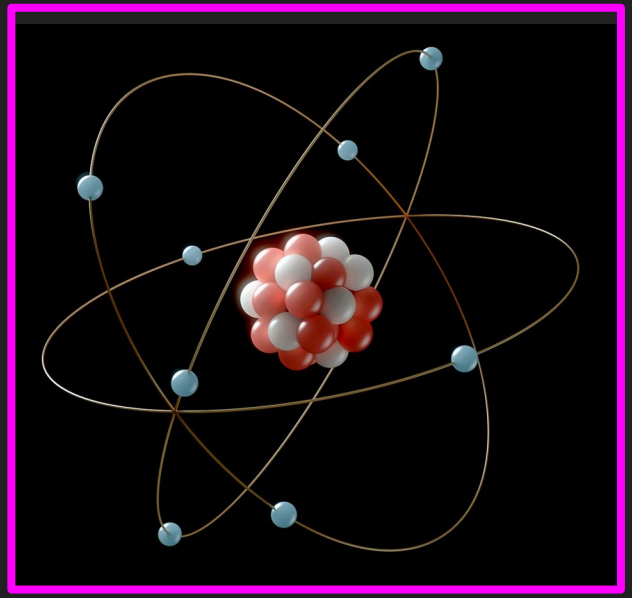

# Investigating Lipid Bilayer Structures with Neutron Reflectometry

By: Ryan Puthumana
Lab: NIST Center for Neutron Research (NCNR)
Mentors: David Hoogerheide and Frank Heinrich

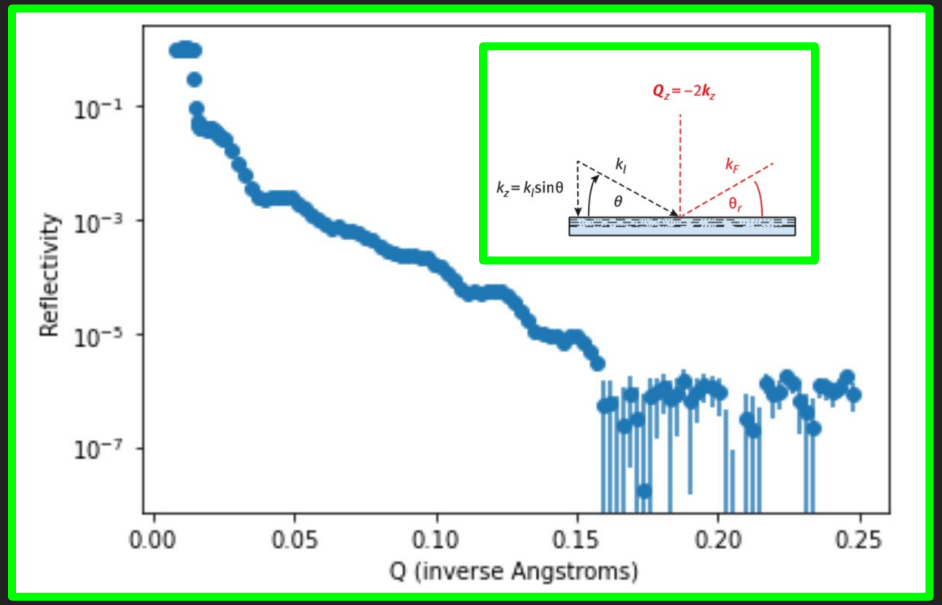
# Presentation Contents

- Introduction
  - What is Neutron Reflectometry?
- Project Workflow
- Results
- Conclusion/Future Directions



# Introduction: What is Neutron Reflectometry?

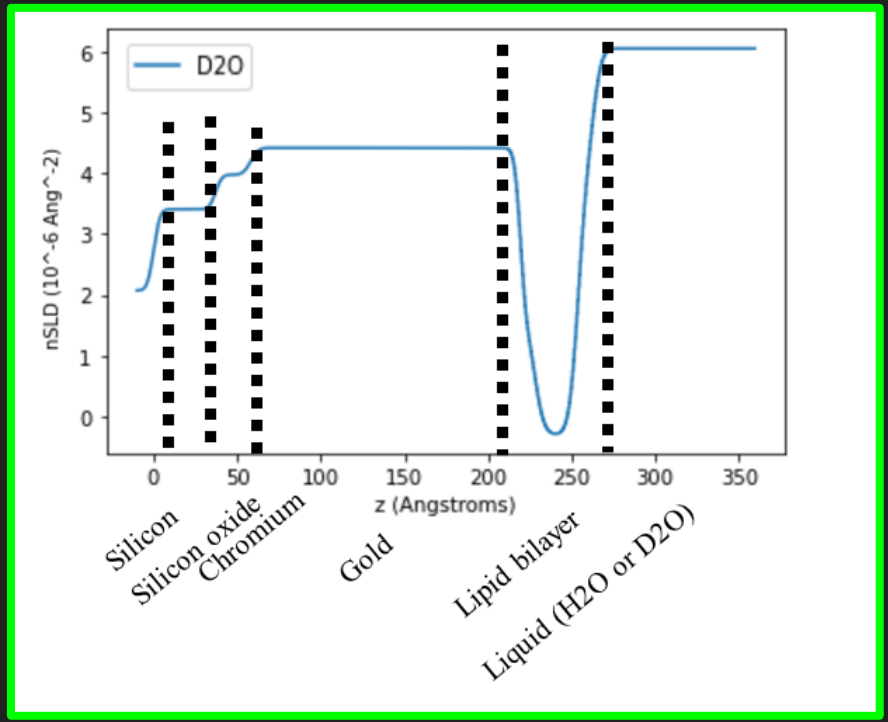
- Neutrons are reflected off a sample of interest
- Measure intensity of neutron reflection relative to incident intensity (reflectivity)
- Measure R (reflectivity) against Q (momentum transferred to neutron from surface).
- Can be used to determine structure of lipid bilayers and membrane proteins.




Eells, R., et al. "3. Structural investigations of membrane-associated proteins by neutron reflectometry". *Characterization of Biological Membranes*, 2019, pp. 87-130.

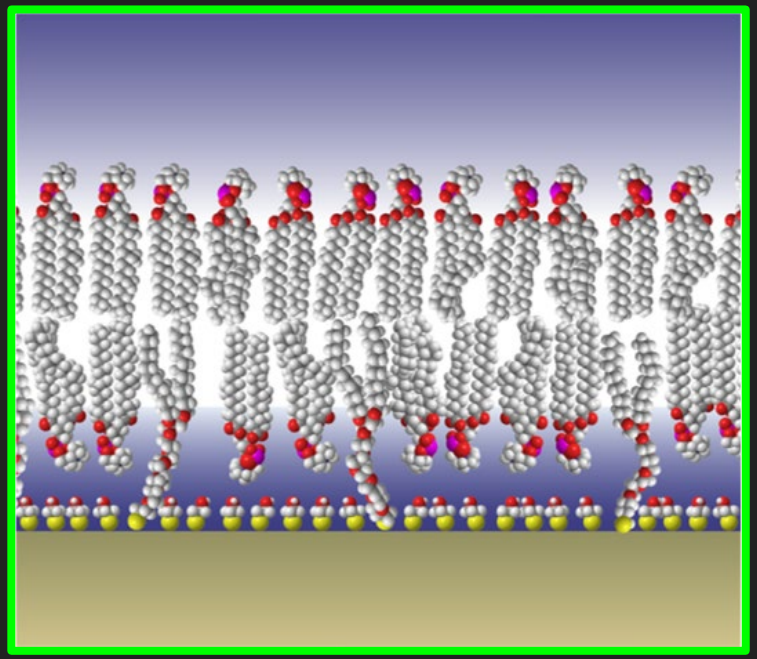
# Introduction: Scattering Length Density

- nSLD encodes the information about the structure of the interface and determines R(Q)
  - Each isotope has a unique scattering length
  - nSLD is material property dependent on the elemental composition and density




Eells, R., et al. "3. Structural investigations of membrane-associated proteins by neutron reflectometry". *Characterization of Biological Membranes*, 2019, pp. 87-130.

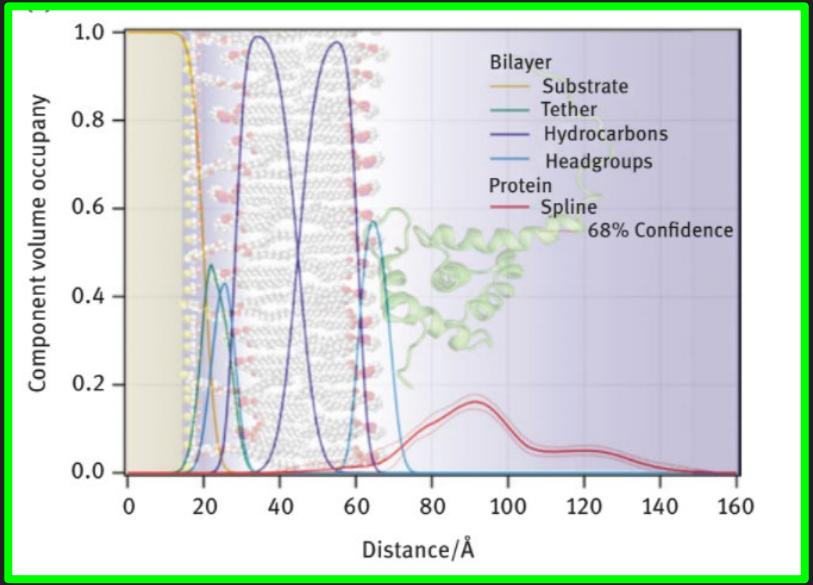
# Introduction: Neutron Reflectometry Experiment



Tethered bilayer lipid membrane (tBLM)

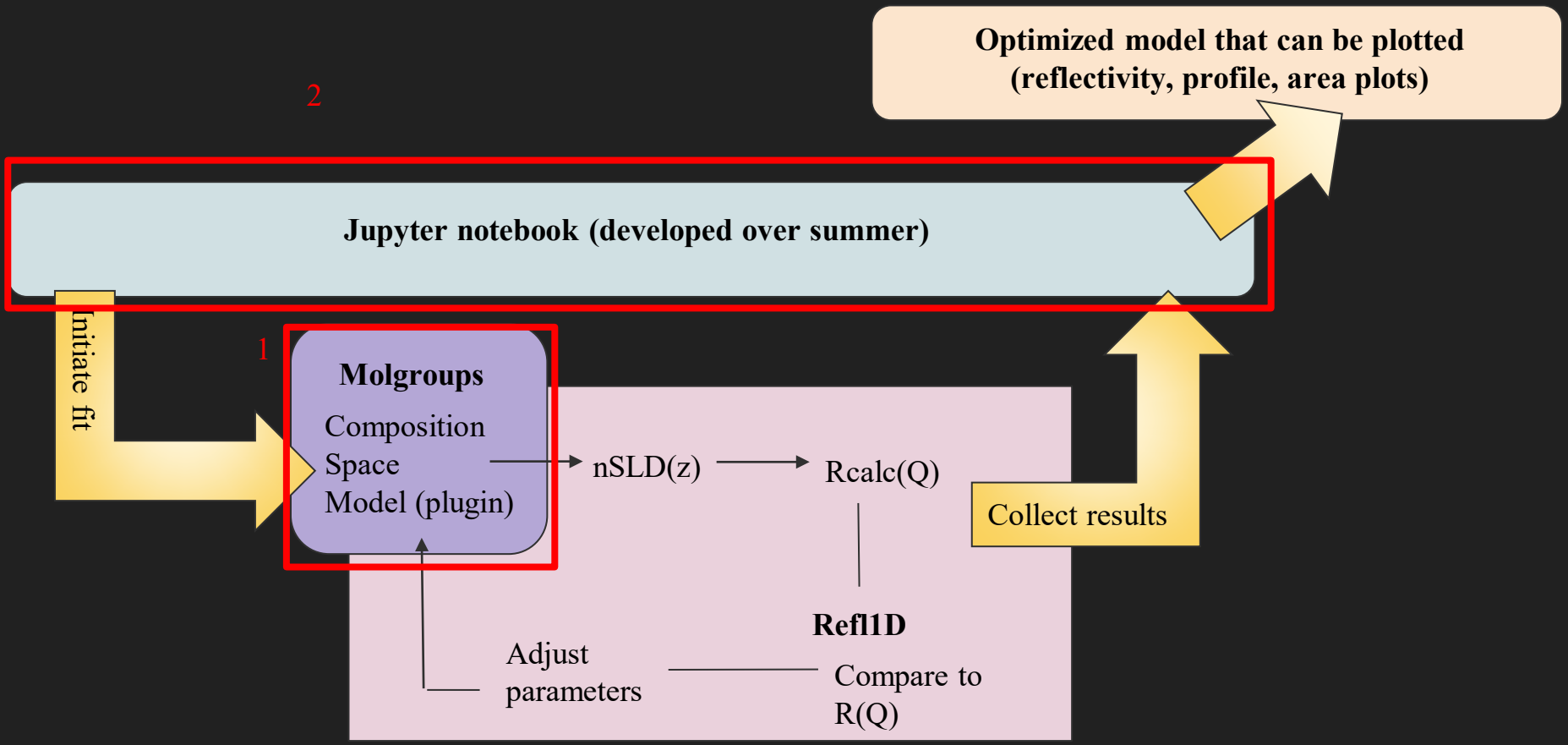
- Usually uses solid substrate to support membrane
  - Directly adsorb lipid bilayer to silicon wafer (ssBLM).
  - Or attach lipid bilayer to gold with tether molecules (tBLM).

# Introduction: Composition-Space Model




- Shows how constituent chemical groups of lipid bilayer are arranged in space.
  - Any empty space filled with water (D2O or H2O)
  - Used to calculate nSLD profiles for optimization of R(Q)

# Project Workflow



# Results: Jupyter Notebook Output (ssBLM)

- Successfully transcribed C++ code into Python for molgroups module.
- Additionally, created a concise shareable Jupyter notebook that is user-friendly and made for the purpose of plotting and fitting real-life reflectometry data (output below).

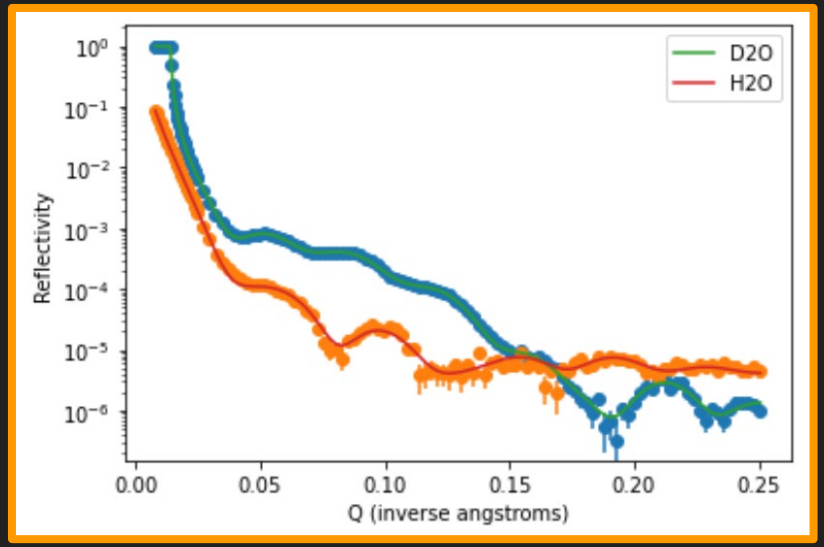



Fig. 1: Reflectivity vs. Q, solid-supported bilayer

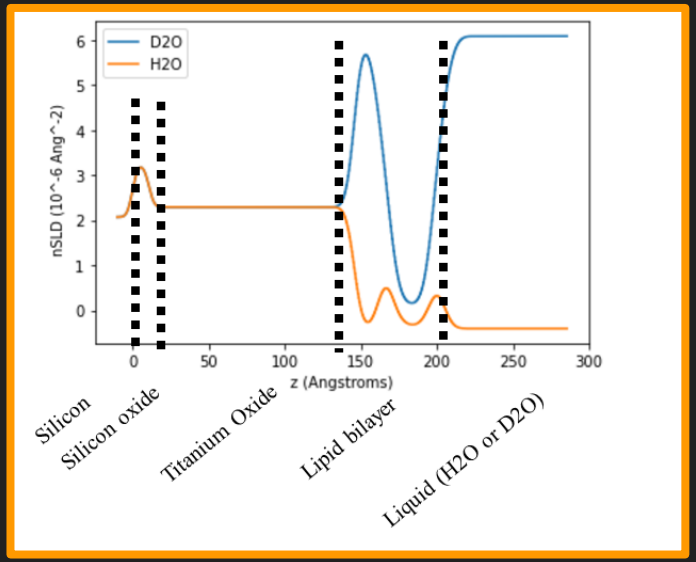



Fig. 2: Profile Data of a Lipid Bilayer (z = distance)

# Results: Composition Space Model (ssBLM)

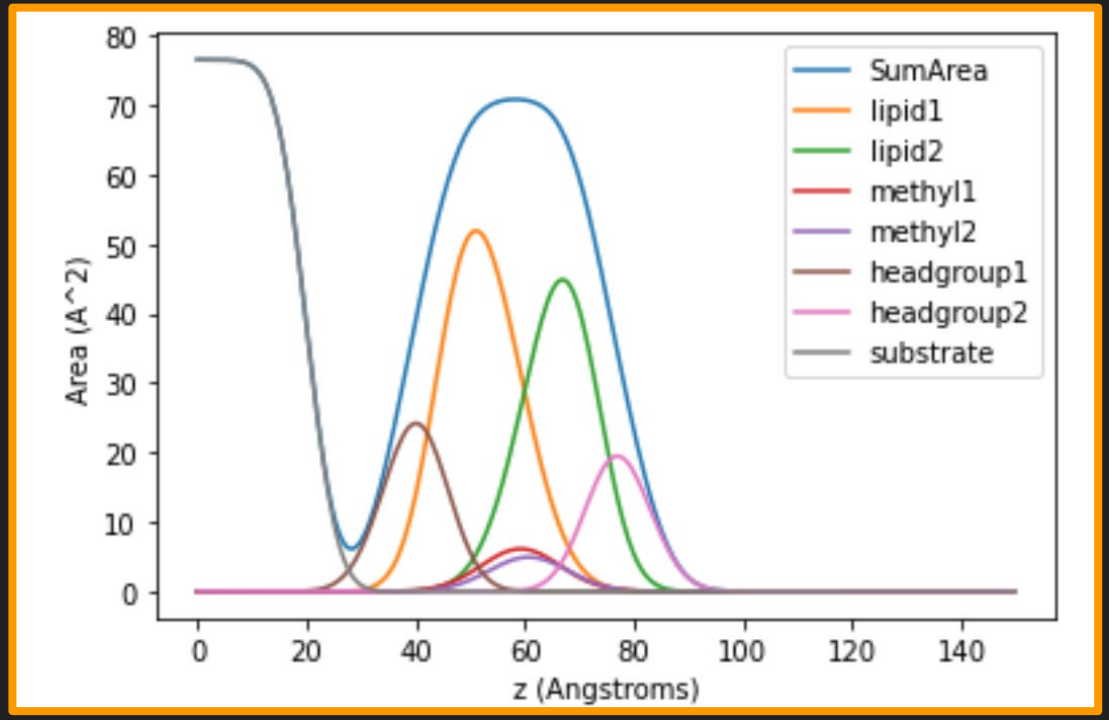
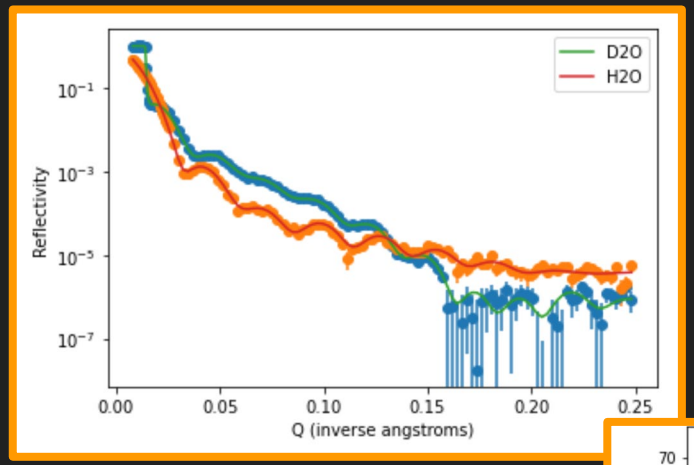
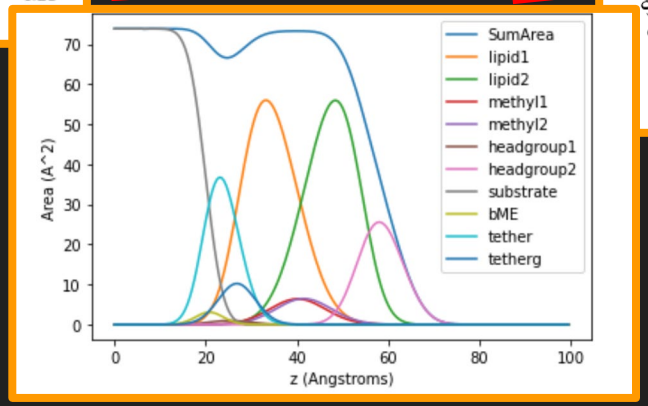
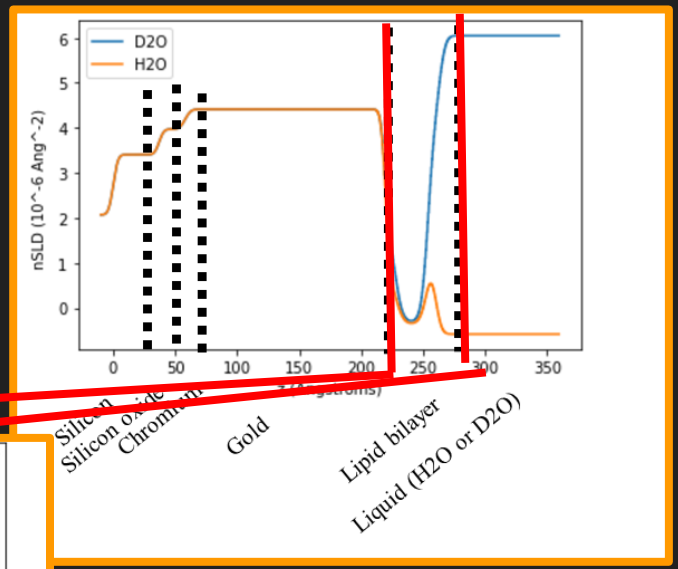



Fig. 3: Area composition space-model of lipid bilayer.

# Results (tBLM)



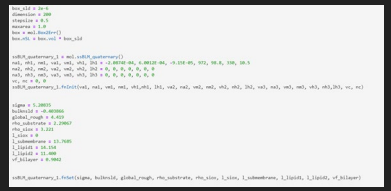



# Results: Final Jupyter Notebook

- 3 major sections in final Jupyter notebook:
  - 1) Set up the composition space model definition

```
!pwd

import matplotlib.pyplot as plt
import numpy as np
import scipy.integrate
import scipy.fft
import molgroups as mol
import math
from numpy import *
```

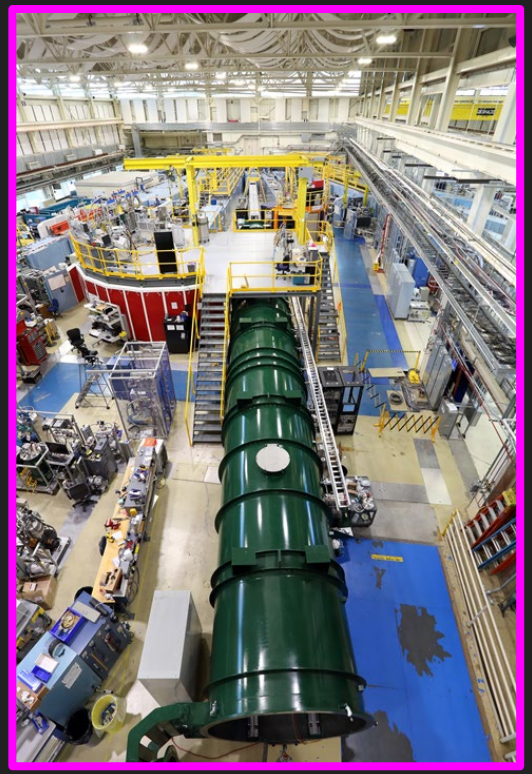


  - 2) Run refl1d fit (need a previously existing run file). Creates a best fit of data

```
!refl1d ssblm_tiox_both.py --fit=dream --burn=200000 --time=8 --steps=200 --store=Output_ssBLM_FINAL --parallel --init=lhs --batch
```

  - 3) Plot the graphs of the resulting refl1d fit (3 graphs output: reflectivity, profile, and space-composition graphs)

# Conclusion and Future Directions



- Conclusion
  - NCNR now has a more user-friendly interface for processing neutron reflectometry data.
  - Future steps could include producing models for proteins.
  - Also, the code could be further streamlined and sped up.

# Acknowledgements

Mentors: David Hoogerheide and Frank Heinrich

Special Thanks to NCNR team and directors Joseph Dura, Julie Borchers, Susana Teixeira

Other acknowledgements to Alyssa Thomas for technical assistance on this project.

Funding courtesy of CHRNS through National Science Foundation.

# Questions?