# Determining a Detector's Saturation Threshold

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## Introduction

The AMOL3416 experiment is focused on the use of coherent diffractive imaging with X-ray Free-Electron Lasers (XFELs) in order to determine high-resolution structures of Carboxysomes, RuBisCO, (an abundant enzyme involved in the first step of carbon fixation) and other nano-scale biological objects. Efforts to discover the functional and structural characteristics of these cell units has potential to facilitate the understanding of major contributors to Earth's carbon fixation, while simultaneously aid in the advancement of the 'diffraction before destruction' method of X-ray imaging. Improvement in determining accurate reconstructions of the X-ray imaged cell-units is achieved by increasing the efficiency of injectors, determining and masking detector artifacts, and refining reconstruction methods. In this case, data usability was aided by the identification of the detector's saturation threshold and the subsequent masking of saturated pixels from scattering patterns. The saturation threshold is found through visual inspection of raw pixel values and represents the detectors limitation of detecting photons.

Keywords: diffractive imaging, XFEL, masking, saturation threshold, scattering patterns

## Procedure

Data collection occurred at the LCLS (Linac Coherent Light Source) XFEL facility at SLAC. Numerous datasets were collected where several different biological objects were imaged by the laser.

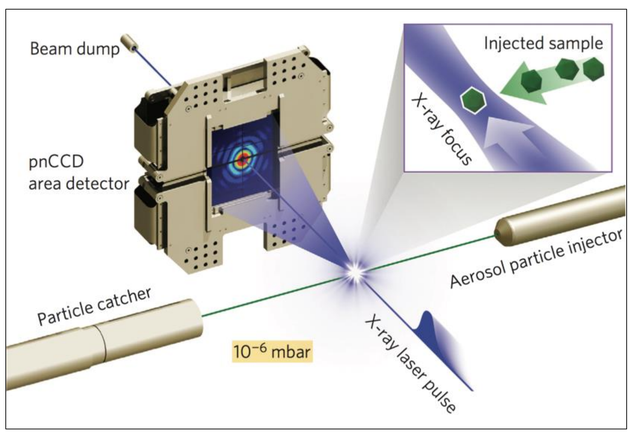


***Fig 1**. Here biological particles are injected into the X-ray beam and a detector records the resulting diffraction patterns. [1]*

The relatively large Japanese P. bursaria chlorella virus 1 (190 nm diameter), was used for testing and creating the saturation mask [2]. This mask exempts over-saturated pixels from the data by accounting for the detector's limitations and focusing solely on the particle's pattern. Larger particles are expected to have more hits at higher intensities, thus making a saturation threshold more distinguishable.

This threshold determines the cut off for which pixel values are past the detectors limits and which actually represent the imaged particle.

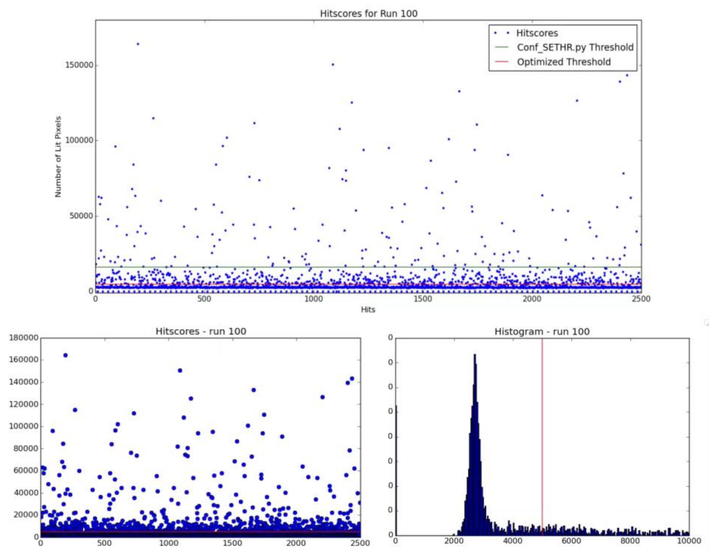


***Fig 2**. Inspection of the lit pixel intensity histogram is used to optimize the hitscore threshold, the cut-off for the number of lit pixels used to determine if a hit has occurred and been recorded.*

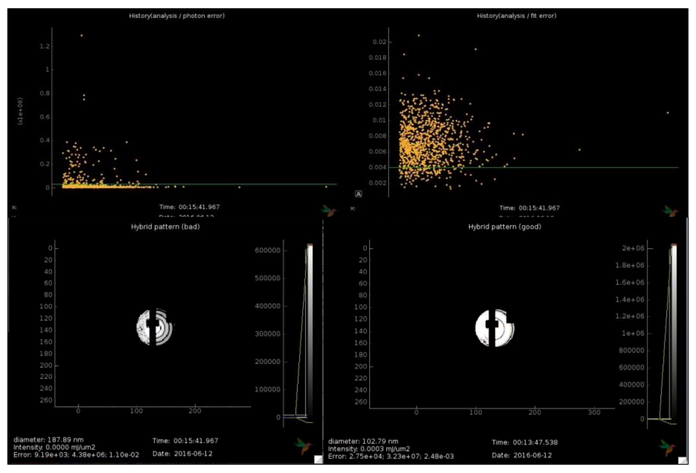


***Fig 3**. The Python package "Hummingbird" [3] uses spherical models (right side) to discern "good" and "bad" hits. Hits are classified as "good" if their photon and fit error are both under the predetermined threshold.*

The most intense hits are expected to have the highest number of lit pixels. We look at "lit" pixels due to the weakness of some shots and to categorize the intensity of the recorded hits. From the top five most intense (total summed intensity) patterns we configure an artificial image of "maximum intensity values".

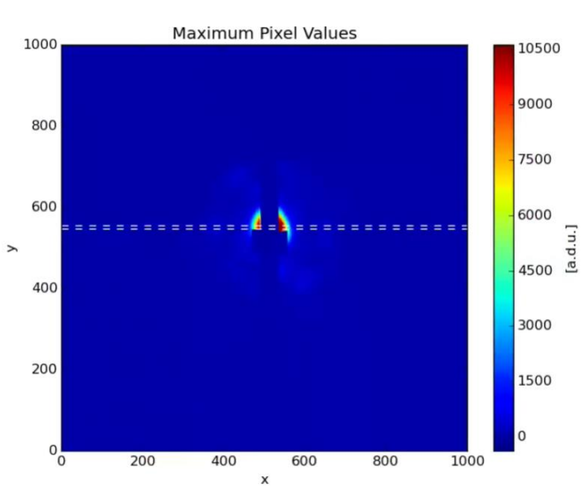


***Fig 4**. Maximum pixel values of the five most intense diffraction patterns. Line scans across the center of the detector (dotted lines) are used to determine the saturation threshold.*

Peak detection in the line scans of the maximum intensity patterns was used to identify the saturation threshold for the four quadrants of the detector:

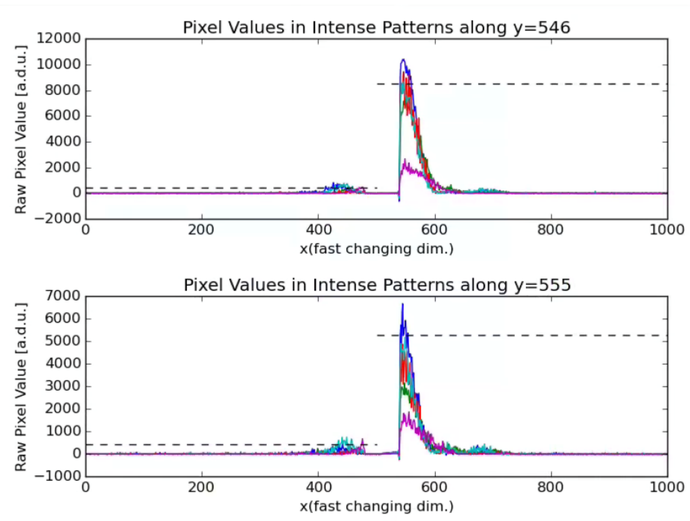


***Fig 5**. Line scan plots corresponding to the dashed lines in Figure 4. Saturation thresholds for the four quadrants of the detector are identified at the peaks (raw pixel values)*

```
[psanagpu102 Saturation-Code(master) 526 13:01:51] python ./saturation_threshold.py 100
[0.0008292800245308978, 0.0007441298339208705, 0.0007185805103316673, 0.0006994982320364
5386, 0.0006223107919305369]
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TOP 5 INTENSITIES [mJ/um2]
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min = 6.22e-04, max = 8.29e-04
mean = 7.23e-04, std = 6.70e-05
median = 7.19e-04
Enter first line scan: 546
Enter second line scan: 555
Enter first quadrant threshold: 430
Enter second quadrant threshold: 8500
Enter third quadrant threshold: 430
Enter fourth quadrant threshold: 5275
```

## Conclusions

This project served to produce and test a method that for finding the saturation threshold in XFEL image data. This threshold reveals the detector's limitation of detecting photons. Refining the mask may occur in the future and lead to a more productive application. Overall, the Uppsala research group, responsible for the AMOL3416 experiment, are on the cusp of diffractive imaging and discovery in the nano-regime, to future sub-nano resolutions.

## Acknowledgments

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## References

[1] Hantke, M. F., Hasse, D., Ekeberg, T., John, K., Svenda, M., Timneanu, N., & ... Martin, A. V. (2014). High-throughput imaging of heterogeneous cell organelles with an X-ray laser. *Nature Photonics*, *8*(12), 943. doi:10.1038/nphoton.2014.270

[2] https://github.com/tepowell14/Saturation-Code

[3] https://github.com/FXIhub/hummingbird

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