Predicting Neutron Scattering Off of Nanoscale Magnetic Elements

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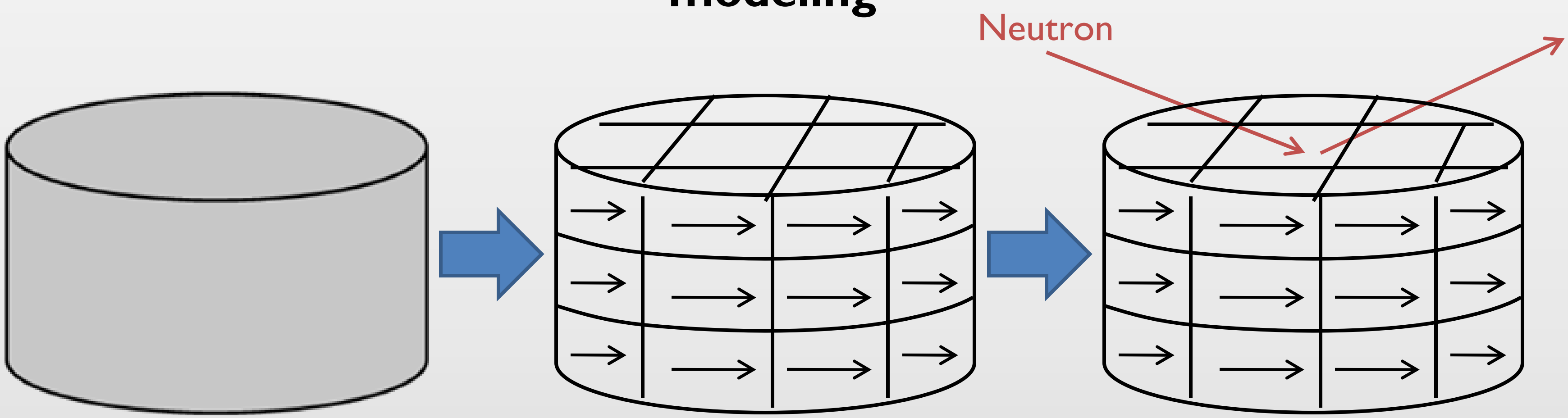
Project Summary

- Calculate the lowest-energy state for magnetic elements
- Write a program to predict magnetic scattering based on scattering properties of neutrons
- Organize a simple, user-friendly system for the entire process:
  - Design an element (or array of elements)
  - Find the element's magnetic moment configuration
  - Determine the neutron scattering off of the element
  - Display the final neutron scattering map

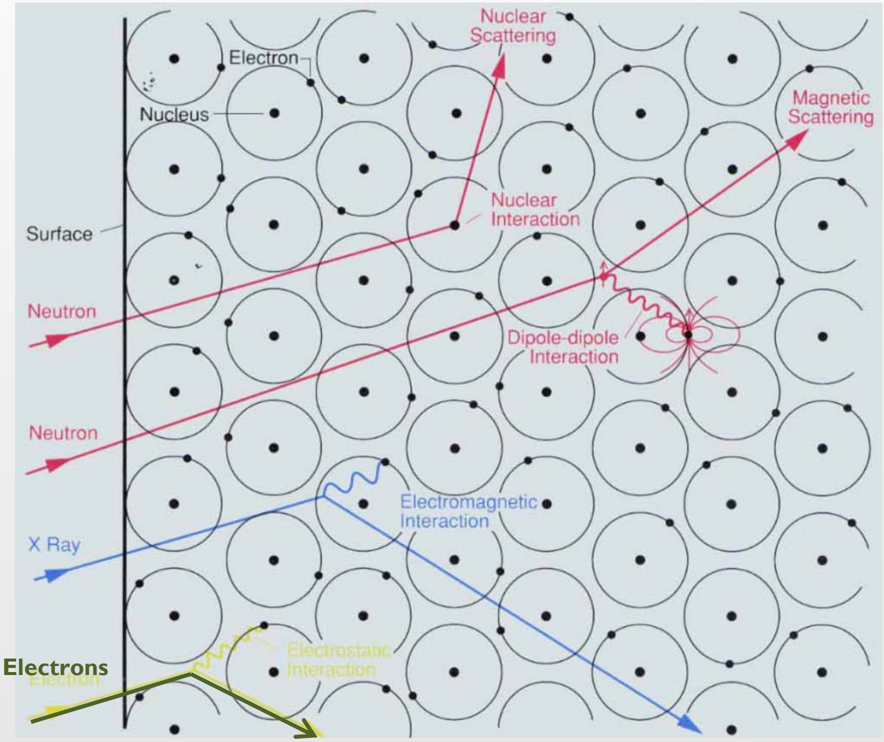
Project Flow Chart

Define shape → **Micro-magnetic modeling** → **Neutron scattering**



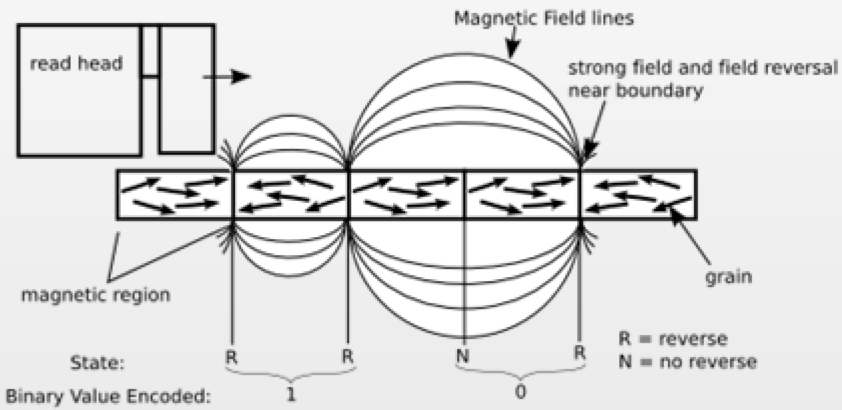
Why Neutrons?

- Neutrons versus x-rays
  - More penetrating
  - Multilayered elements
- Analyzing magnetic elements
  - Neutral, no charge
  - Possesses a magnetic moment



Why Nanoscale Magnetic Elements?

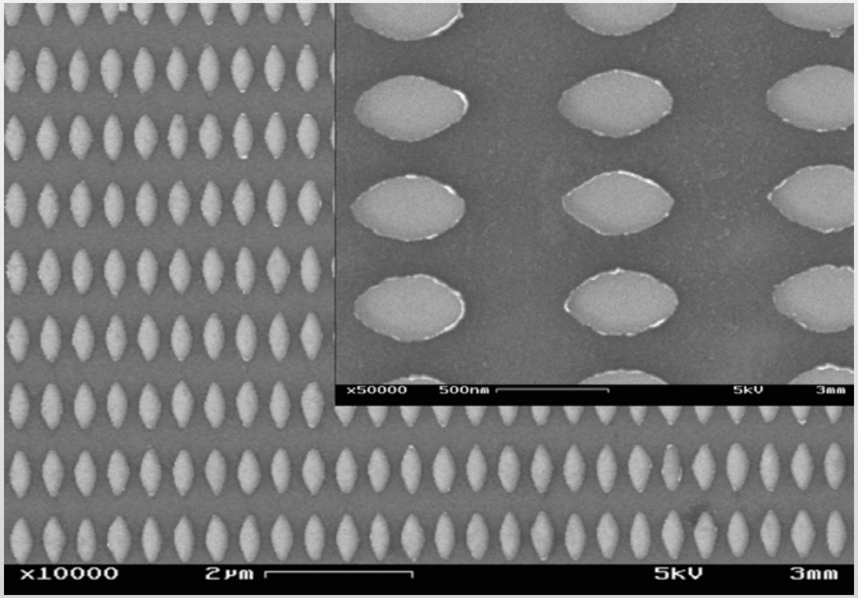
- Hard drives
  - Magnetic direction stores data
  - Nanoscale elements for space-efficiency
  - Read heads
- Cancer treatments
  - Magnetic elements used to detect or treat cancer
  - Nanoscale elements to focus solely on harmful cells in the body



Data to Model

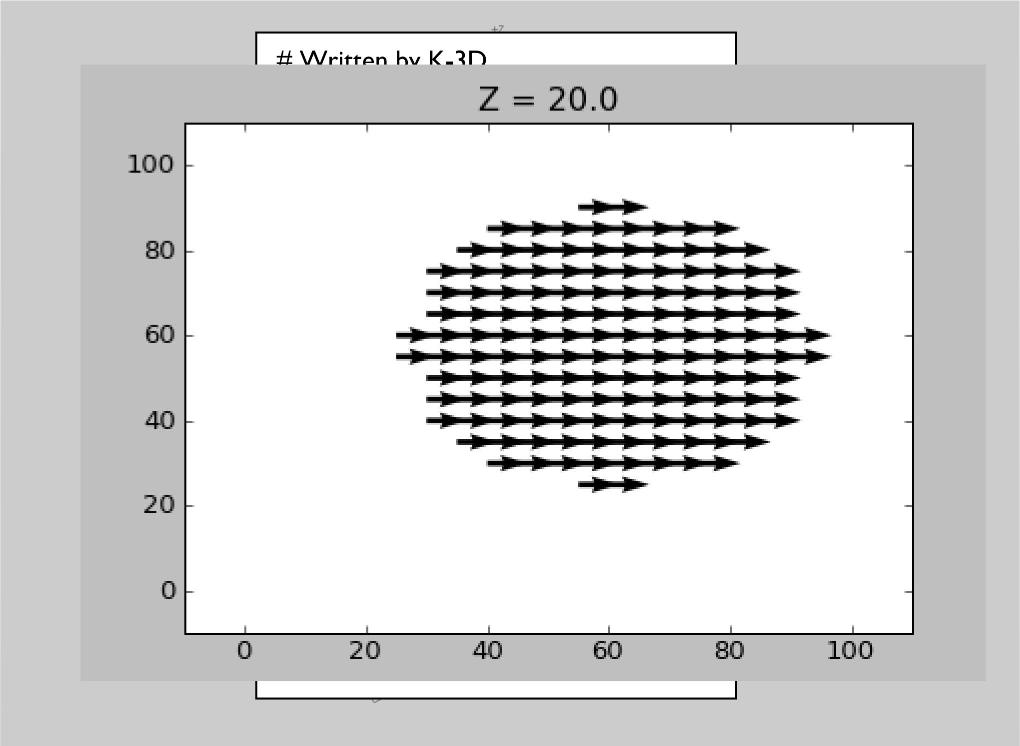
- 3D analysis
- Sample analyzed by Kathryn
- Series of elliptical columns
  - 550 nm x-diameter
  - 350 nm y-diameter
  - 20 nm high along z-axis

Direction	Dimensions	Measurements
Long	Length	550 nm
	Period	900 nm
	Spacing	350 nm
Short	Length	350 nm
	Period	450 nm
	Spacing	100 nm



K3D: Defining shapes

- Modeling software useful for designing more complex nanoscale elements
- Export as raw, output in a text file
- Interpreted and discretized by Python program



NIST

: Micro-magnetic modeling

- Object Oriented Micro-Magnetic Framework
- Micro-magnetic solver
- Discretizes imported element into desired number of magnetic domains
- Calculates magnetic moments for each discretized cell

Micromagnetic Equations

Landau-Lifshitz-Gilbert:

$$\frac{d\mathbf{M}}{dt} = \frac{-\omega}{1+\lambda^2}\mathbf{M}\times\mathbf{H}_{\text{eff}} - \frac{\lambda\,\omega}{(1+\lambda^2)M_s}\mathbf{M}\times(\mathbf{M}\times\mathbf{H}_{\text{eff}})$$

$$\mathbf{H}_{\text{eff}} = -\frac{1}{\mu_0}\frac{\partial E_{\text{density}}}{\partial\mathbf{M}}$$

Energies:

$$E_{\text{exchange}} = \frac{A}{M_s^2}\left(|\nabla M_x|^2 + |\nabla M_y|^2 + |\nabla M_z|^2\right)$$

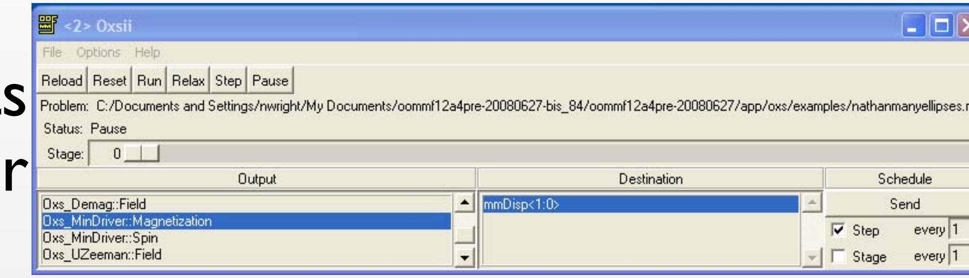
$$E_{\text{anis,cubic}} = \frac{K_1}{M_s^4}(M_x^2M_y^2 + M_y^2M_z^2 + M_z^2M_x^2)$$

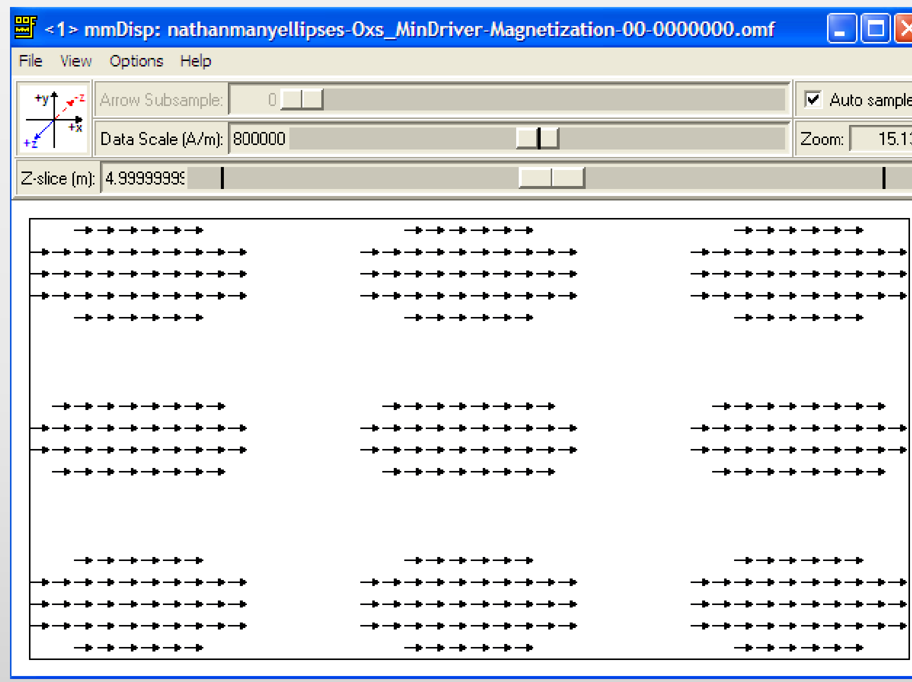
$$E_{\text{demag}} = \frac{\mu_0}{8\pi}\mathbf{M}(r)\cdot\left[\int_V \nabla\cdot\mathbf{M}(\mathbf{r}')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\,d^3r' - \int_S \hat{\mathbf{n}}\cdot\mathbf{M}(\mathbf{r}')\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\,d^2r'\right]$$

$$E_{\text{Zeeman}} = -\mu_0\mathbf{M}\cdot\mathbf{H}_{\text{ext}}$$

: continued

- Calculate the ground magnetic state of elements imported from MIF files or K3D
- Runs through a simulation and displays ground magnetic state of the element as a collection of 3D vectors
- Export final output magnetic configuration to Python as a text file





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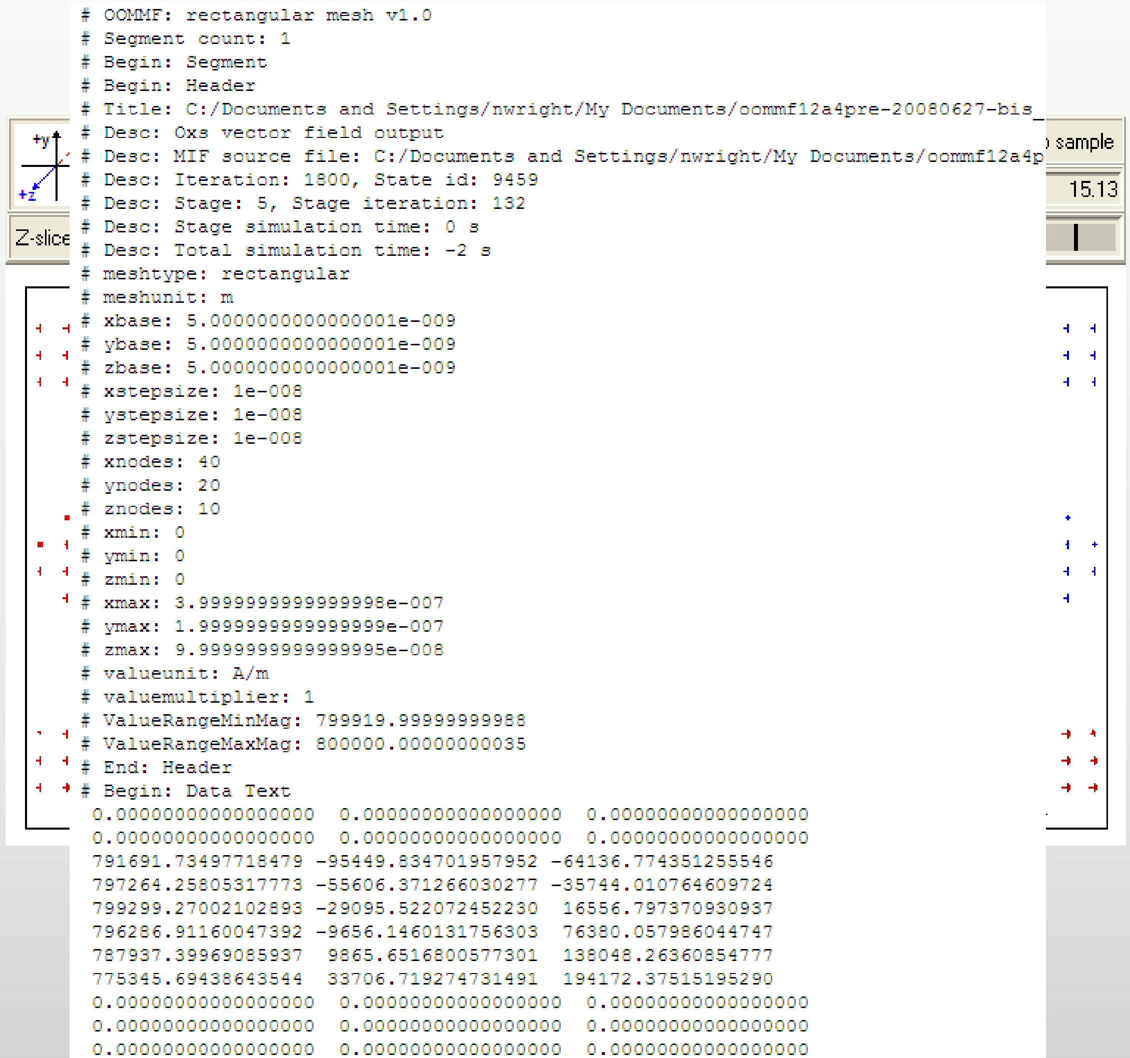
OOMMF Reader

- Read the text file output from OOMMF
- Enter magnetic vectors into an array
- Format data for SLD calculator and Born Approximation



```
# OOMMF: rectangular mesh v1.0
# Segment count: 1
# Begin: Segment
# Begin: Header
# Title: C:/Documents and Settings/nwright/My Documents/oommf12a4pre-20080627-bis_
# Desc: Oxs vector field output
# Desc: MIF source file: C:/Documents and Settings/nwright/My Documents/oommf12a4p
# Desc: Iteration: 1800, State id: 9459
# Desc: Stage: 5, Stage iteration: 132
# Desc: Stage simulation time: 0 s
# Desc: Total simulation time: -2 s
# meshtype: rectangular
# meshunit: m
# xbase: 5.0000000000000001e-009
# ybase: 5.0000000000000001e-009
# zbase: 5.0000000000000001e-009
# xstepsize: 1e-008
# ystepsize: 1e-008
# zstepsize: 1e-008
# xnodes: 40
# ynodes: 20
# znodes: 10
# xmin: 0
# ymin: 0
# zmin: 0
# xmax: 3.9999999999999998e-007
# ymax: 1.9999999999999999e-007
# zmax: 9.9999999999999995e-008
# valueunit: A/m
# valuemultiplier: 1
# ValueRangeMinMag: 799919.99999999988
# ValueRangeMaxMag: 800000.00000000035
# End: Header
# Begin: Data Text
 0.0000000000000000  0.0000000000000000  0.0000000000000000
 0.0000000000000000  0.0000000000000000  0.0000000000000000
 791691.73497718479 -95449.834701957952 -64136.774351255546
 797264.25805317773 -55606.371266030277 -35744.010764609724
 799299.27002102893 -29095.522072452230  16556.797370930937
 796286.91160047392 -9656.1460131756303  76380.057986044747
 787937.39969085937  9865.6516800577301  138048.26360854777
 775345.69438643544  33706.719274731491  194172.37515195290
 0.0000000000000000  0.0000000000000000  0.0000000000000000
 0.0000000000000000  0.0000000000000000  0.0000000000000000
 0.0000000000000000  0.0000000000000000  0.0000000000000000
```

SLD Calculator and Born Approximation

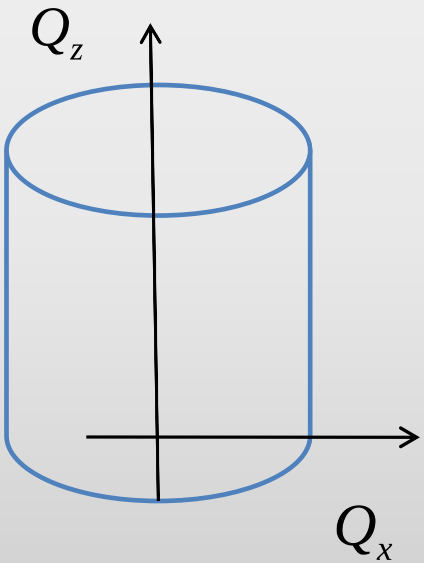
$$\vec{q} = \vec{M} - \vec{Q}(\vec{Q} \bullet \vec{M})$$

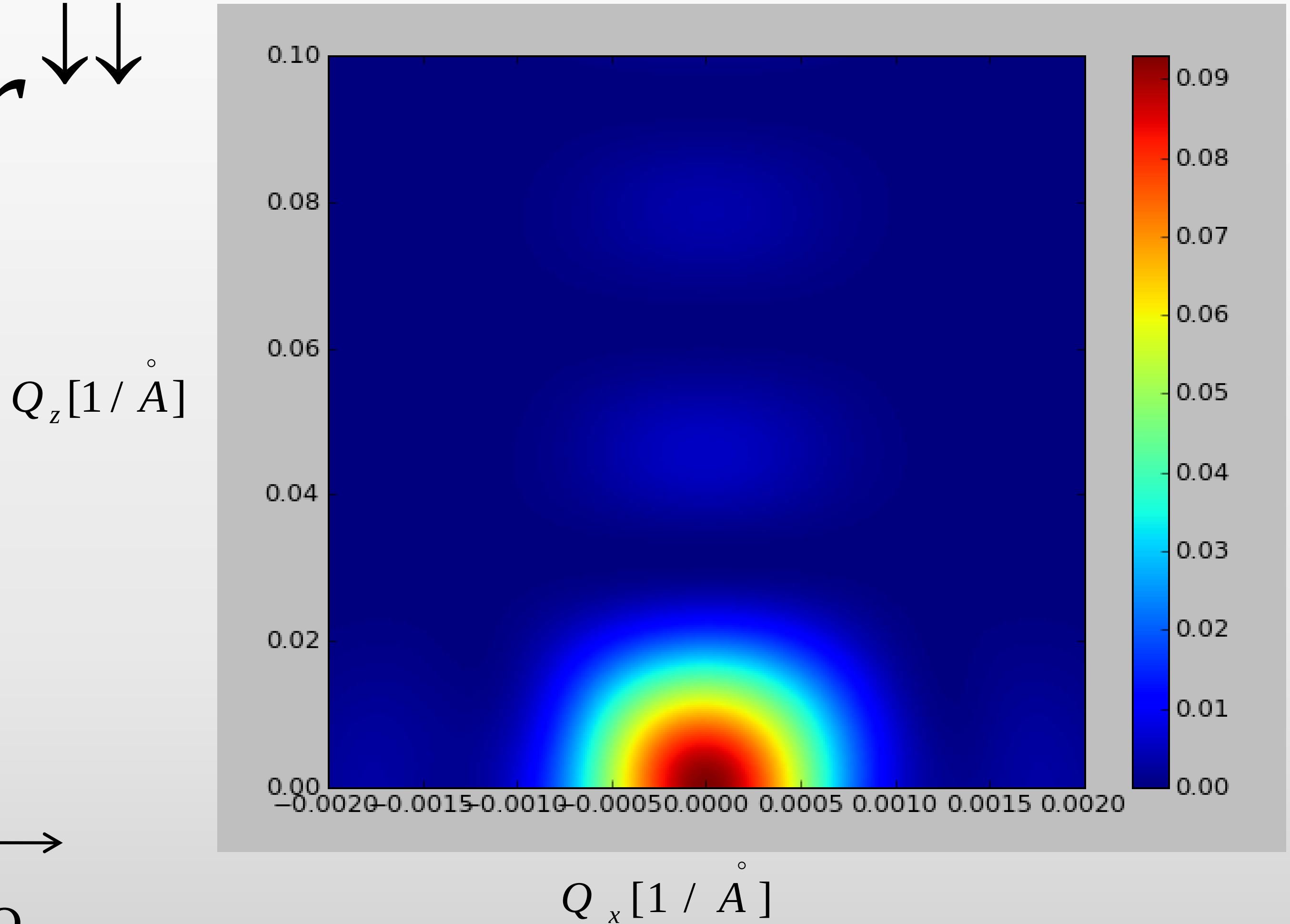
$$r^{\uparrow\uparrow,\downarrow\downarrow} = \sum_j [(\rho_{nj} \mp q_a \rho_{mj}) e^{i\vec{Q} \bullet \vec{R}_j}]$$

$$r^{\uparrow\downarrow,\downarrow\uparrow} = \sum_j [(q_b \pm i q_c) \rho_{mj} e^{i\vec{Q} \bullet \vec{R}_j}]$$

Scattering Maps

$r^{\uparrow\uparrow}$ $r^{\downarrow\downarrow}$





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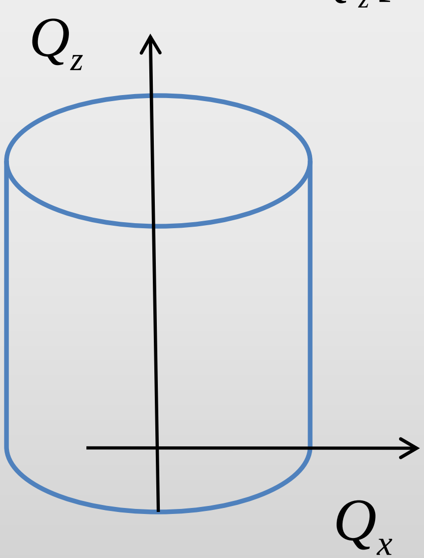
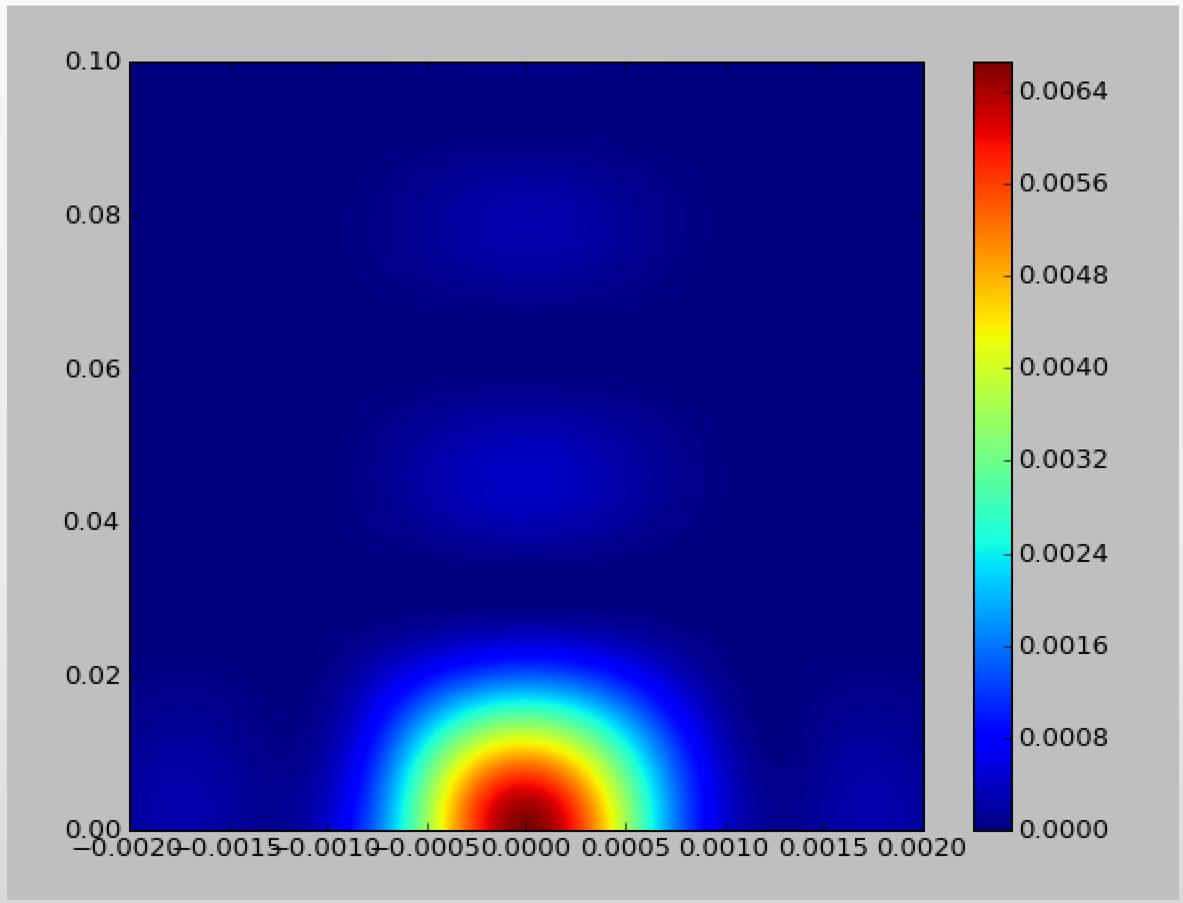
Scattering Maps (continued)

$$r^{\uparrow\downarrow}$$



$Q_z\,[1/\mathring{A}]$



$Q_x\,[1/\mathring{A}]$

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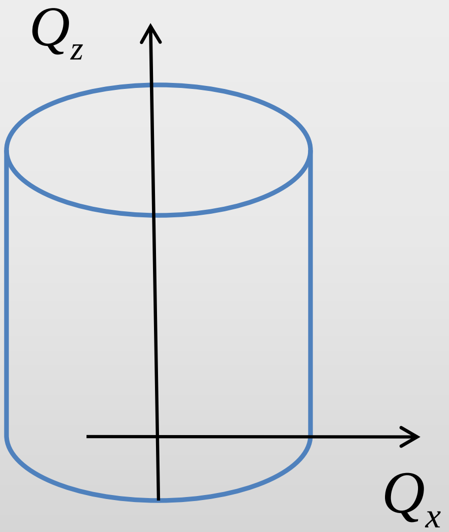
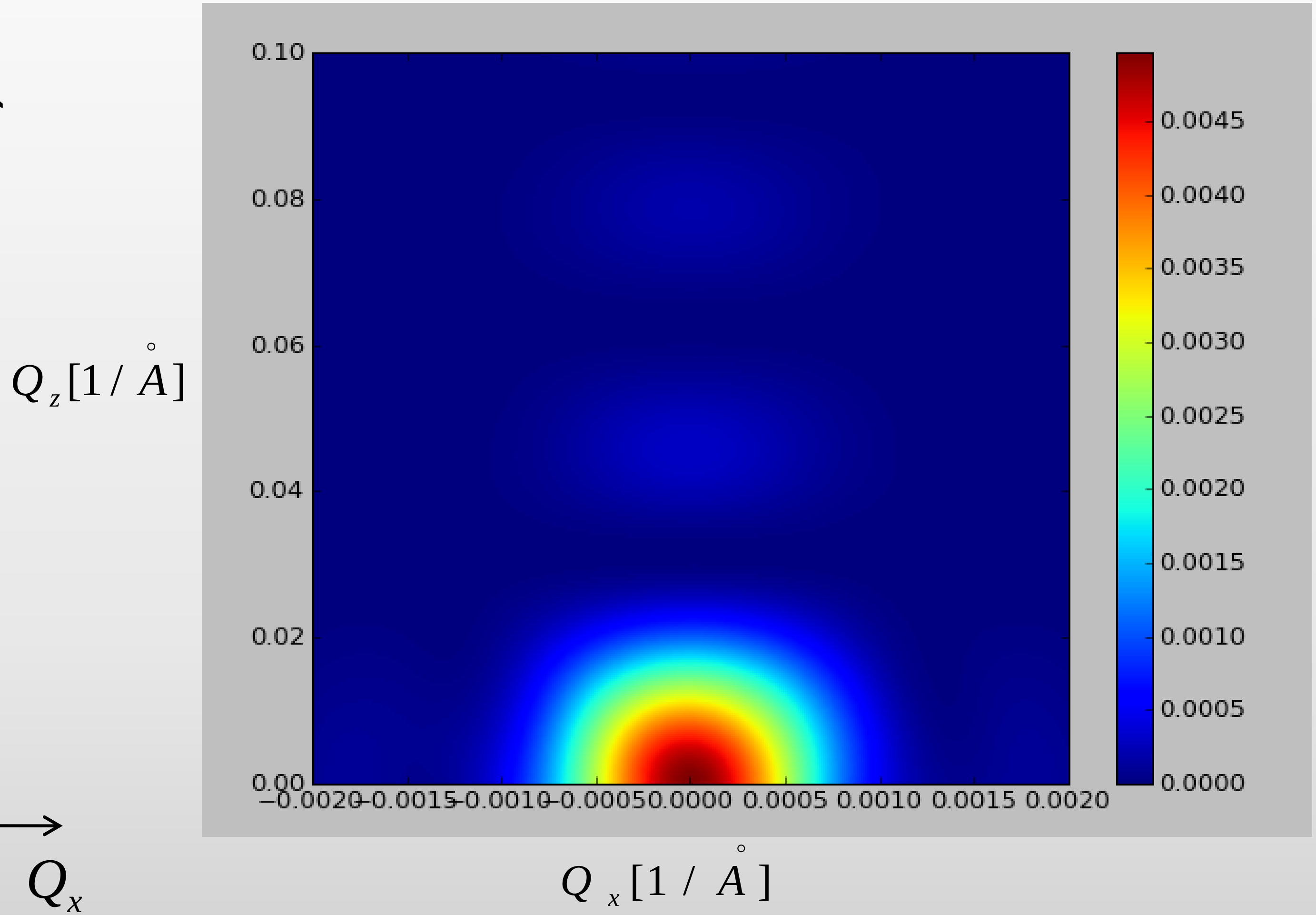
Scattering Maps (continued)

$$r^{\downarrow\uparrow}$$





Conclusion

Successes

- Determined significant magnetic contribution to neutron scattering
- Completed basic progression from defining shapes to neutron scattering
- Established an effective method of analyzing magnetic elements

Challenges

- Real data/shapes
- Complex elements
- Debugging
- Interpreting output

Future Directions

- Define more diverse/complex elements
- Debugging
  - Check Magnetic Scattering Length Density calculator
  - Optimize the code
- Complete the progression
  - Define shapes to micro-magnetic modeling
- Ready for use
  - Make code more user-friendly
  - Document code

Acknowledgements and Thanks

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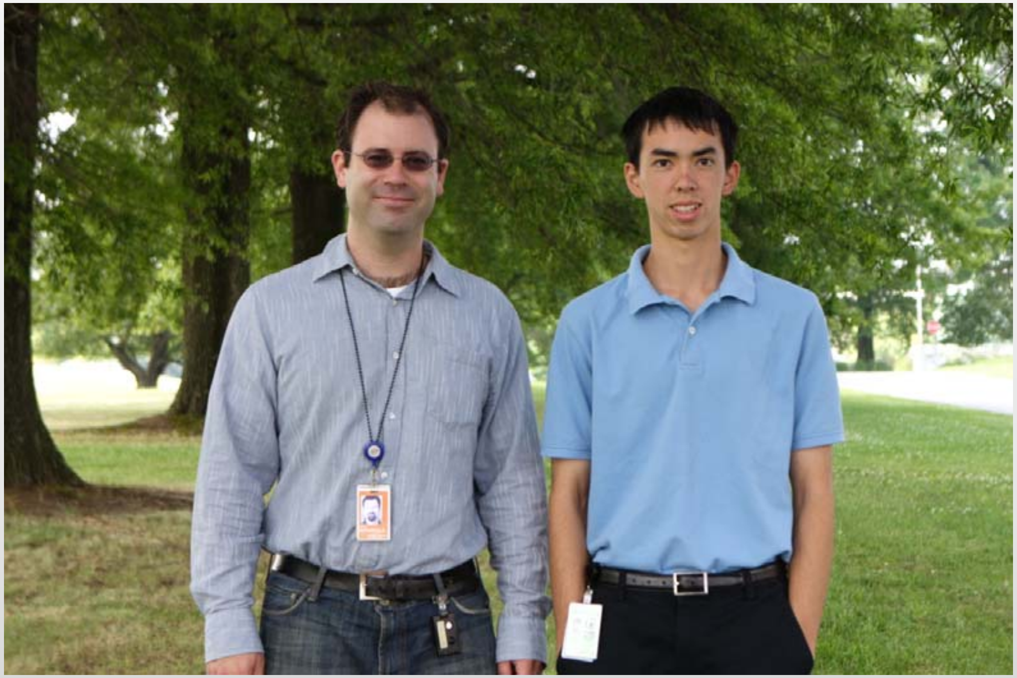
- Julie Borchers
- Fellow SURFers
- NIST SURF
- CHRNS



Thank you
Questions?

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