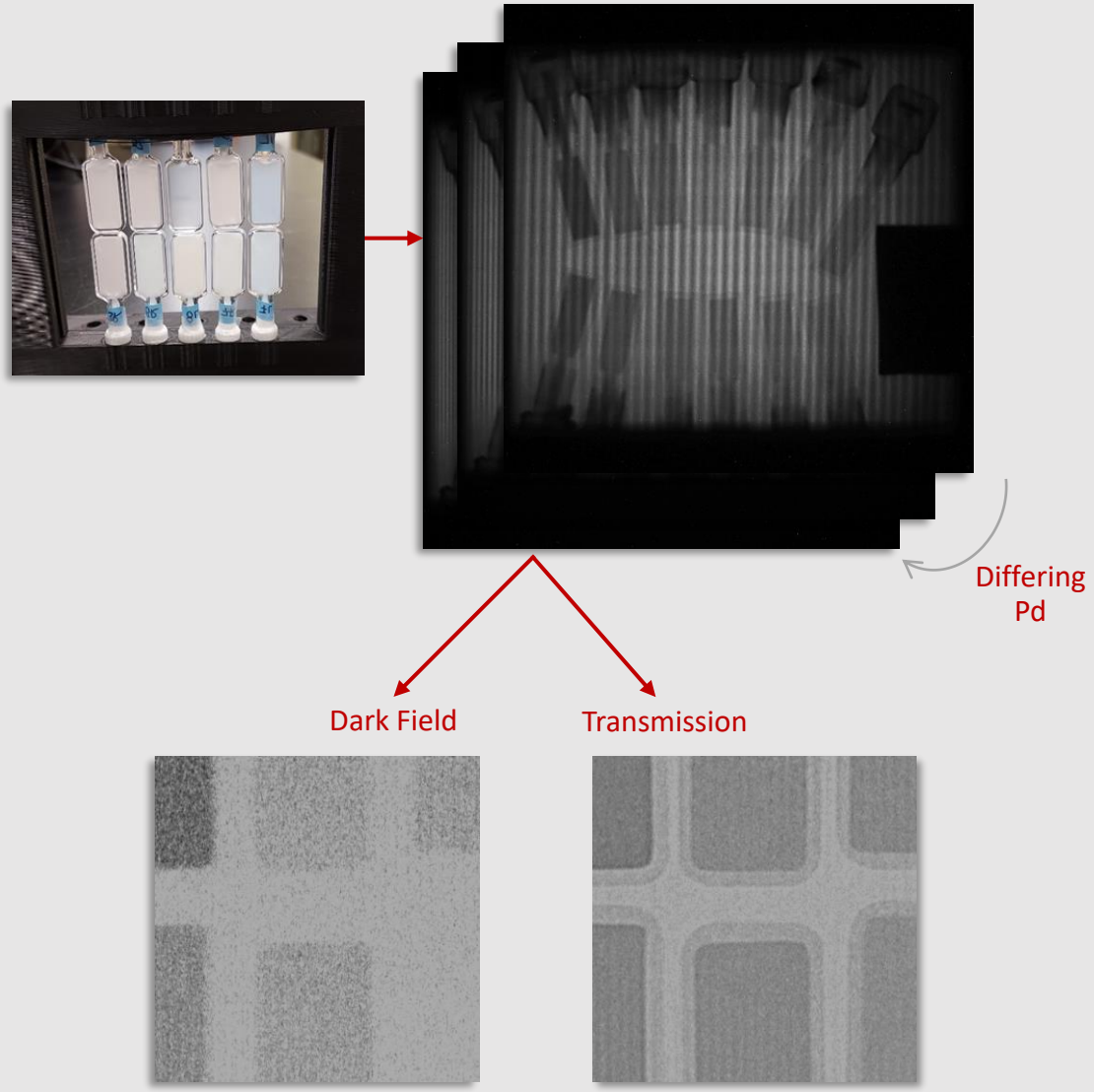


SasView Intensity graph for 100nm SpereNodQ

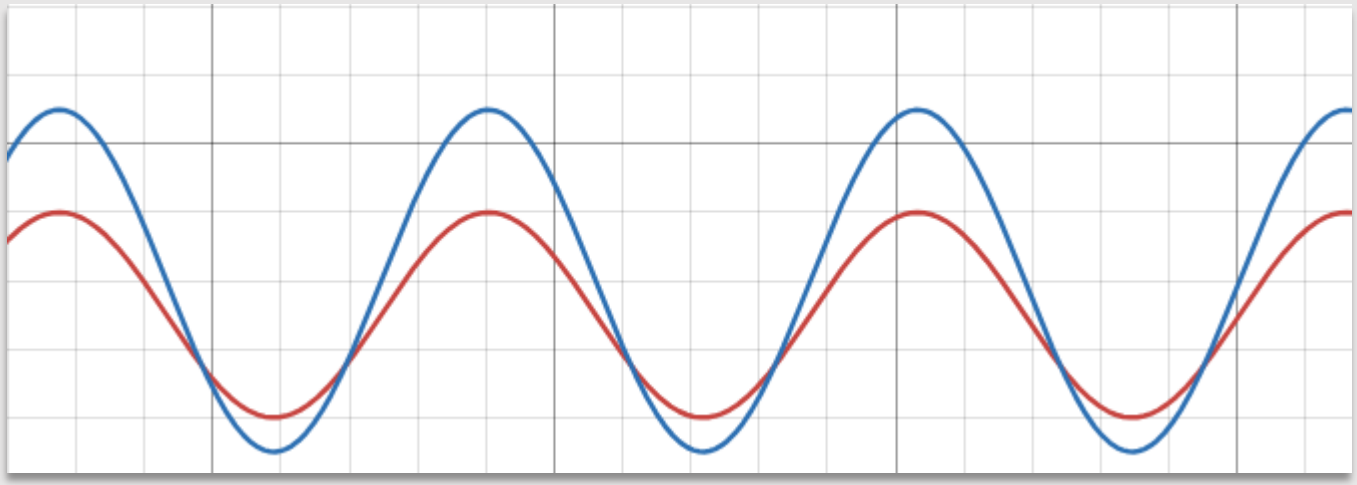
Hankel Transform
(Assuming same Data)

My Code Dark Field spectra for Polystyrene DF

IMAGING

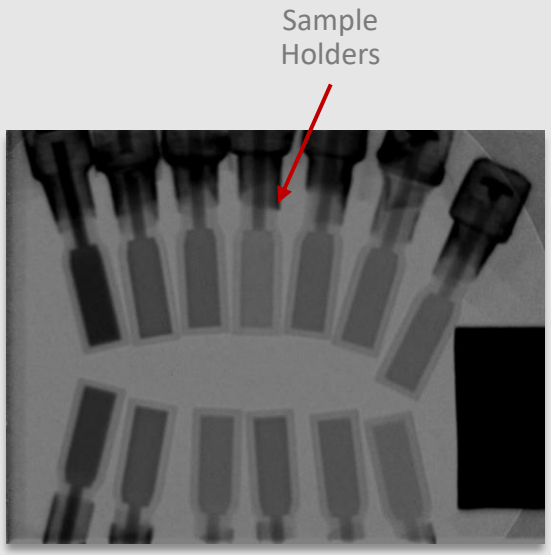


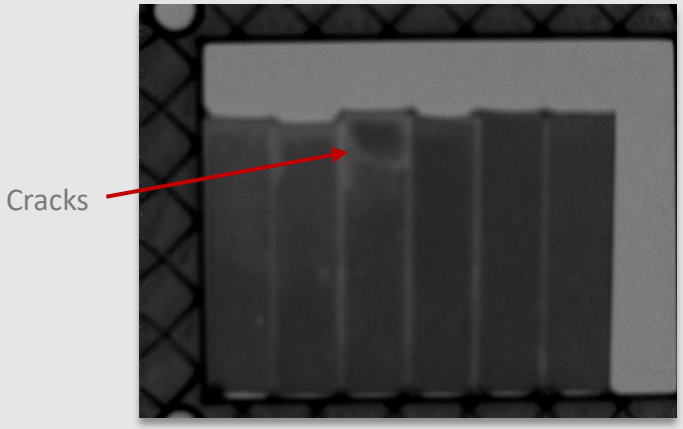
- Moire Pattern on the sample
- Spatial Resolution(Interferometry)
- Dark Field Images are compilations of other images
- Images are captured of more than one sample.

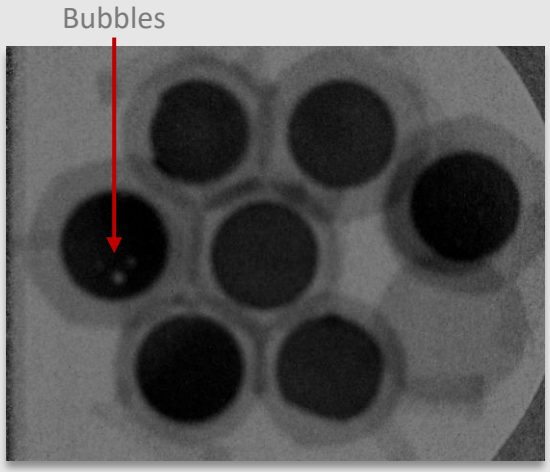


ILL data for the INFER team 2024-5 & LANL data from INFER team 2022-12

OBJECTIVE



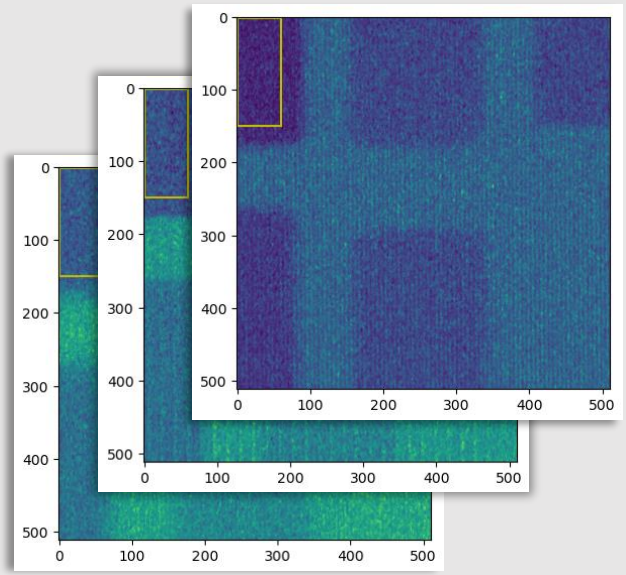




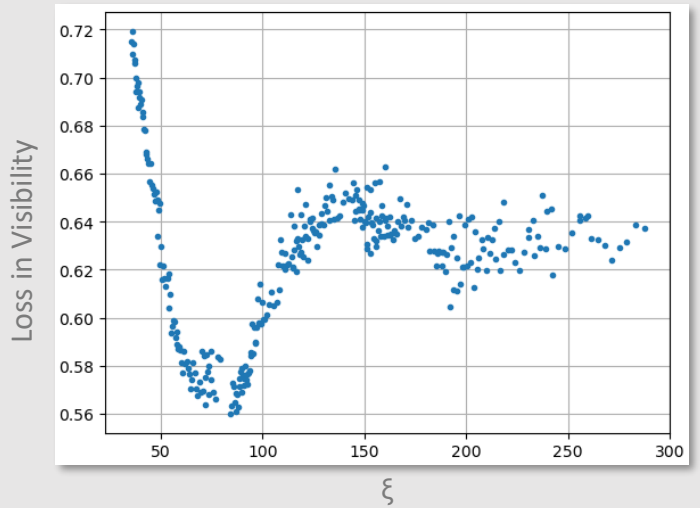
The goal of this project is to create a user interface that allows researchers to just select the region of interest (ROI) and fit the graph to models to analyze the data.

ILL data for the INFER team 2024-5

GRAPHING



Code

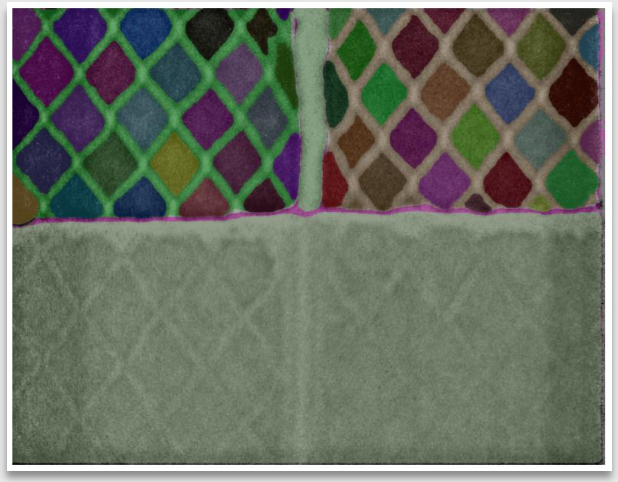


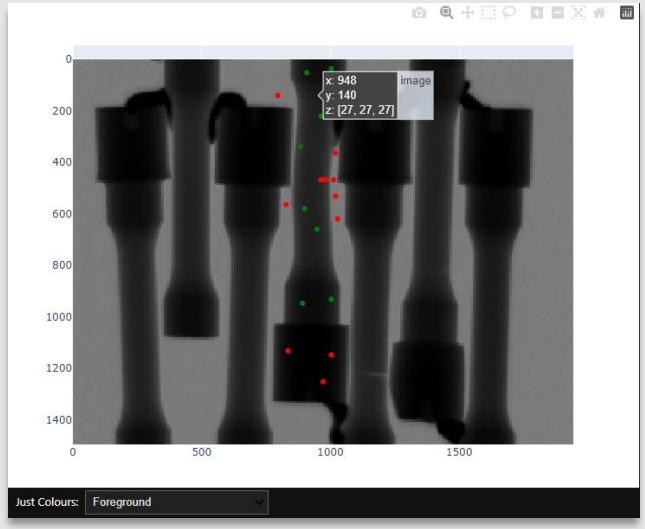
- Re-creating the code for extracting Dark Field Spectra.

  - Same ROI Selection as Previous Method

LANL data from INFER team 2022-12

SEGMENTATION





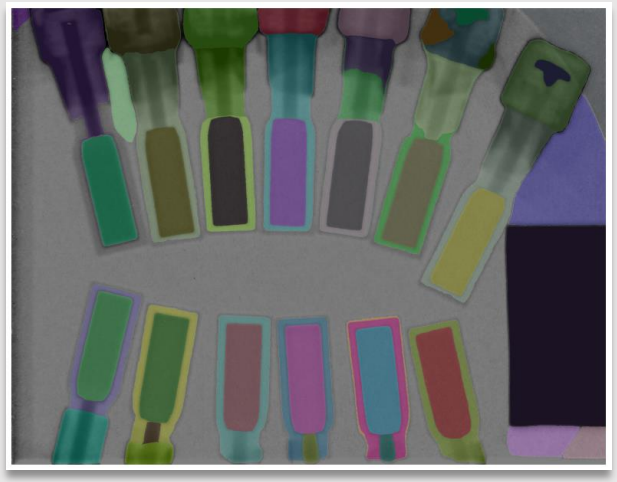
- Segment Anything Model(SAM) code packages

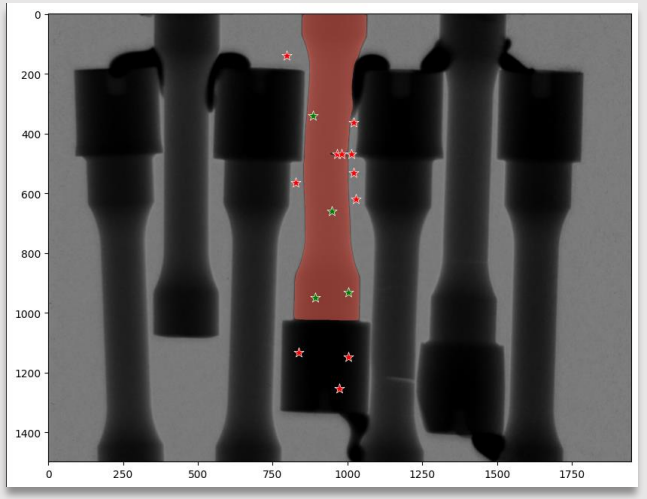
- Automatic Segmentation Vs. Prompted Segmentation

- Mask Generation and the manipulation of data

- Mask Exportation

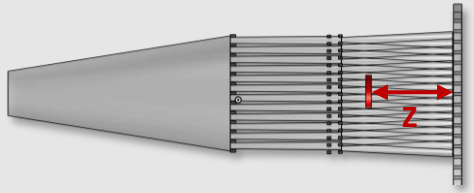
Meta

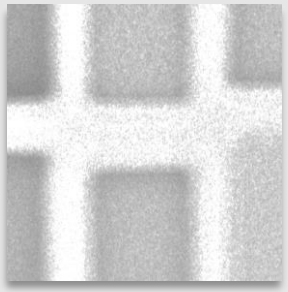


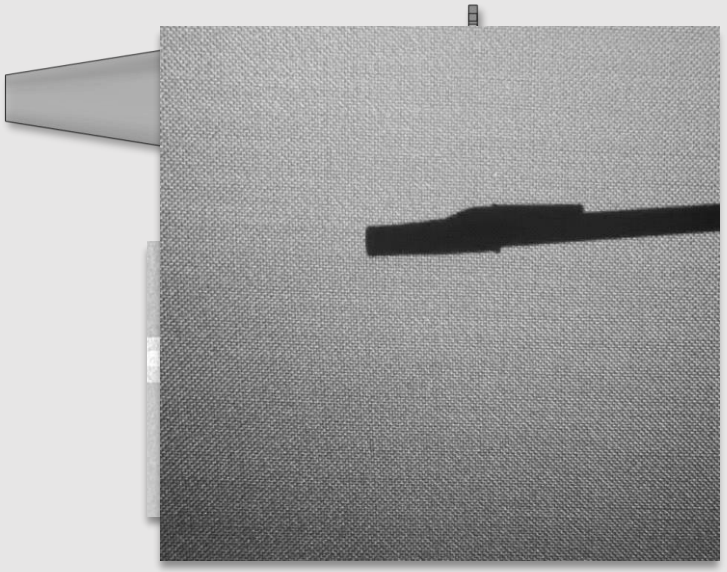


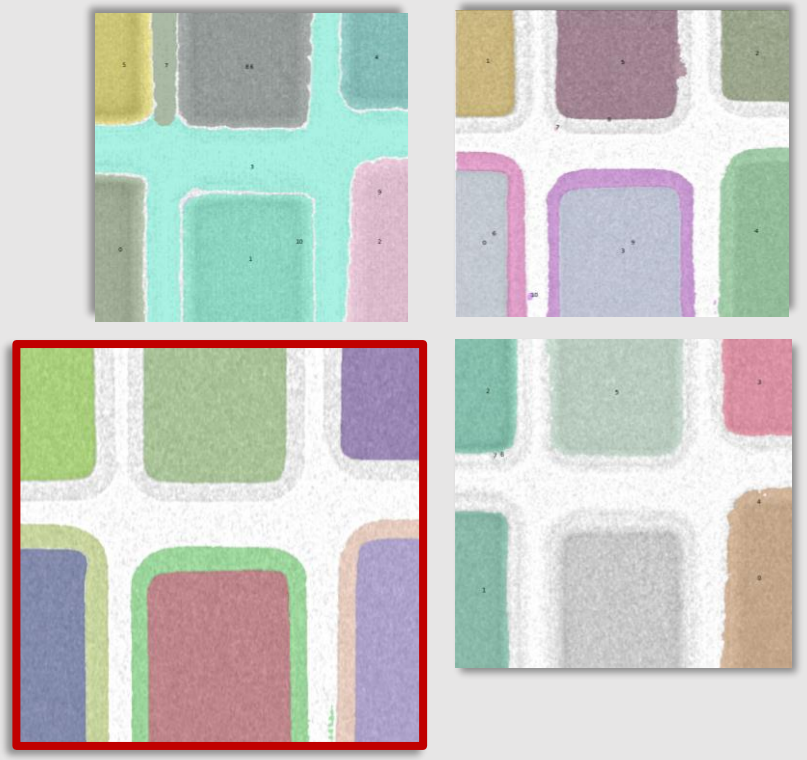
ILL data for the INFER team 2024-5 & LANL data from INFER team 2022-12

THE DATA SET





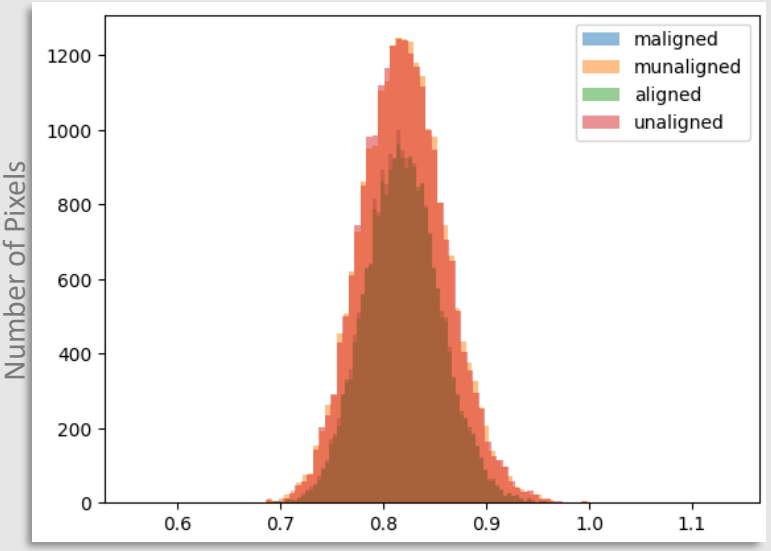


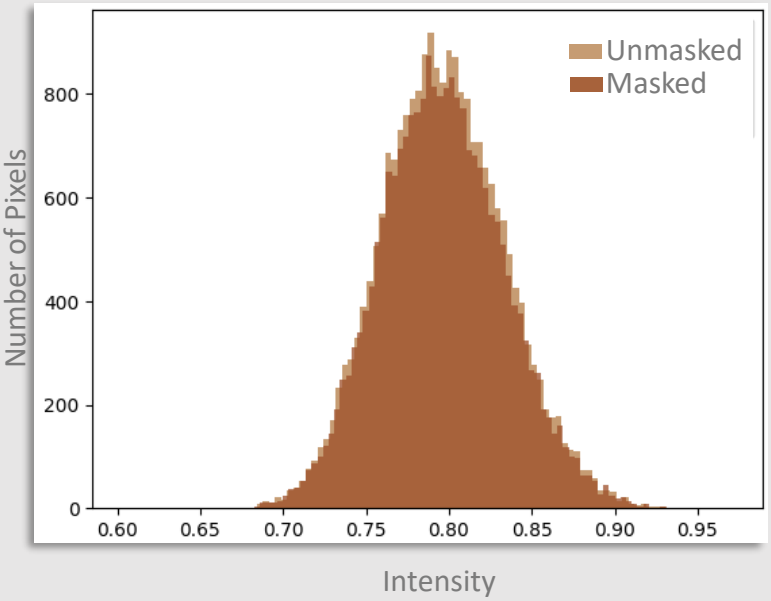


- One Mask per Image (Impractical)
- A single Mask for the whole data set
- Image for Mask Selection

Smallest Z distance transmission image

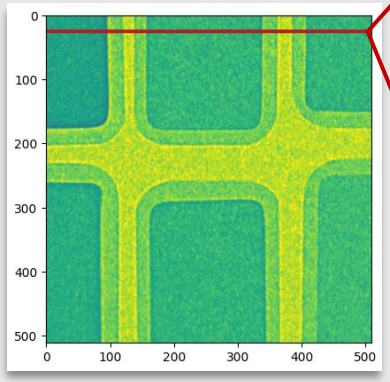
RESCALE

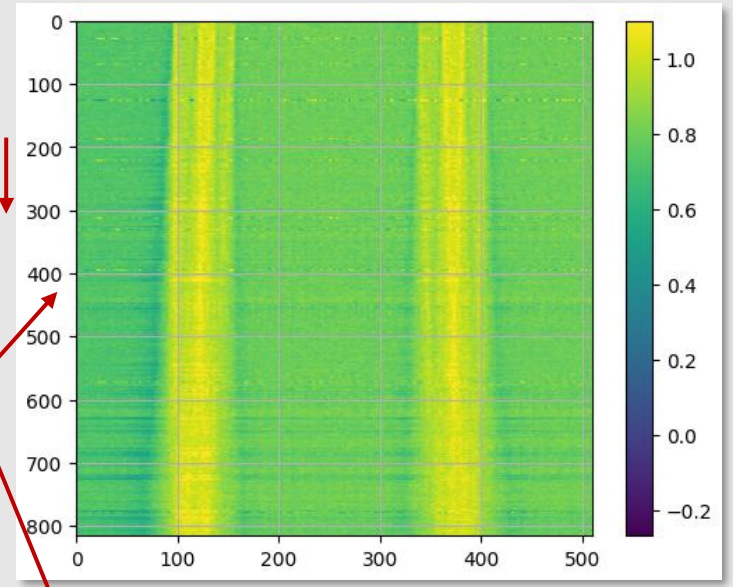


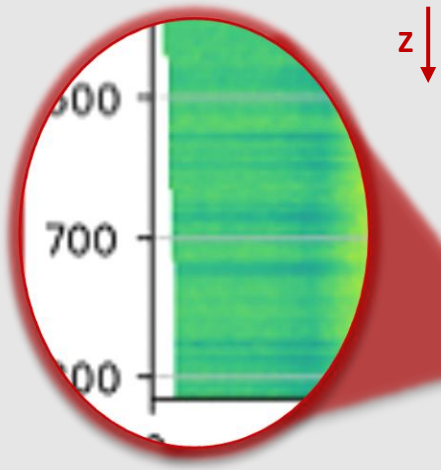


- Image Rescale Function shifts and squeezes
- Replacement pixels
- Difference minimalization

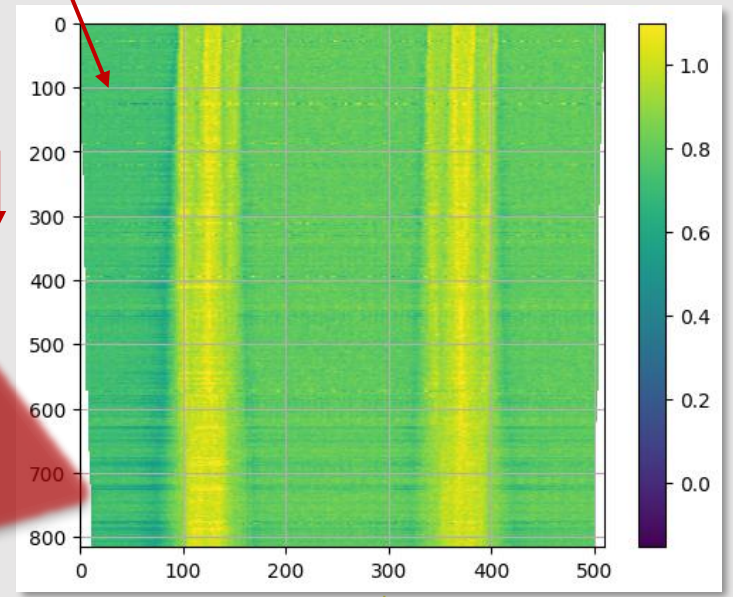
Unaligned





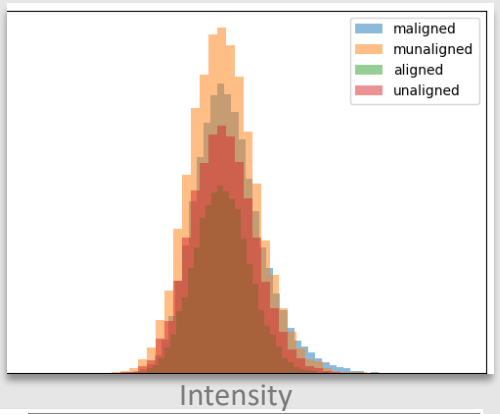


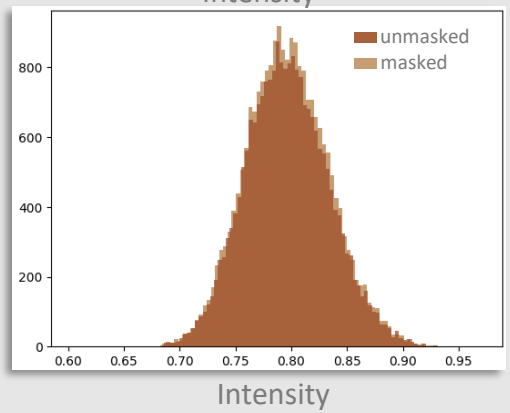
Aligned

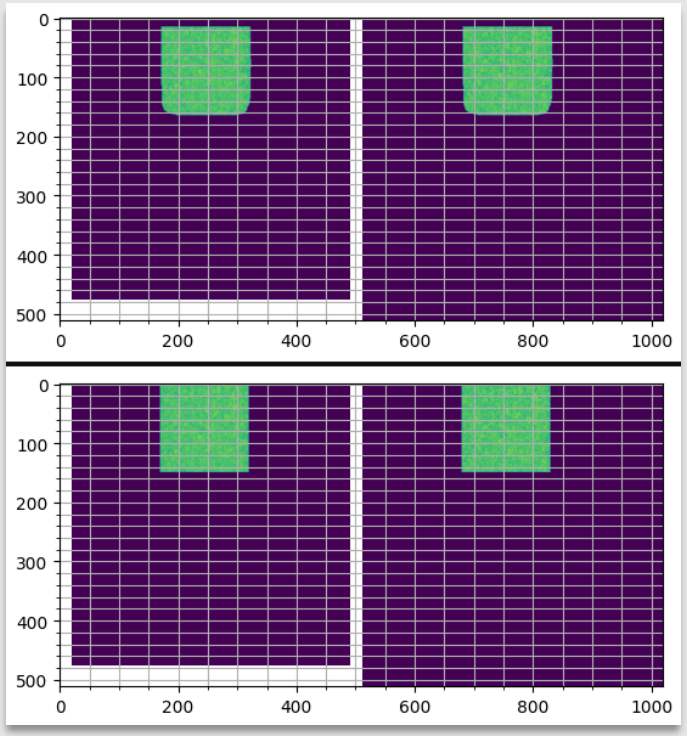


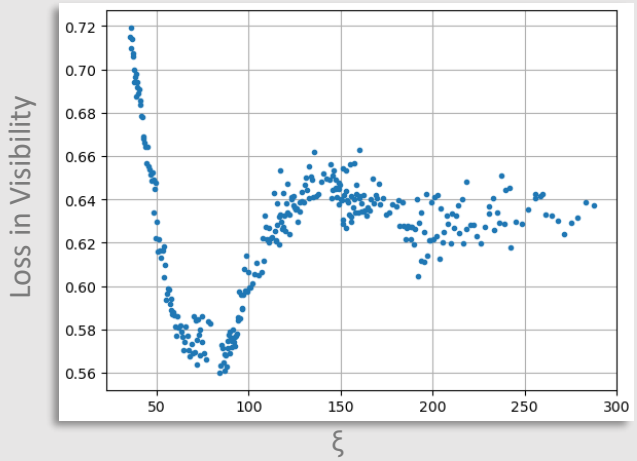
MASK

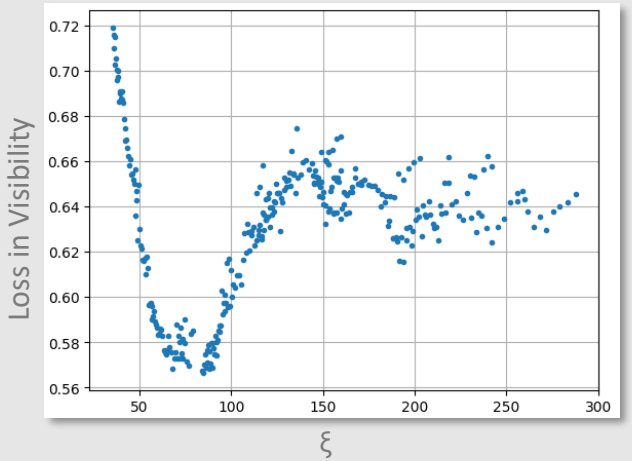
- Mask Erosion
- Minimization of difference
- Dark Field spectra from new ROI

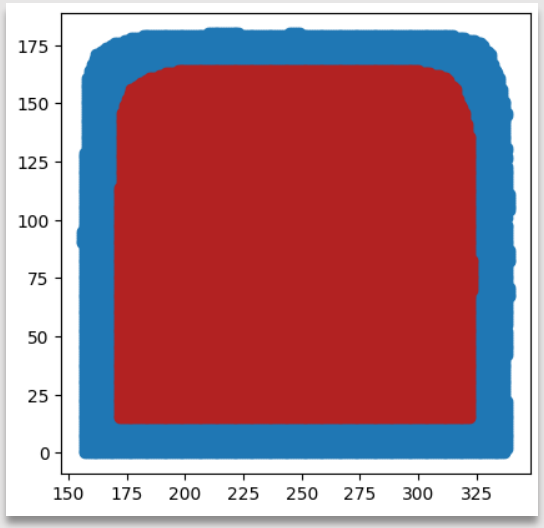




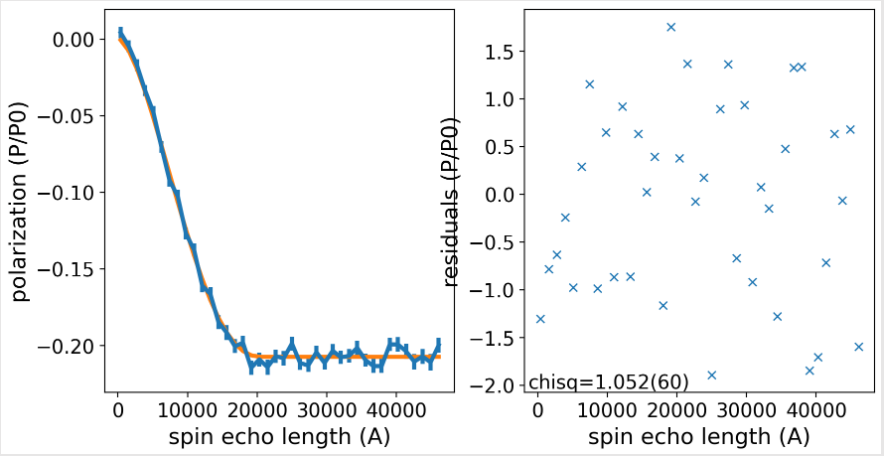


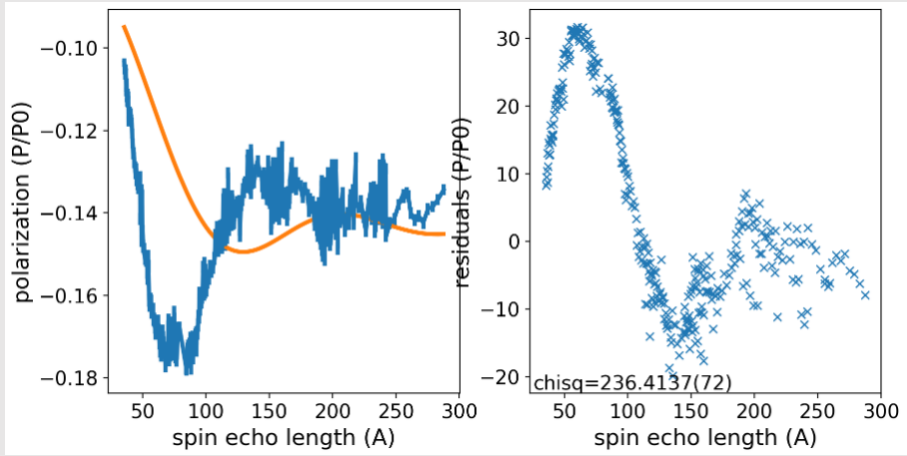






FITTING





- Fitting Models to Data Using SasView packages
- Storing the spectra points as SESANS data
- Parallel GUI

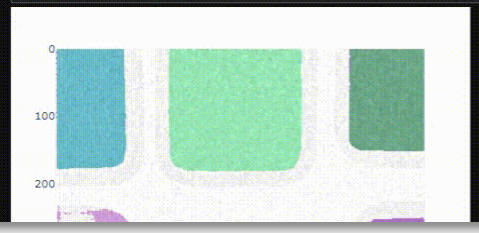
SasView

USER INTERFACE


```
import matplotlib.pyplot as plt
import random
import cv2
import requests
import plotly.express as px
import plotly.graph_objects as go
import os
from pycocotools import mask as mask_util
from unittest import mock
import math
import pandas as pd
# Mock pyautogui to prevent it breaking on import
sys.modules["pyautogui"] = mock.MagicMock()
import pyautogui
from scipy.ndimage import binary_erosion
```

```
[2]: import ipynb.fs.full.Automatic_Segmentation as automatic
     import ipynb.fs.full.SCopy as spectra
     import ipynb.fs.full.ImageReg as imagereg
     path = Path(r"/storage/pkienzle/data/2022-12-LANL-polystyrene")
     reference_ID = 4
     df = imagereg.uniform_images(path,reference_ID)
```

```
[11]: image = cv2.cvtColor(df.iloc[reference_ID]['atten_im'], cv2.COLOR_BGR2RGB)
      masks,x,y = automatic.pick_mask(image)
      plt.figure(figsize=(20,10))
```



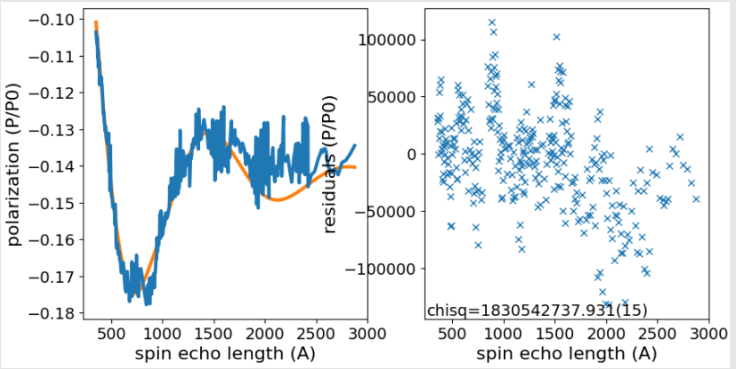

```
loaded_data_list = Loader().load('DarkFieldSpectra.ses')
data = loaded_data_list[0]
#data.SESANS = True
print(data)
#data = np.loadtxt("DarkFieldSpectra.txt", skiprows=2)
params = {
    "radius": 442.8,
    "background": 0, # always set to 0 for sesans data fits!
    'radius_pd_n':200,
    'radius_pd_nsigma':5,
    'radius_pd_type': 'gaussian',
    'radius_effective_mode': 1,
    'charge': 1,
    'temperature':293,
    'concentration_salt': 0.0035,
    'dielectconst': 79.755
}
kernel = sasmodels.core.load_model("sphere@hayter_msa")
model = sasmodels.bumps_model.Model(model=kernel, **params)

model.scale.range(0, 1)
model.radius.range(0, 20000)
model.radius_effective.range(0,1000)
model.volfraction.range(0,1)

experiment = sasmodels.bumps_model.Experiment(data=data, model=model)

problem = bumps.fitproblem.FitProblem(experiment)

results = bumps.fitters.fit(problem, verbose=True)
plt.figure(figsize=(10, 5))
problem.plot()
```



- The Current User Interface is on Jupyter notebooks
- Only Incorporates Automatic Segmentation
- Future: Dash

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jupyter → plotly | Dash

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THANK YOU!

To My Mentors: Caitlyn Wolf, Paul Kienzle, Katie Weigandt
To SHIP directors: Julie Borchers & Leland Harriger
The INFER Team
The NCNR
Family & SHIP Students!

Any Questions?