Computational Analysis of Neutron Scattering Data

PhD Dissertation Defense

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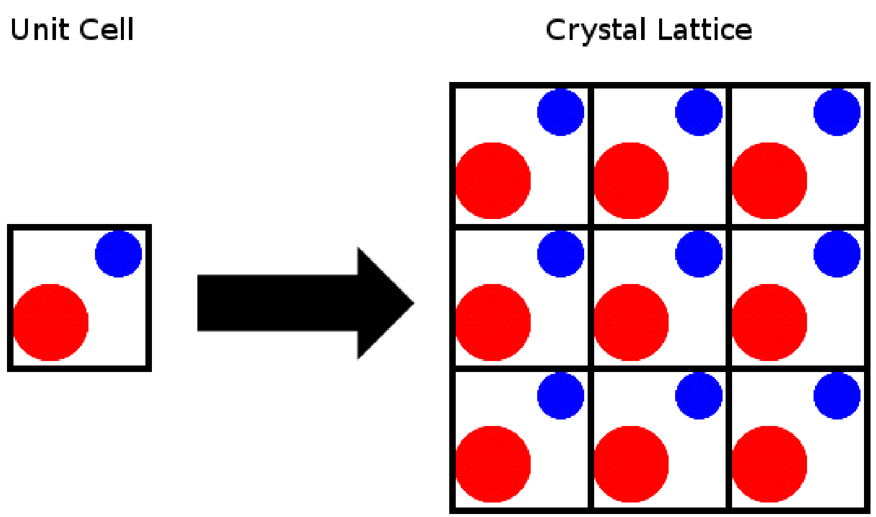
About Me

- B.S. Computer Engineering 2009
- M.S. Computer Engineering 2012
- Intern at ORNL for 5 years
  - Worked on satellite image processing using machine learning for most of ORNL internship
- Some of my more recent research has involved data processing for neutron scattering experiments
  - Shared many similarities with my satellite imagery work
  - Focus on crystal defect detection
  - Joint effort between some of the computational groups at ORNL and groups at SNS

Quick Recap from Proposal

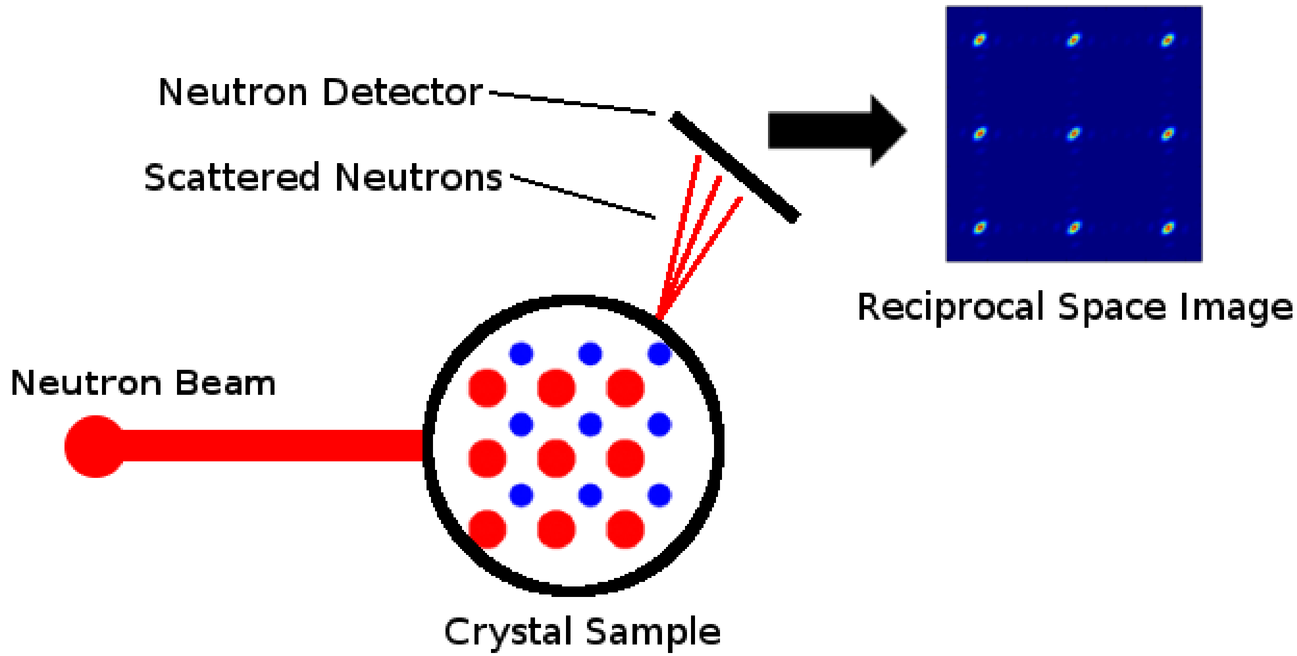
Crystal Structures

- Crystals are repeating structures of "unit cells" of atoms
  - Atoms are the same for all cells
  - Repeating structure is called "long-range order"
- A defect occurs when the periodic structure is disrupted
  - These defects affect material strength, thermal conductivity, pharmaceutical properties, and more.



Neutron Scattering Background

- Looking at diffuse neutron scattering
  - Used for analysis of crystal lattice structures
  - Neutrons pass through sample and create diffraction patterns
  - Diffraction patterns create reciprocal space image
    - Discrete Fourier transform for cell structure factors

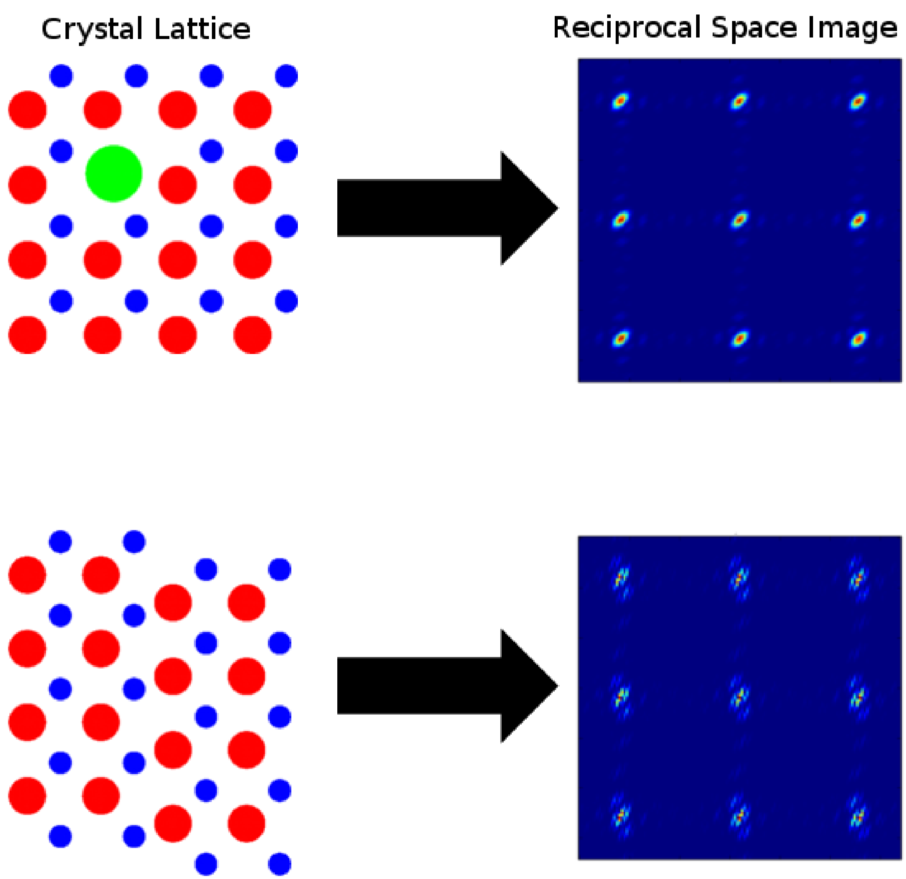


Neutron Scattering Background

- Two parts of reciprocal space images:
  - Bragg peaks
    - High-intensity diffraction patterns
    - Describe average crystal structure
  - Diffuse scattering
    - Low-intensity diffraction patterns
    - Describe <u>deviations from</u> average crystal structure
- <u>Goal:</u> Analyze textures in the reciprocal space imagery to identify defects in simulated crystal structures
  - Single crystal neutron scattering
  - Diffuse scattering patterns will be the primary focus as they describe deviations from the average crystal structure

Neutron Scattering Background

- Different defects create different diffraction patterns
- Can be viewed as a “fingerprint” for the defect



Preliminary Work from Proposal

- Goal: Automatically detect defects in simple simulated crystal structures for single crystal scattering experiments
- General Approach:
  - Extract texture features from reciprocal space images
  - Look at problem as a generic data classification problem
  - Minimal knowledge of underlying crystal structure needed
  - No need for system changes if crystal structure changes

Preliminary Work from Proposal

- Experimental results:
  - 2-class defect classification accuracy: 98.05%
  - 3-class defect classification accuracy: 76.12%
    - Lower accuracy due to similarities between substitution classes
- Extra proof of concept work since proposal
  - Increasing class separation margin for substitutions had little to no effect on classification accuracy in 3-class problem
  - System was able to also detect substitution location
    - 64-class substitution location accuracy: 95.67%
  - Random forests were found to perform better than SVMs
    - Both in accuracy and computational complexity
- Details for this preliminary work are available in dissertation

Large Structure Analysis

Overview

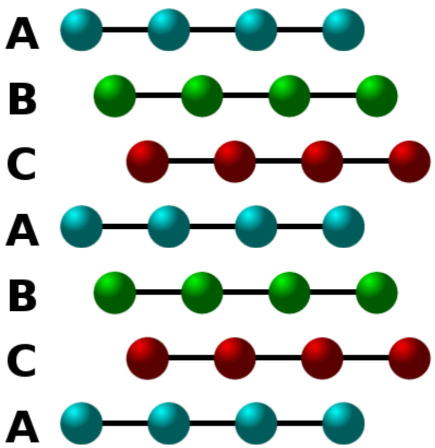
- Preliminary work was a proof of concept
  - Tested if defect detection methodology works at all
  - Dataset was for a toy problem
  - Crystal structure was not realistic
  - Defects were very, very simplistic
- Next step: Scale up to a larger structure
  - Defects can be more complex
  - Larger reciprocal space image size
  - Intensity range is much larger than small structure data range

Large Structure Data Properties

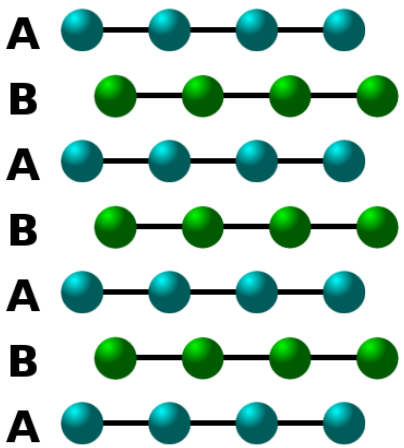
- Data is for close-packed crystal structures
- Simulated using the DISCUS simulator
  - Developed by Los Alamos National Laboratory
  - Uses similar methodology to (Butler and Welberry, 1992)
  - Adds extra variables to make simulation more realistic
- Crystal structure is a 100 cell by 100 cell silicon lattice
- Image size is 501 pixels by 501 pixels
  - Single-band intensity maps
- Comparison to preliminary data:
  - Lattice was 8 cells by 8 cells
  - Image size was 129 pixels by 129 pixels

Close-Packed Crystal Structures

- Close-packed crystal structures are created by stacking layers of atoms to form a crystal lattice
  - Layers denoted as letters (A, B, C, etc.)
  - Stacks are represented by strings (ABC)
- Two stacking configurations:



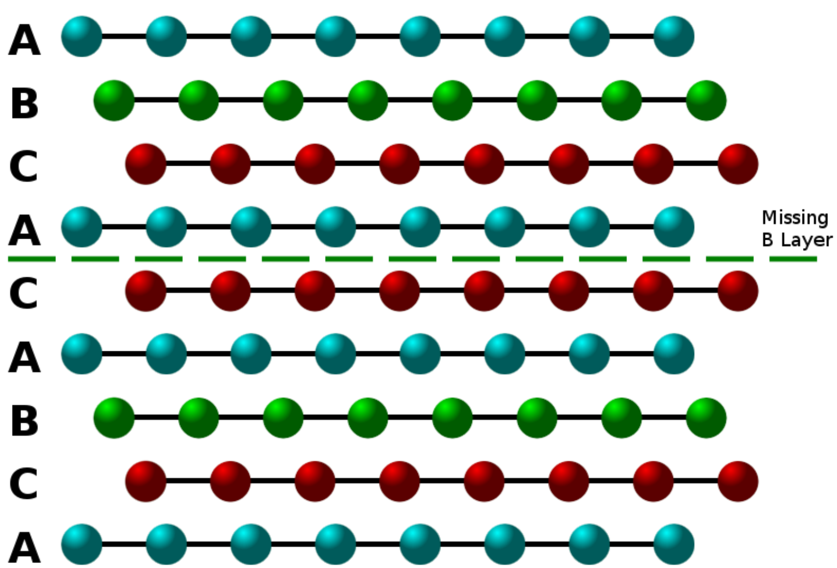
Cubic close packed (CCP)
3-layer configuration

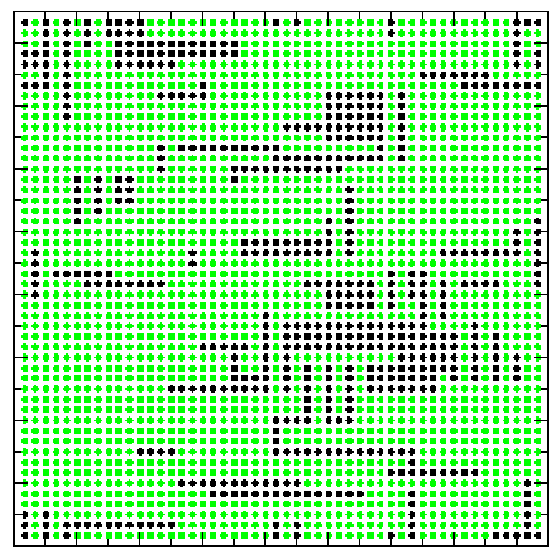


Hexagonal close packed (HCP)
2-layer configuration

Close-Packed Structure Defects

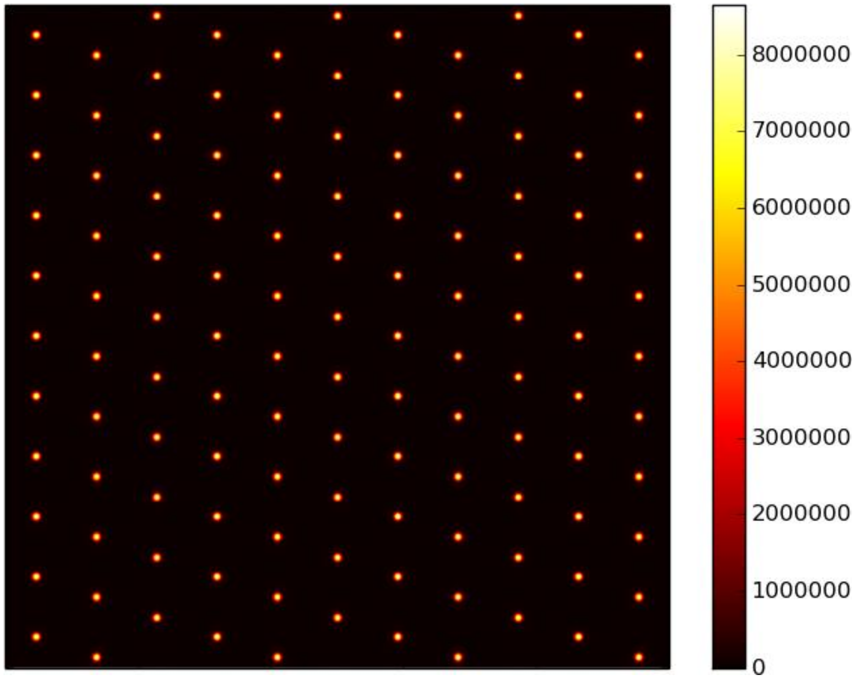
- Two types of defects considered
  - Stacking faults
    - Switching from cubic to hexagonal structure (or vice-versa)
  - Short-range order (SRO)
    - Small areas of disorder within the crystal



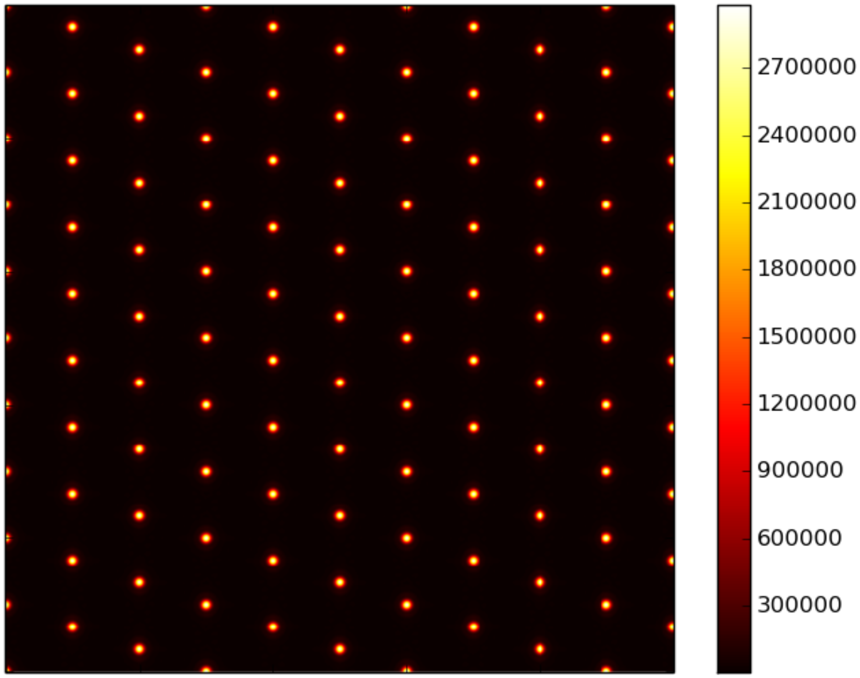


Close-Packed Structure Defects

- Defects can be similar in appearance



No Defect



SRO

Close-Packed Structure Defects

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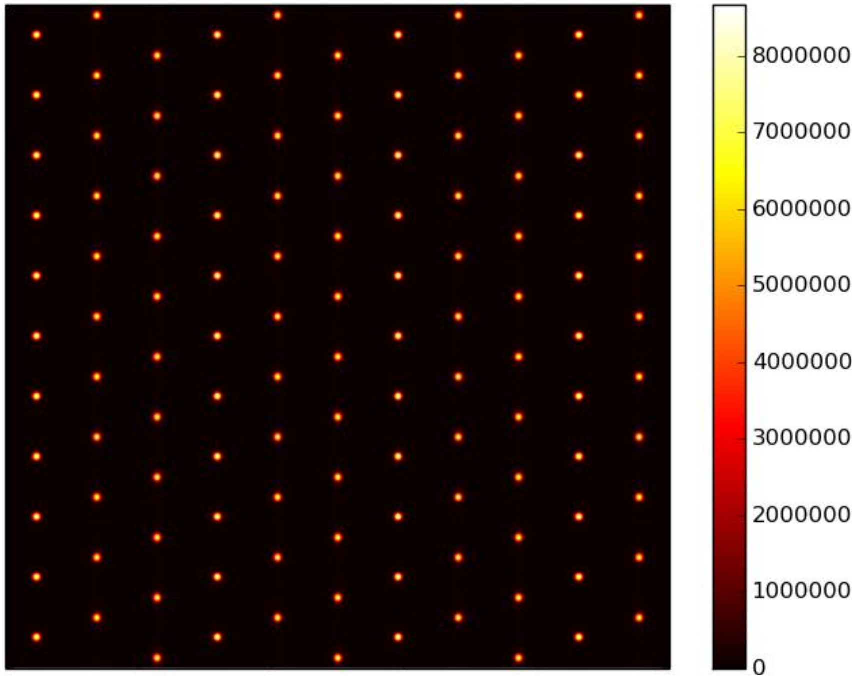
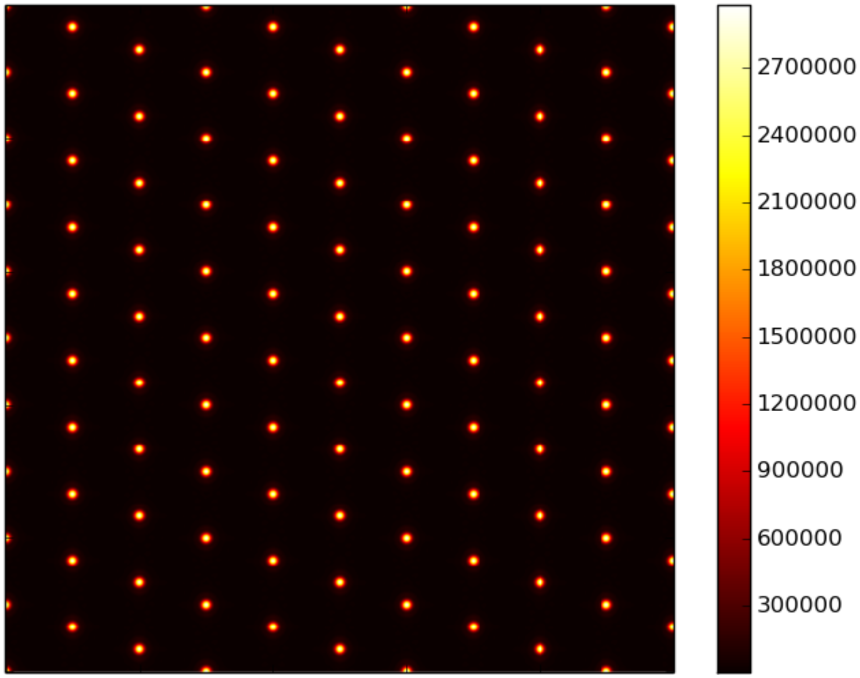


Stacking Fault



SRO

Image Feature Extraction

- Keypoint features
  - Automatically detect keypoints (regions of interest) within the image and generate a descriptor for each keypoint location
  - Descriptor is feature vector describing the texture of the image at the keypoint location

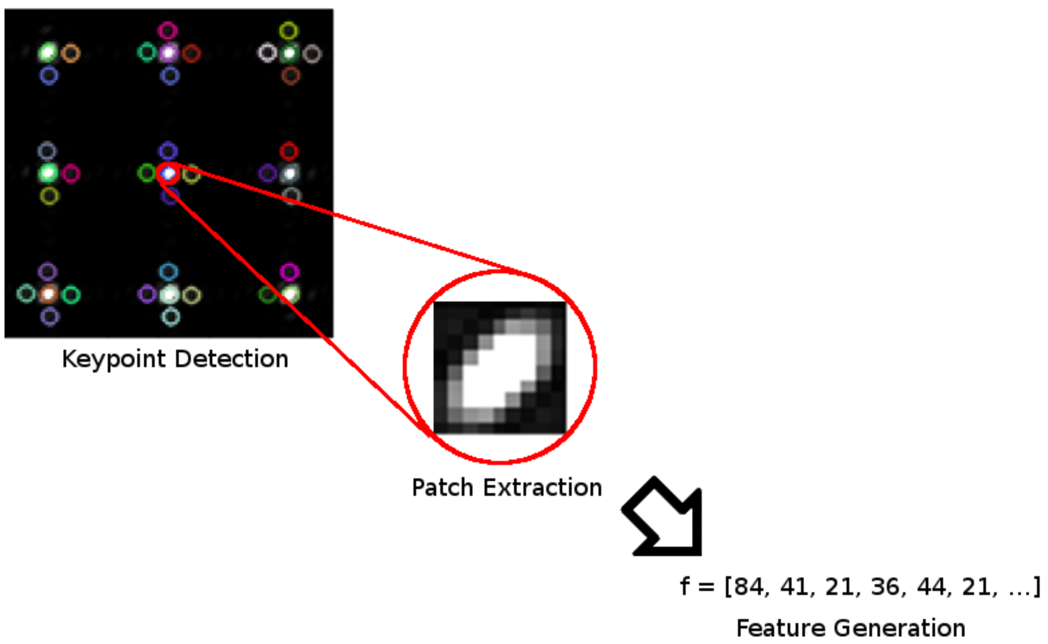
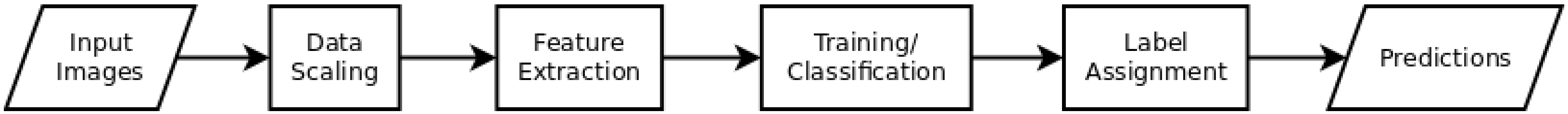


Image Keypoint Extractors

- 3 keypoint extraction algorithms evaluated:
  - SIFT
    - 128-dimensional feature vectors
    - Advertised benefits: "Gold standard" for keypoint features
  - SURF
    - Similar to SIFT, slightly different features (approximations)
    - 64-dimensional feature vectors
    - Advertised benefits : Faster than SIFT
  - ORB
    - Open-source alternative to SIFT and SURF
    - 256-dimensional binary feature vectors
    - Advertised benefits : Real-time performance, high noise robustness

Defect Detection Methodology

- Two challenges were posed by the new data:
  - Large image intensity range
  - Increased volume of detected keypoints due to larger image size
- In order to accommodate for the large range, a preprocessing step was added that scales the data before keypoint extraction
  - Improved keypoint detection for diffuse textures
- The increased number of detected keypoints was addressed by training on only 10% of the keypoints for each image
  - Reduced time required to train classifier without significantly affecting accuracy



Defect Detection Methodology

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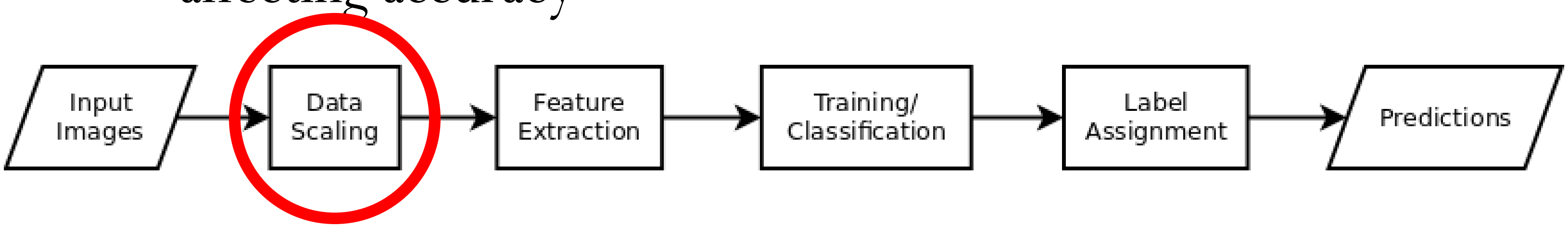


Image Preprocessing

- Large structure data intensity range is huge
  - Typically in the ballpark of $[0, 10^6]$
  - Range for preliminary data was approximately [0, 650]
- <u>Problem:</u> Causes problems during keypoint extraction
  - Makes keypoint detection difficult
  - Scaling is needed as a preprocessing step
- Common practice seems to be thresholding intensities at 10%–15% of the maximum intensity value
  - Percentage seems to be “eyeballed”
  - Still not good enough for keypoint extraction

Image Preprocessing

- The large data range was due to the Bragg peaks
- Goal: Reduce Bragg peak intensity without affecting diffuse scattering patterns
- GUI developed to assist with scaling scheme for Bragg peaks
- Result: Scaling methodology developed that thresholds the intensity *I(p)* at pixel *p* in the image such that:

$$I_{new}(p) = \min(I(p), t)$$

where threshold *t* is the mean intensity for the image

Image Preprocessing

- GUI Screenshot (Intensity Mode)

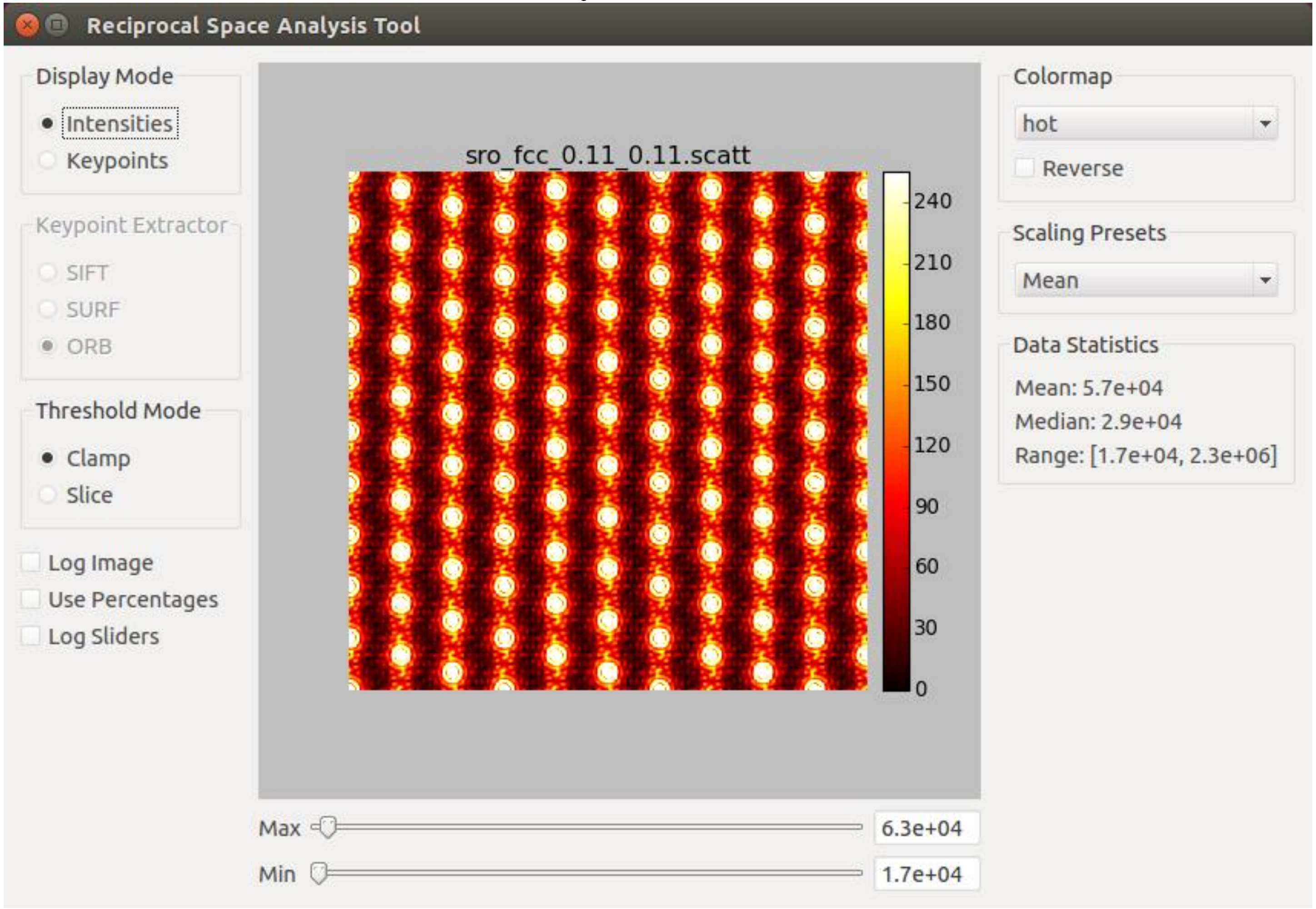


Image Preprocessing

- GUI Screenshot (Keypoint Mode)

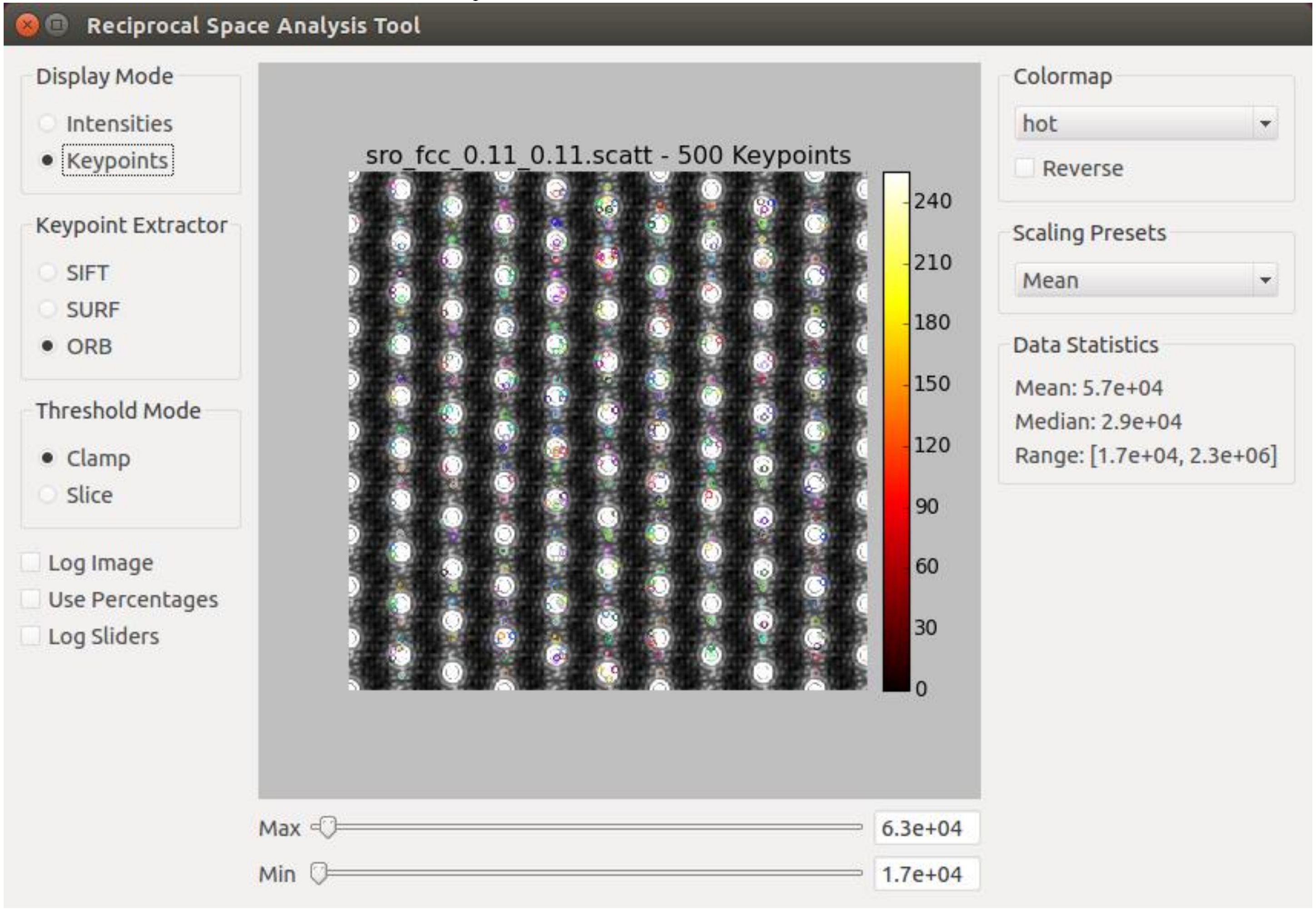
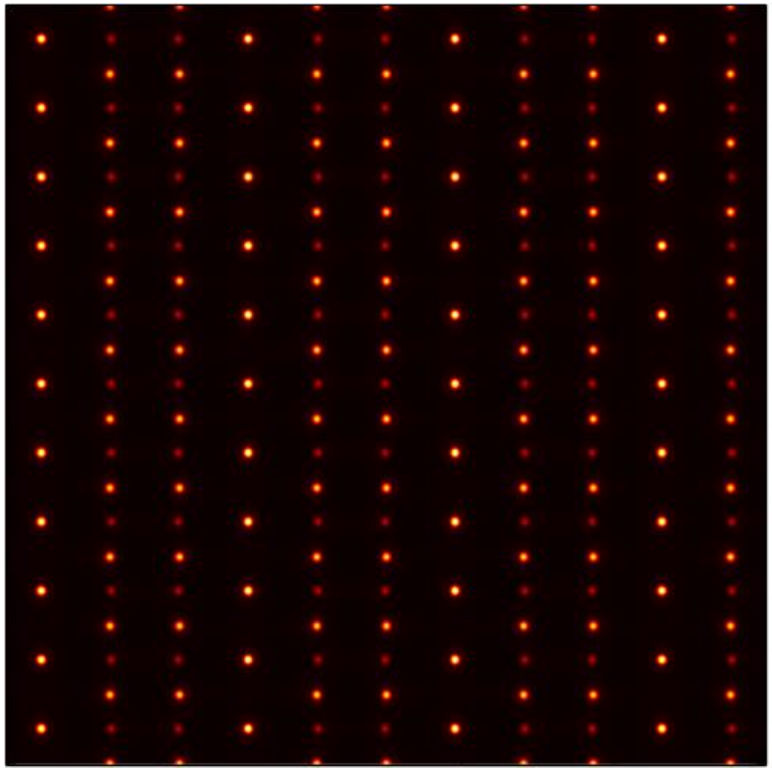


Image Preprocessing

- Fixed Percentage Scaling (1% max)



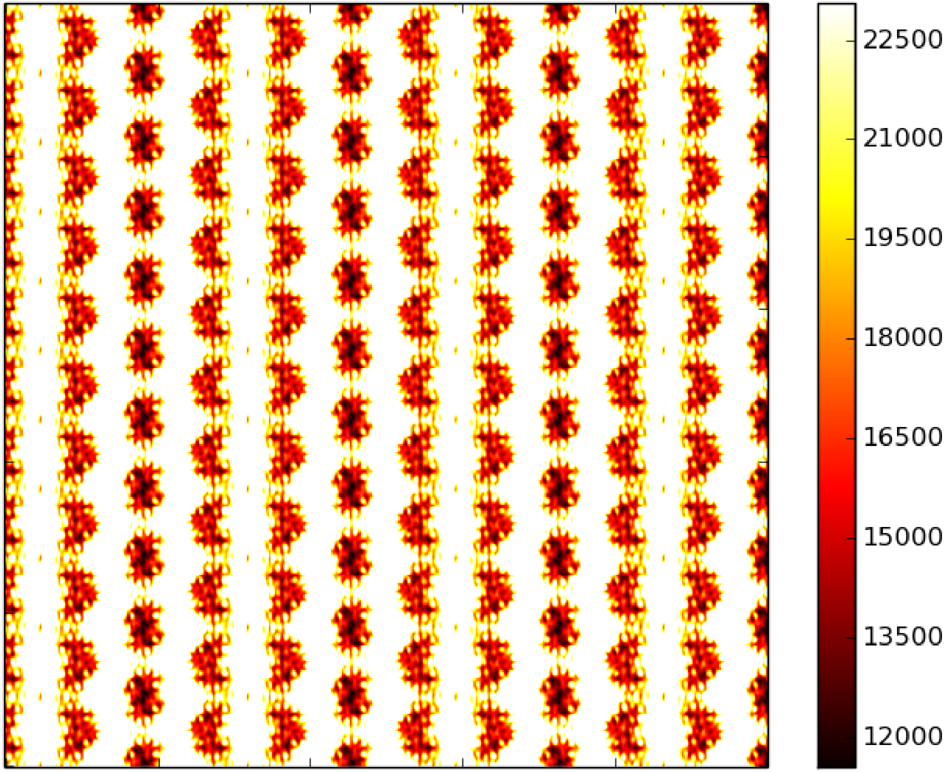
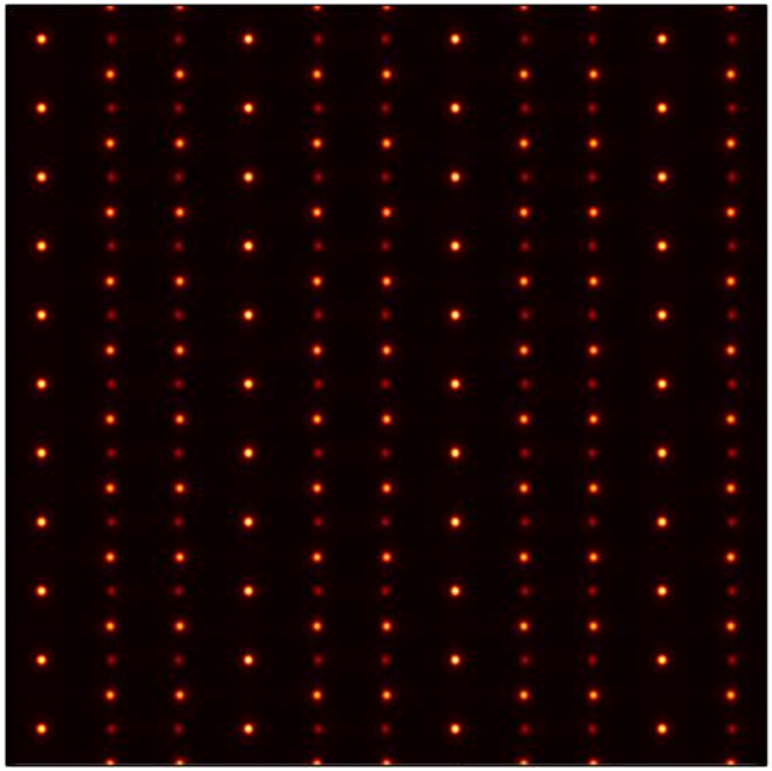
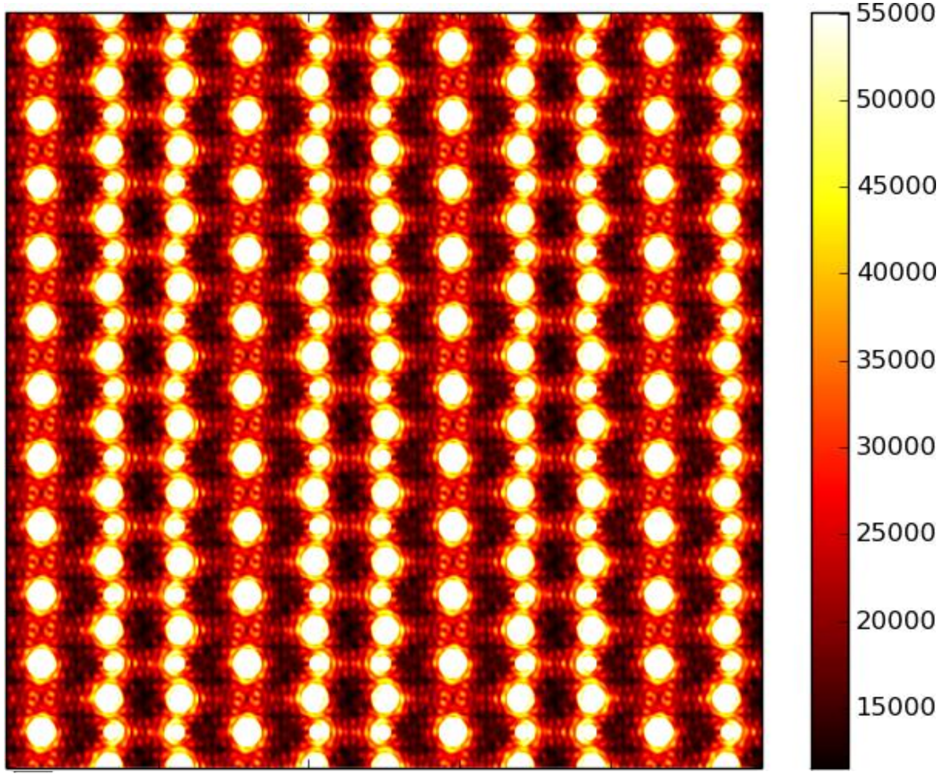


Image Preprocessing

- Mean Scaling





Large Structure Experiment

- Goal: Classify image as belonging to 1 of 3 defect classes:
  - "No Defect", "Stacking Fault", "SRO"
  - Classes suggested by neutron scientists as hard to distinguish visually
- 600 images simulated via DISCUS
  - 200 No Defect (100 CCP/100 HCP)
  - 200 Stacking Fault (100 CCP/100 HCP)
  - 200 SRO (100 CCP/100 HCP)
- Note: No distinction was made between CCP and HCP samples during training
  - Learning to ignore stacking configuration and just focus on the defects was left to the learning algorithm

Large Structure Experiment

- Preprocessing:
  - Images scaled via mean scaling method
  - Linear scaling to [0,255] then performed as required by keypoint extractors
- 3 keypoint extractors tested: SIFT, SURF, and ORB
- Training:
  - Random forest classifier
  - Used 10% of the images in the dataset
  - Random 10% of the keypoints in each image used for training
- Keypoint voting used to classify test images
- Results averaged over 100 independent experiments

Large Structure Experiment

- Results:

Keypoint Extractor	Accuracy
SIFT	**96.36%**
SURF	93.04%
ORB	92.59%

- Conclusions:
  - This "difficult" defect detection problem was rather easy to solve using the computational defect detection methodology
  - SIFT had highest accuracy of the keypoint extractors
    - More on keypoint extractor evaluation in a moment…

Prediction Evaluation Criteria

- Question: How to evaluate the quality of a prediction?
  - What happens if there is a voting tie or general uncertainty?
- Goal is to reduce need for human evaluation
  - Cannot expect classifier to be perfect
  - A heuristic may be misleading
- Solution: Assign confidence measure to each prediction
  - Defined as the percentage of keypoints that belong to the class that "won" the vote
  - Samples with confidence falling below a predefined threshold can be flagged for human evaluation

Prediction Evaluation Criteria

- Mean confidence for experiment

Keypoint Extractor	Mean Confidence
SIFT	75.98%
SURF	81.61%
ORB	79.39%

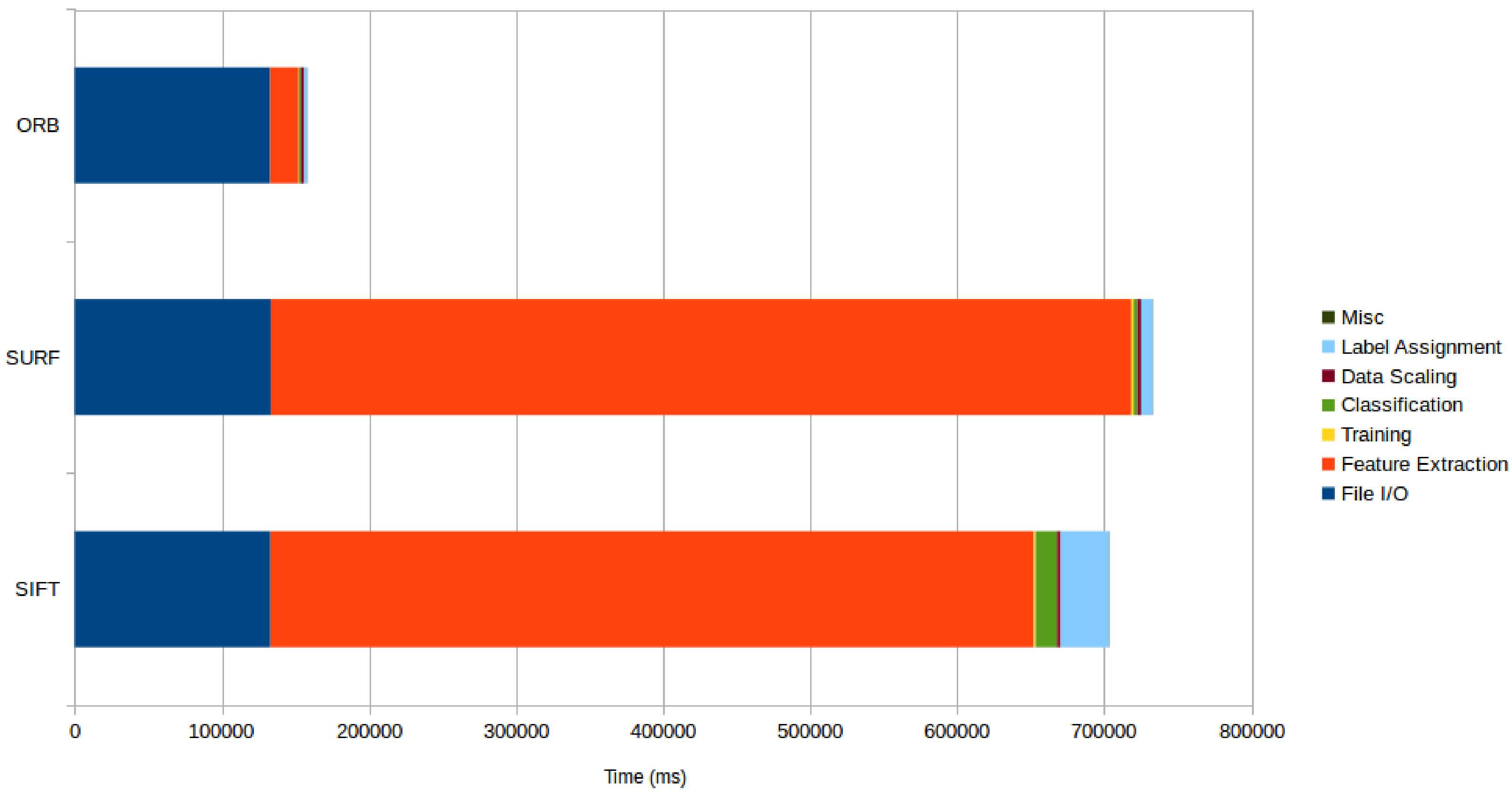
- Word of Caution: A high mean confidence does not imply high accuracy
  - Primary goal is to maximize accuracy
  - Only then can confidence be maximized

Keypoint Extractor Evaluation

- The keypoint extractors were evaluated using two criteria:
  - Classification accuracy
  - Computational complexity with respect to image size
- Classification accuracy
  - SIFT had higher accuracy than SURF or ORB
- Computational complexity
  - All three extractors have complexity $O(mn)$ for an image of dimensions m pixels by n pixels
    - Detailed ORB analysis is available in dissertation appendix
  - **However**, there is more to consider…

Keypoint Extractor Evaluation

- Benchmark graph for keypoint extractors:



Keypoint Extractor Evaluation

- Computational complexity observations:
  - Computational complexities are the same, but the running times are very different
  - Times required to process a single image vary by algorithm
  - Longer feature vectors cause subsequent processing steps to require more time to complete
- <u>Summary:</u>
  - SIFT has higher accuracy at the cost of longer running times
  - ORB runs faster than SIFT at the cost of lower accuracy
  - A researcher will need to consider the tradeoff between higher accuracy and shorter completion time

Conclusion

Conclusion

- Crystal defects can be detected using image processing and machine learning methods
  - Detection methodology presented and verified using a series of increasingly difficult problems
  - Scaling methodology developed to handle large intensity ranges
  - Method to handle larger image sizes also evaluated
- Random forests most effective in detecting defects
- SIFT and ORB were the top performing keypoint extractors
- Confidence measure can be used to address uncertainty

Future Work

- Real data analysis
  - What modifications will need to be made when using real data?
- Experimentation with multiple defects
  - Is it possible to detect two different defect types in an image?
- Defect texture analysis
  - What textures are unique to a specific type of defect?
    - Could help with classifying subtle differences
- Sensitivity quantification
  - How subtle must defects be before they cannot be detected?
    - First step: Determine which types of defects are hardest to detect
  - Does sensitivity change across periodic table?
- Future publication expected through ORNL/SNS

Summary of Contributions

- Evaluation of data processing methodologies for scattering data
- Analysis of reciprocal space imagery characteristics
- Development of scaling methodology for scattering data
- Creation of GUI to aid in reciprocal space analysis
- Formalization of defect detection methodology evaluated using following test cases
  - Classification of simple defect types in small structures
  - Prediction of defect properties in small structures
  - Detection of more complex faults in larger structures
- Comparison of keypoint extractor and machine learner performance in the context of reciprocal space imagery
  - Including detailed complexity analysis for ORB keypoint extractor

Goals from Proposal

- All goals from proposal completed
  - Small structures: Analysis of substitution class separation
  - Small structures: Detection of substitution location
  - Large structures: Analysis of data properties
  - Development of scaling methodology
  - Defect detection for large crystal structures
  - Evaluation of feature extractors and machine learning methods
    - Including computational complexity analysis
    - Detailed analysis for ORB
  - Study of tie-breaking and confidence for defect predictions

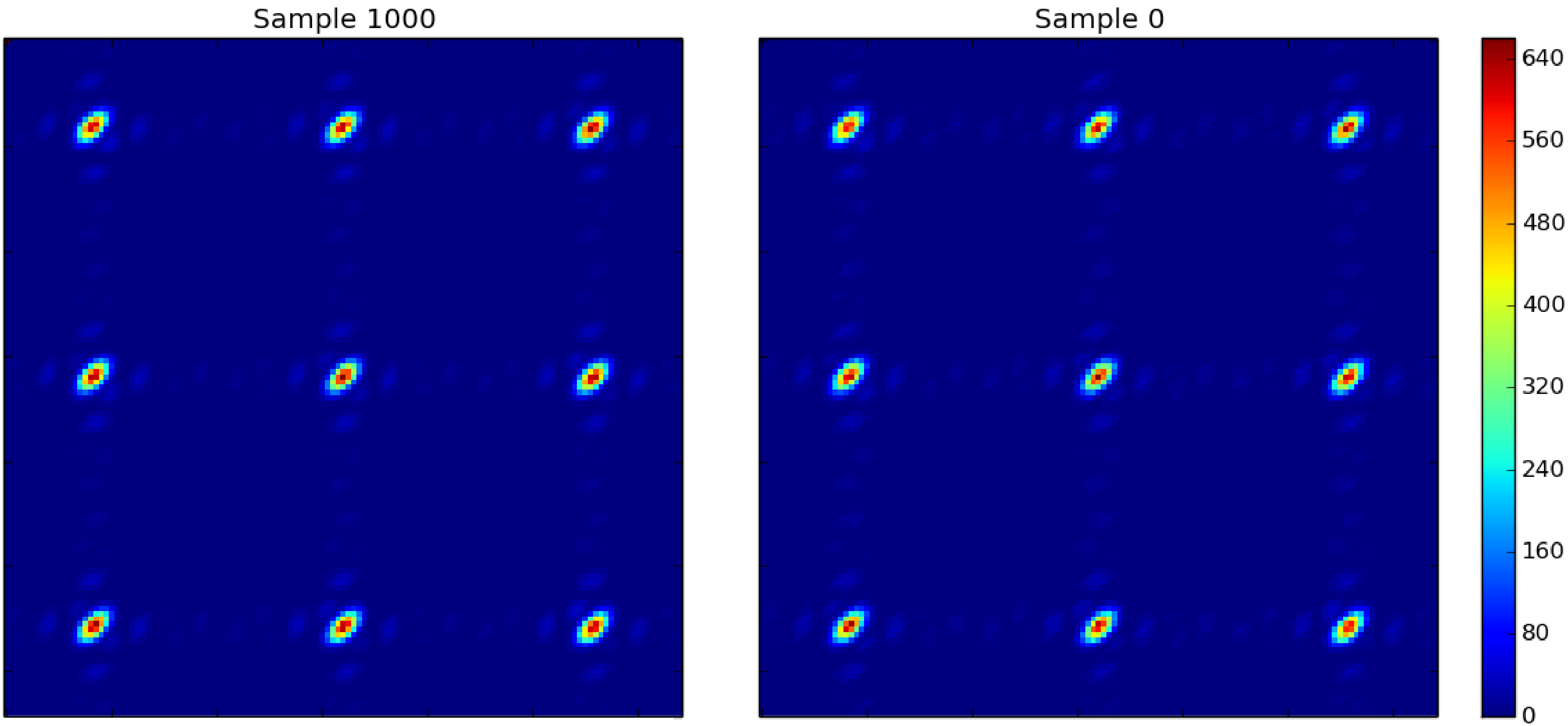
Thank You

Questions?

Extra Slides

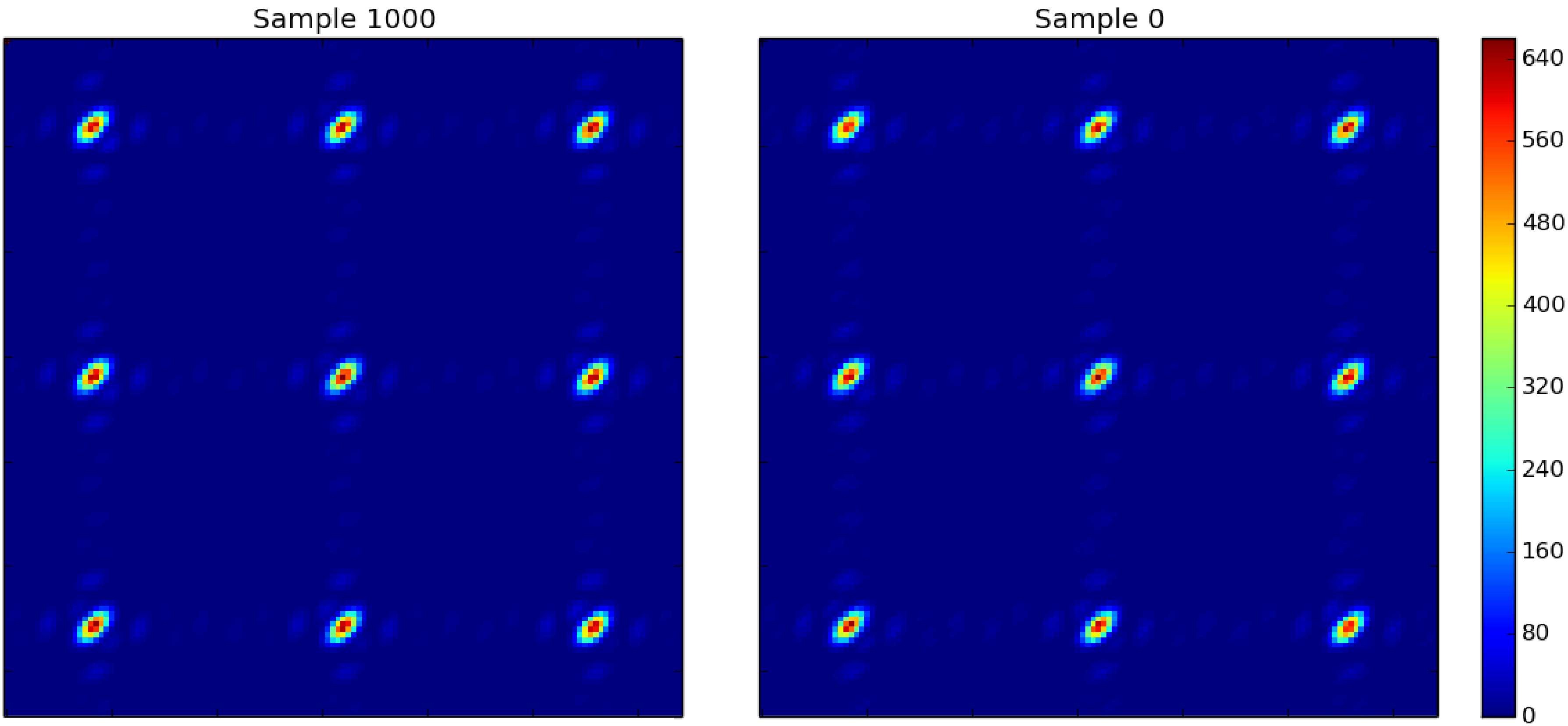
Current Detection Methodology

- State-of-the-art crystal defect detection:



Current Detection Methodology

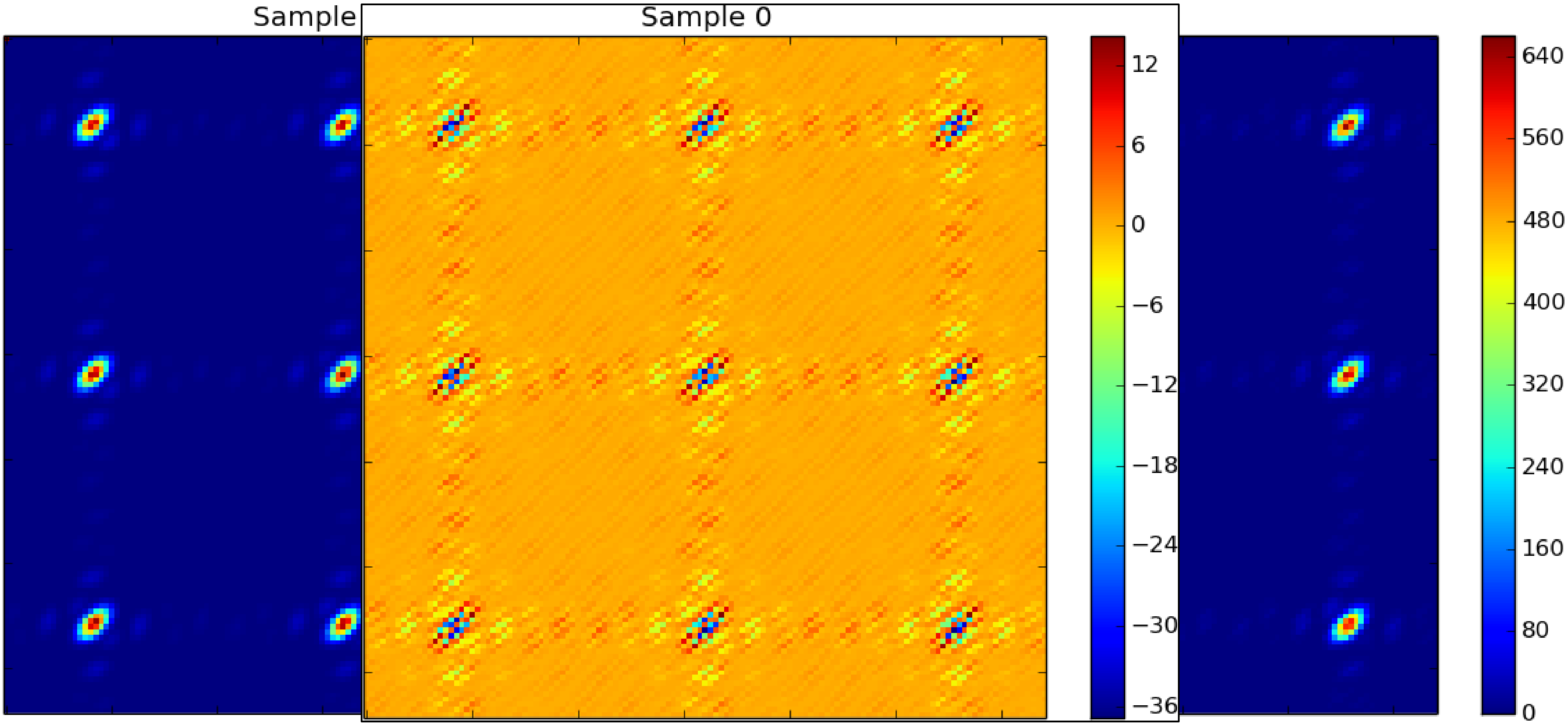
- State-of-the-art crystal defect detection:



SPOT THE DIFFERENCE

Current Detection Methodology

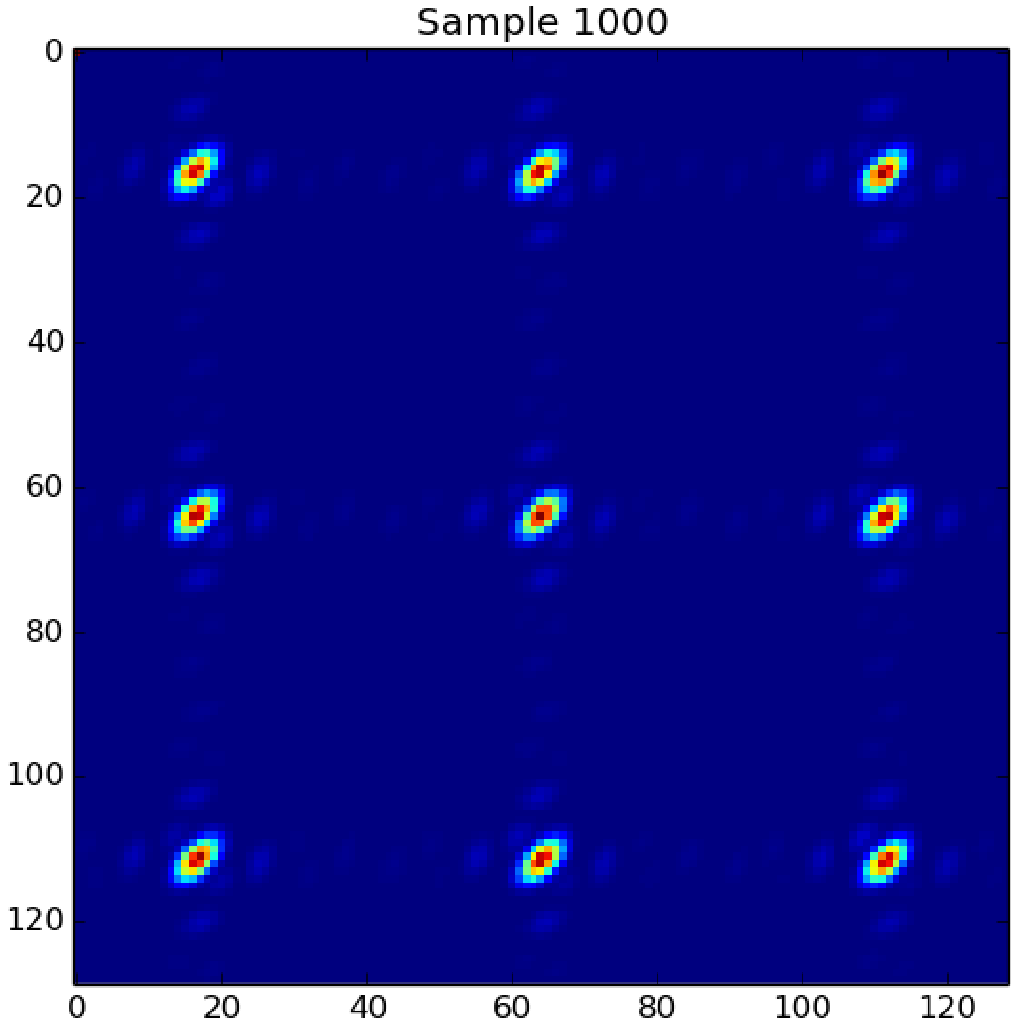
- State-of-the-art crystal defect detection:



SPOT THE DIFFERENCE

(HINT: HERE'S A DIFF)

Sample Reciprocal Space Image



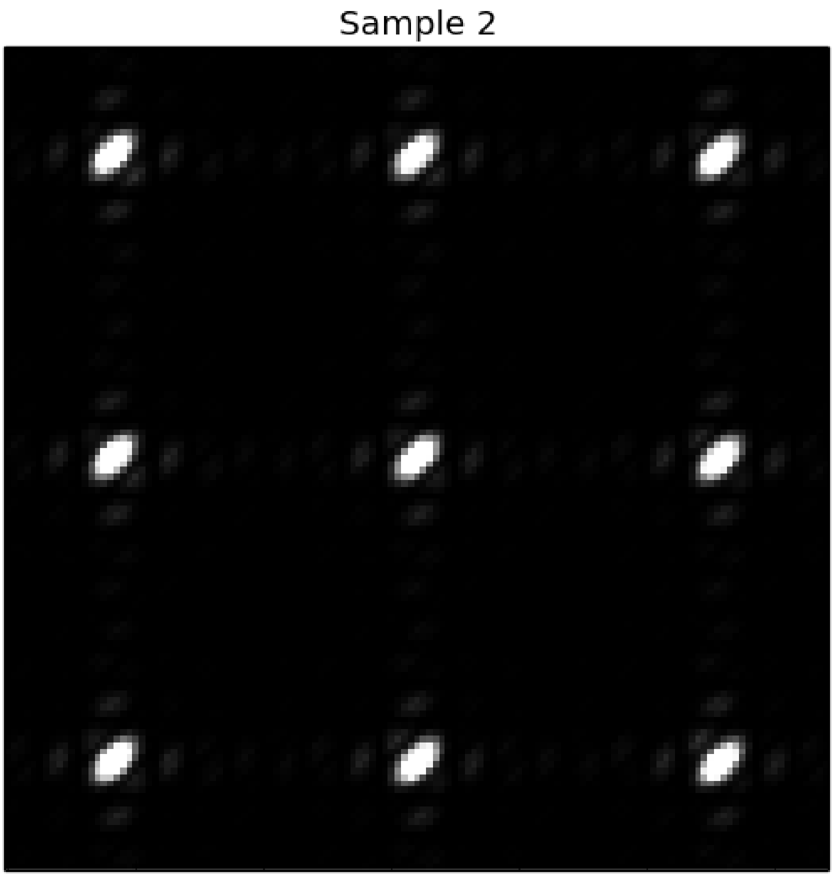
Reciprocal Space Definition

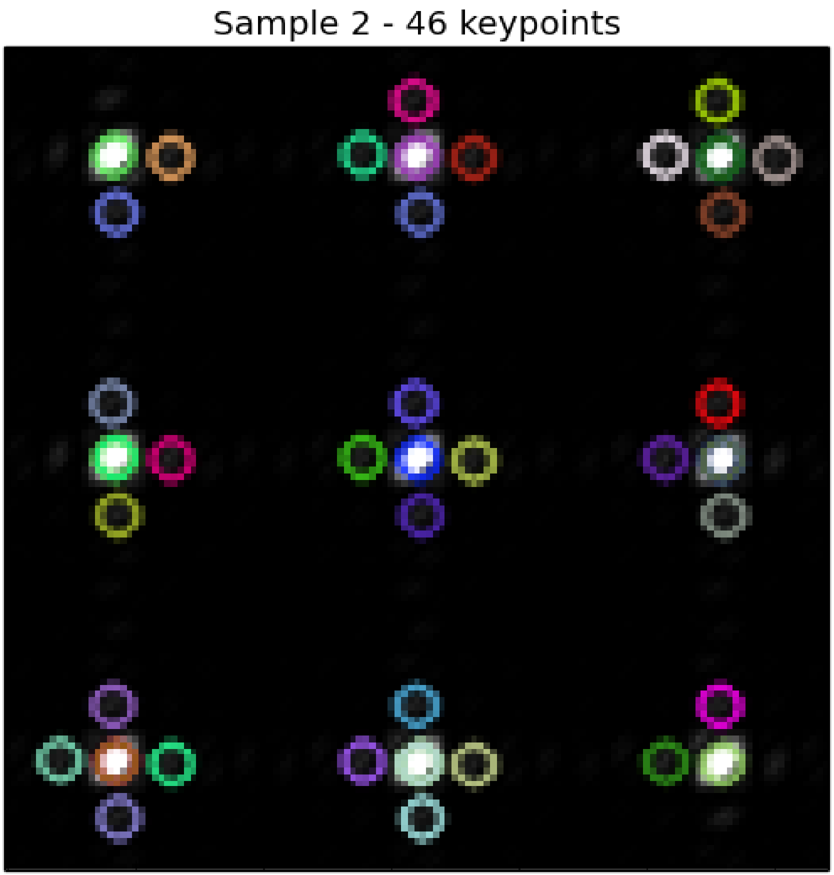
- Total complex scattered amplitude:
  - $A(\boldsymbol{k}) = \sum_{m=1}^{N} F_m \exp(i\boldsymbol{k} \cdot \boldsymbol{R}_m)$ where:
    - N = number of cells in the lattice
    - F_m = structure factor for m$^{\text{th}}$ cell (listed below)
    - $\boldsymbol{k}$ = diffraction wave vector
    - $\boldsymbol{R}_m$ = position vector of m$^{\text{th}}$ cell

- Structure factor:
  - $F_m = \sum_{n=1}^{N_m} f_n \exp(i\boldsymbol{k} \cdot \boldsymbol{r}_n)$ where:
    - f_n = scattering factor for atom n
    - $\boldsymbol{r}_n$ = location of atom n within the cell

- Reciprocal space intensity at $\boldsymbol{k}$:
  - $I(\boldsymbol{k}) = A(\boldsymbol{k})A^*(\boldsymbol{k})$
  - Reciprocal space images are basically the DFT magnitude for the structure
  - Phase problem: Phase data lost = Unable to do inverse transform

Feature Extraction Example





Data Information

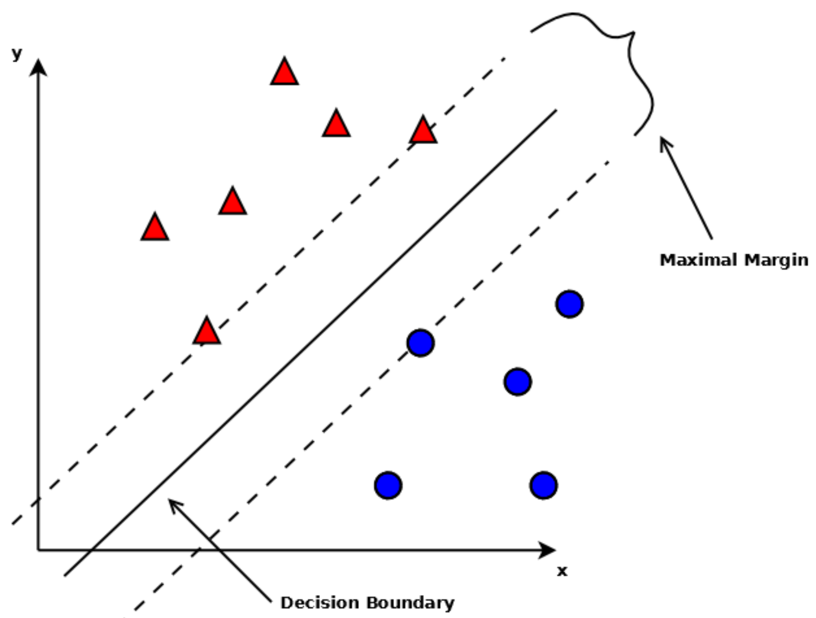
- Toy dataset
  - 8 cell by 8 cell crystal lattice
  - 129 pixel by 129 pixel intensity maps
  - Cells contain two atoms with different scattering factors
  - Crystal is for proof of concept
    - Not intended to represent a realistic crystal
- Reciprocal space images: Single band pixel intensity maps
- Simulated dataset
  - Generated with the help of ORNL staff using methodology presented in (Butler and Welberry, 1992)
  - Simulations are apparently very accurate and seem to be a common step before performing neutron scattering experiment

Feature Classification

- Any classifier can be used at this point
- Three types of classifiers were evaluated in the experiments:
  - Support vector machine (Linear kernel)
  - Support vector machine (RBF kernel)
  - Random forest
- Input data points:
  - Keypoint descriptors
  - Corresponding label for the image they were extracted from
- Classification of a new image involves:
  - Collecting predictions for all of the keypoints in the image
  - Assigning a final label via a majority vote of the keypoints

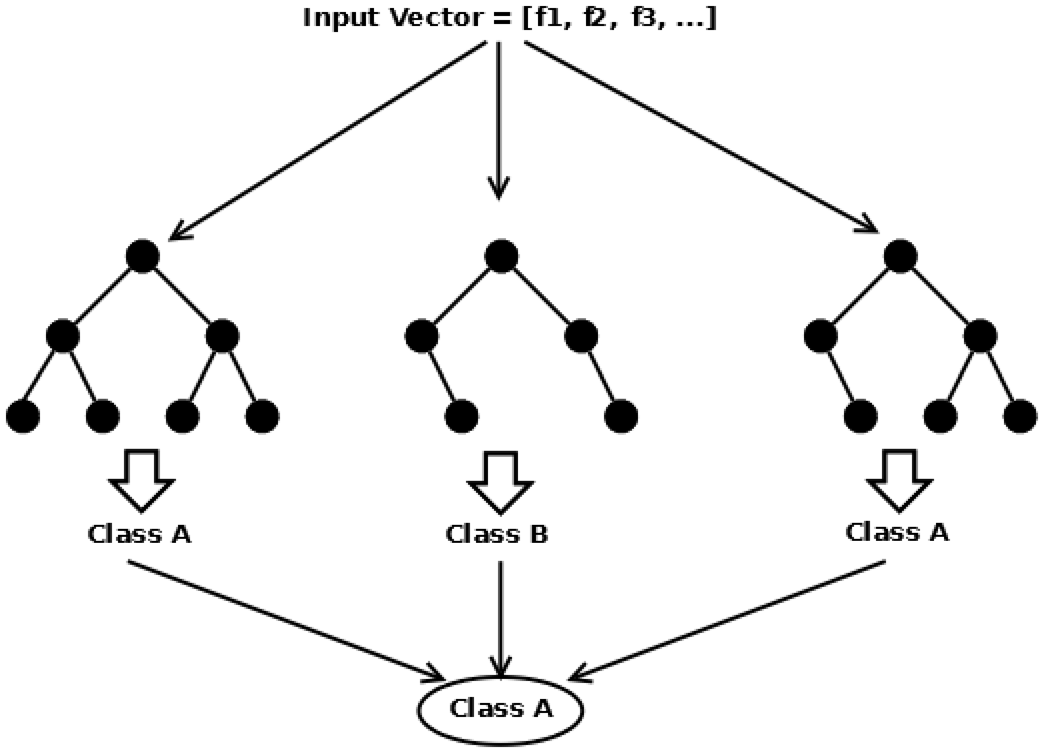
Support Vector Machines

- SVMs seek to create a decision boundary that maximizes the margin between two classes
- They are a standard baseline method
- A kernel functions can be used to aid in separation
  - Linear and radial basis function (RBF) evaluated



Random Forests

- Random forests are ensembles of decision trees
  - Each tree uses a different subset of the data
  - Each tree node uses a subset of features to make decision
  - Final classification is via vote or average of tree classifications

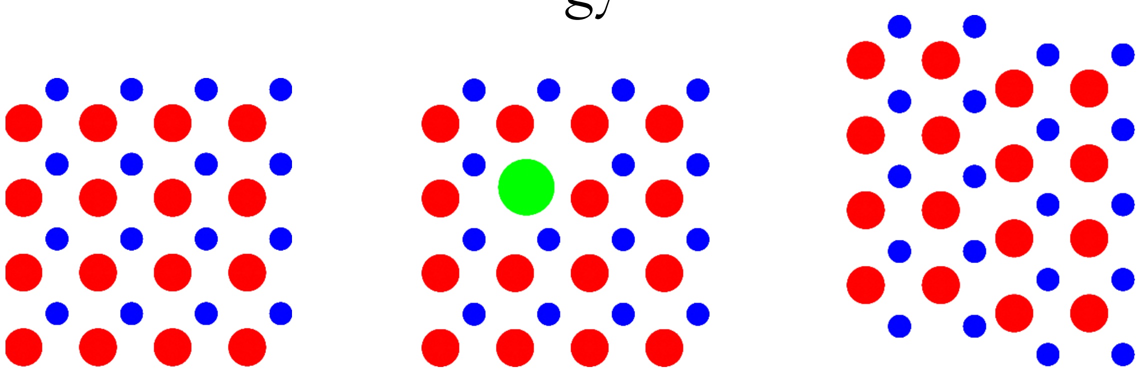


Comparison of Learning Algorithms

- Learning algorithms evaluated using two criteria:
  - Classification accuracy
  - Computational complexity with respect to training sample volume
- Classification accuracy
  - Random forests had consistently higher classification accuracy
- Computational complexity for *N* training samples
  - SVM training: $O(N^2) - O(N^3)$
  - Random forest training: $O(N*log(N))$
- Conclusion: Random forest is the better choice
  - It had higher accuracy in the experiments
  - It has lower computational complexity for training

Experiment: 2-class Problem

- <u>Goal:</u> Classify a crystal containing one of two defect types:
  - Substitution (small and large)
    - Small - scattering factor on [0,1]
    - Large - scattering factor on (1,2)
  - Shear
- Simple problem to evaluate the effectiveness of the proposed defect detection methodology



No Defect **Substitution** **Shear**

Experiment: 2-class Problem

- 600 images
  - 400 substitution (200 large, 200 small)
  - 200 shear
- SIFT descriptors extracted from each image
  - Extractor requires images to be scaled to range [0,255]
- Training procedure:
  - 3 learners tested: SVM (linear), SVM (RBF), and random forest
  - Learner trained using keypoint descriptors
    - Trained on 10% of images
    - Image label is assigned to each keypoint
- Class of test image determined via majority vote of its keypoints
- Results averaged over 20 independent experiments

Experiment: 2-class Problem

- Results:

Learning Algorithm	Accuracy
SVM (linear)	97.31%
SVM (RBF)	95.92%
Random Forest	**98.05%**

- Conclusion:
  - Methodology does good job of detecting defects
  - All classifiers performed very well in this experiment

- Next step: Test using a more difficult problem

Experiment: 3-class Problem

- Goal: Present harder problem to classifier to test the sensitivity of the defect detection methodology
- Split substitution class into "large substitution" and "small substitution" subsets
  - Harder to distinguish between these classes
- 600 images
  - 200 large substitution
  - 200 small substitution
  - 200 shear
- Training and classification procedure was the same as the previous 2-class experiment

Experiment: 3-class Problem

- Results:

Learning Algorithm	Accuracy
SVM (linear)	70.87%
SVM (RBF)	70.56%
Random Forest	**76.12%**

- Conclusions:
  - Methodology is precise enough to predict subtle defect differences
  - Random forest performed much better than the SVMs
  - Lower overall accuracy was due to confusion between large and small substitution classes
    - Increasing class separation did not significantly affect results

Experiment: Substitution Location

- Goal: Evaluate whether classification methodology can be used to detect other specific properties of a defect
  - Can location of substitution be predicted?
- 1000 large substitution images
  - Substitution can be in 1 of 64 possible cell locations
- Feature extraction and machine learning set-up was the same as the other defect classification experiments
  - Classification label is the integer index [0,63] for the cell containing the substitution defect

Experiment: Substitution Location

- Results:

Learning Algorithm	Accuracy
SVM (linear)	94.80%
SVM (RBF)	73.76%
Random Forest	**95.67%**

- Conclusions:
  - It is possible to predict specific defect properties
  - Random forest and linear SVM performed very well
  - SVM with RBF kernel did not perform as well