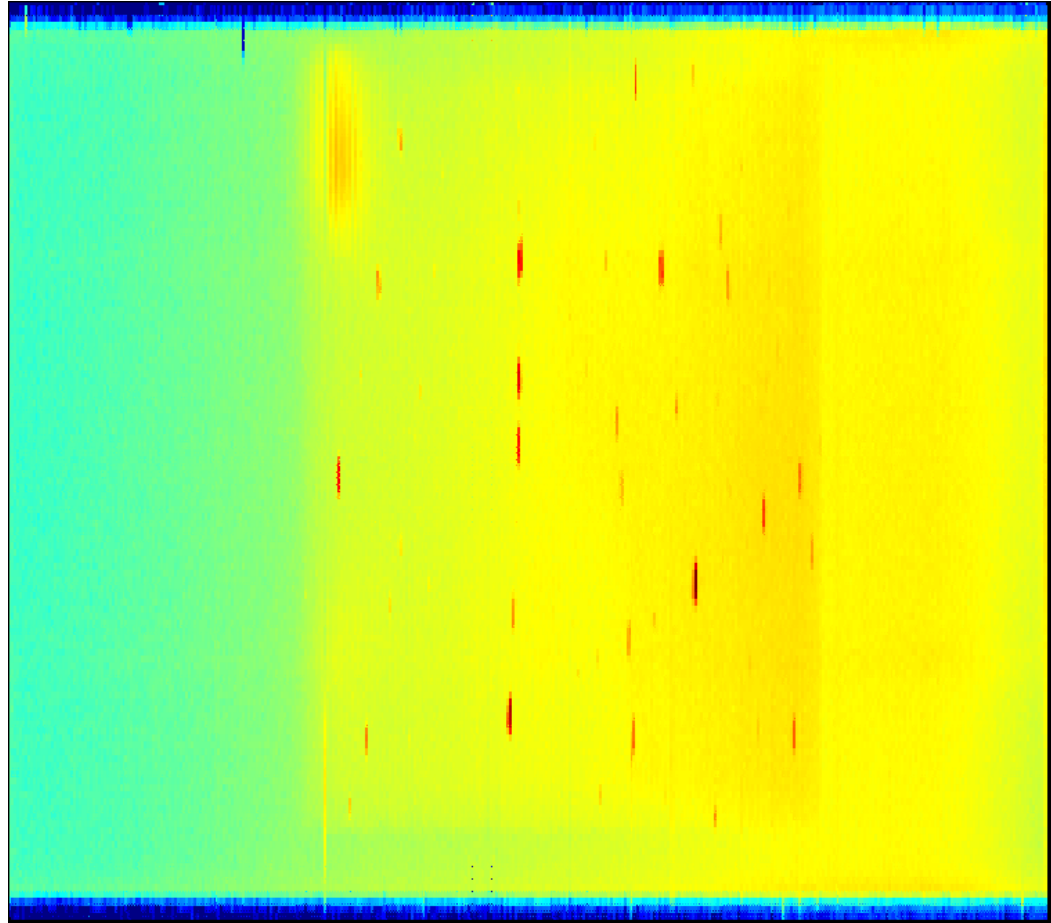


Finding Single Crystal Peaks

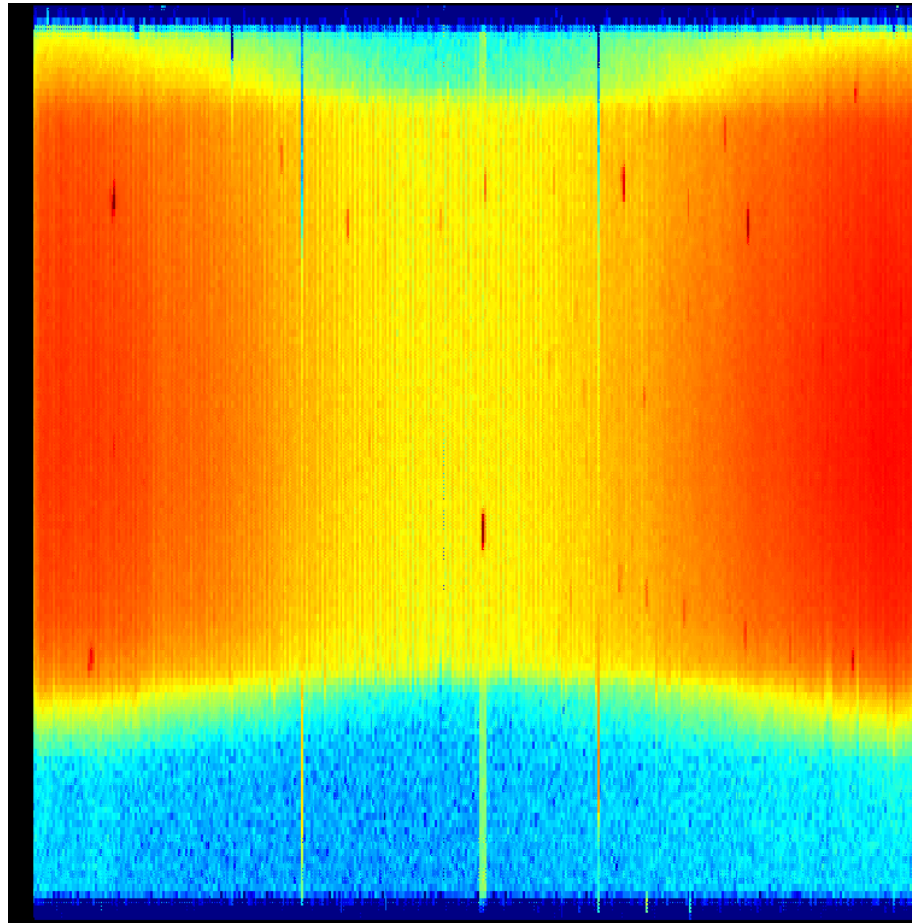
WISH Clear Peaks



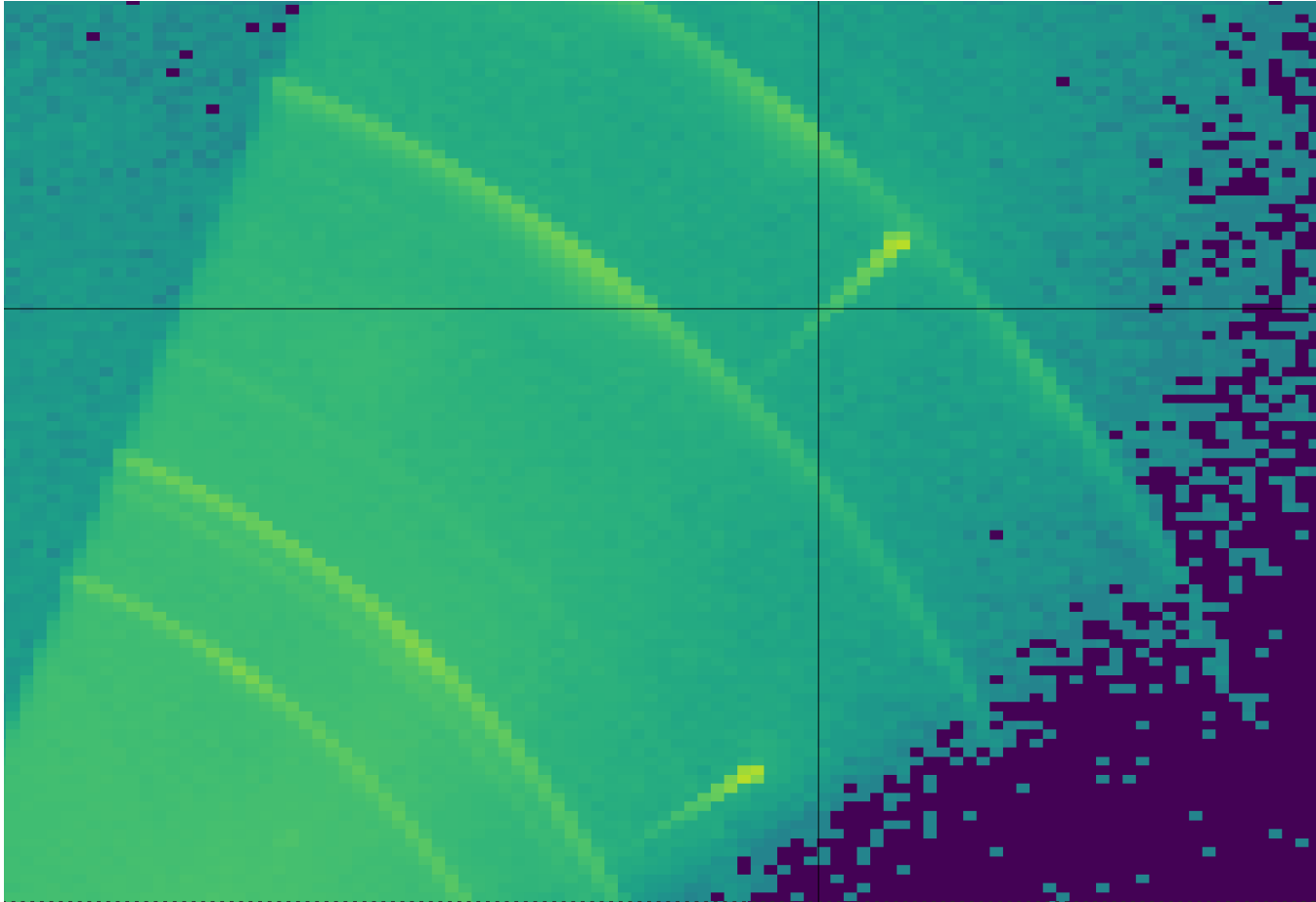
Description of Problem

- A lot of Instrument Scientist time is spent identifying or correcting peaks
- Current density-based algorithm too unreliable when heavy noise is involved
- For a human, the process is easy but tedious and wasteful
- Could machine learning be used to better identify peaks in the presence of noise?

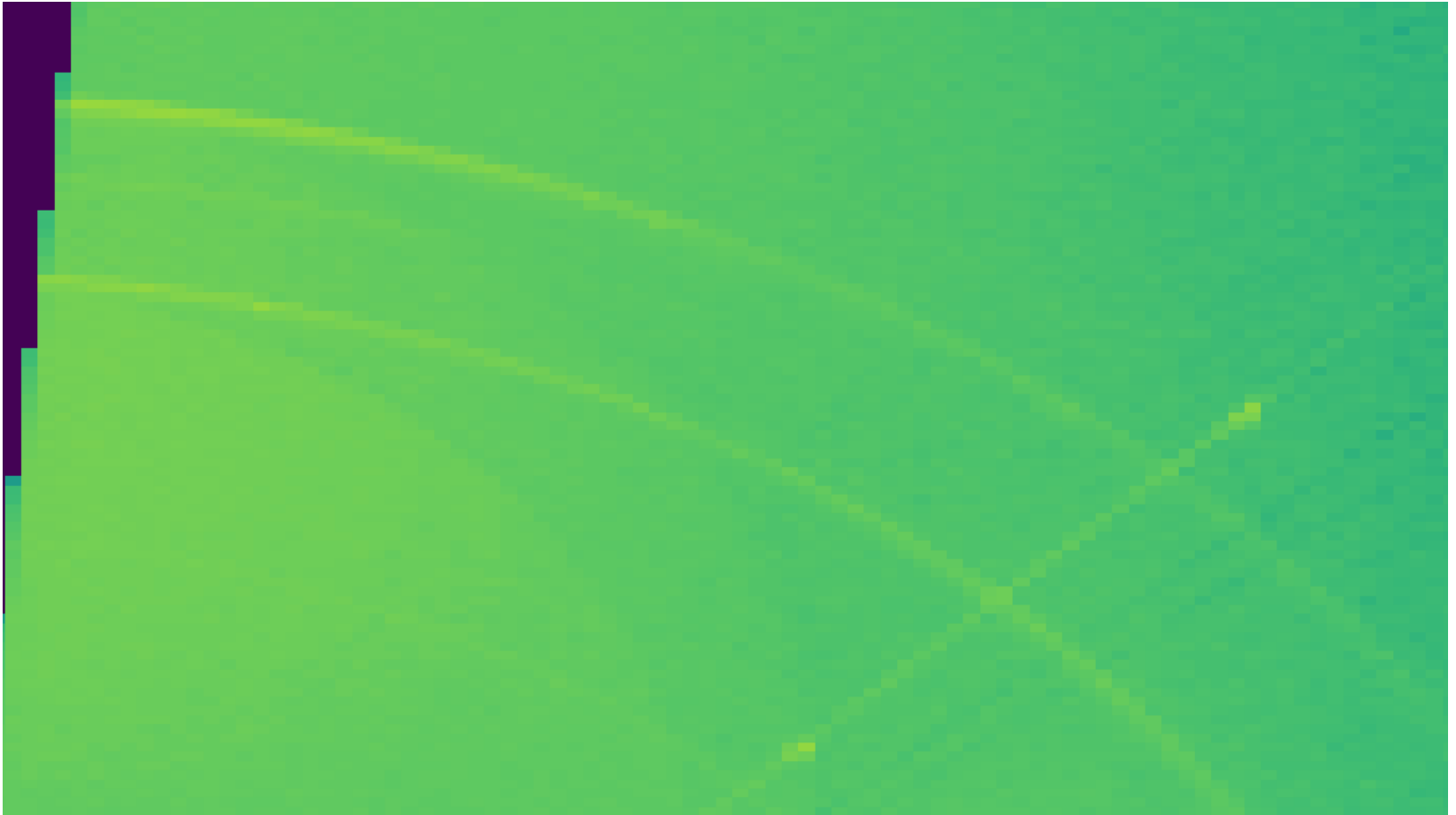
WISH Noisy Peaks



Peaks and Rings



Noise



Weak Peaks



Goals

- Ideally, we want:
 - Automatic identification with minimal error
 - Confidence estimate
 - Classification by shape and size
 - Continuous learning based on corrections

Thoughts and Challenges

- Considering:
 - Hand-crafted ROI + SVM or Random Forest
 - Neural Network(s) for ROI and classification
- Data is 3-dimensional
 - To slice or not to slice
- Data can be huge (~10GB+ in memory)
- Lack of correctly identified data for training
 - Considering simulated data as substitute

Plan Going Forward

- Next steps to find a solution
 - Generate simulated training data set
 - Much faster than trying to gather enough manually labelled real data
 - Evaluate performance of current algorithm against simulated data set
 - Develop prototype(s) using new approach
 - Evaluate performance of prototype(s) against simulated data set

Questions We Have

- Feasibility of Problem
 - Is this something ML can solve?
- Most Appropriate Models
- Do the next steps we plan to take make sense?
- How best to measure effectiveness of model & simulated data?