Photon Centroiding for High-Resolution RIXS Experiments Using Richardson–Lucy Deconvolution

Chuzida Chen – cchen@slac.stanford.edu (1, 2, 3), Lingjia Shen (1)

1. SLAC National Accelerator Laboratory, USA. 2. University of California, Berkeley, USA. 3. Advanced Light Source, Lawrence Berkeley National Laboratory, USA.

SLAC NATIONAL ACCELERATOR LABORATORY U.S. DEPARTMENT OF ENERGY Stanford University

INTRODUCTION

Resonant inelastic X-ray scattering (RIXS) is a technique that offers promising utilities for the study of condensed matter systems at high energy resolutions. However, one of the limiting factors of RIXS resolving power is the effective detector pixel size [1, 2, 3], being technologically challenging to minimize its effects. This project offers a viable solution towards such problem via Richardson-Lucy (RL) Deconvolution. Upon determination of the CCD's point spread function (PSF), the algorithm demonstrates effective 'thinning' of one-photon droplets down to a single pixel along the dispersion axis. This project reveals the potential utility of this algorithm towards research involving photon-hungry processes such as RIXS and XPCS

RICHARDSON-LUCY DECONVOLUTION

The detector's PSF F blurs the ground truth image W by a convolution such that one observes instead H. With an initial guess of $W^{(0)}$, W can be solved iteratively by generating improved estimates of the reciprocal kernel G, which satisfies $W = G * H$. At the r-th iteration of RL:

$$H^{(r)}(x,y) = \iint W^{(r)}(\xi,\eta)F(x-\xi, y-\eta)\,d\xi d\eta$$

The r-th approximation of G is then:

$$G^{(r)}(x-\xi, y-\eta) = \frac{W^{(r)}(x,y)F(x-\xi,y-\eta)}{H^{(r)}(\xi,\eta)}$$

Finally, the $(r+1)$-th approximation of the ground truth image is:

$$W^{(r+1)}(x,y) = W^{(r)}(x,y)\iint \frac{H(\xi,\eta)}{H^{(r)}(\xi,\eta)}F(x-\xi, y-\eta)\,d\xi d\eta$$

The algorithm is shown to [6]:

1. Preserve nonnegativity and normalization
2. Yield unique solution when elements of H $\geq$ to that of W
3. Converge to a maximum likelihood solution

Figure 1: Example of RL algorithm in context of astro-imaging. Image credit: https://clarkvision.com/articles/image-restoration3/

MOTIVATION

- Charge Diffusion in CCD compromises spatial resolution
- High resolution detectors enhance RIXS experiments [4]
- Existent photon centroiding algorithms are controvertible due to biases [5]

LOOKING FOR POINT SPREAD FUNCTION

- Charge diffusion modeled by 2D Gaussian
- Effective pixel size is 40 μm vertical and 10 μm horizontal
- The PSF size (L_x, L_y) limits the number of affected pixels while the standard deviations (σ_x, σ_y) of the Gaussian determine the value
- Maximum correlation approach
- Data: RIXS at Copper L_3-edge of sample La_2CuO_4

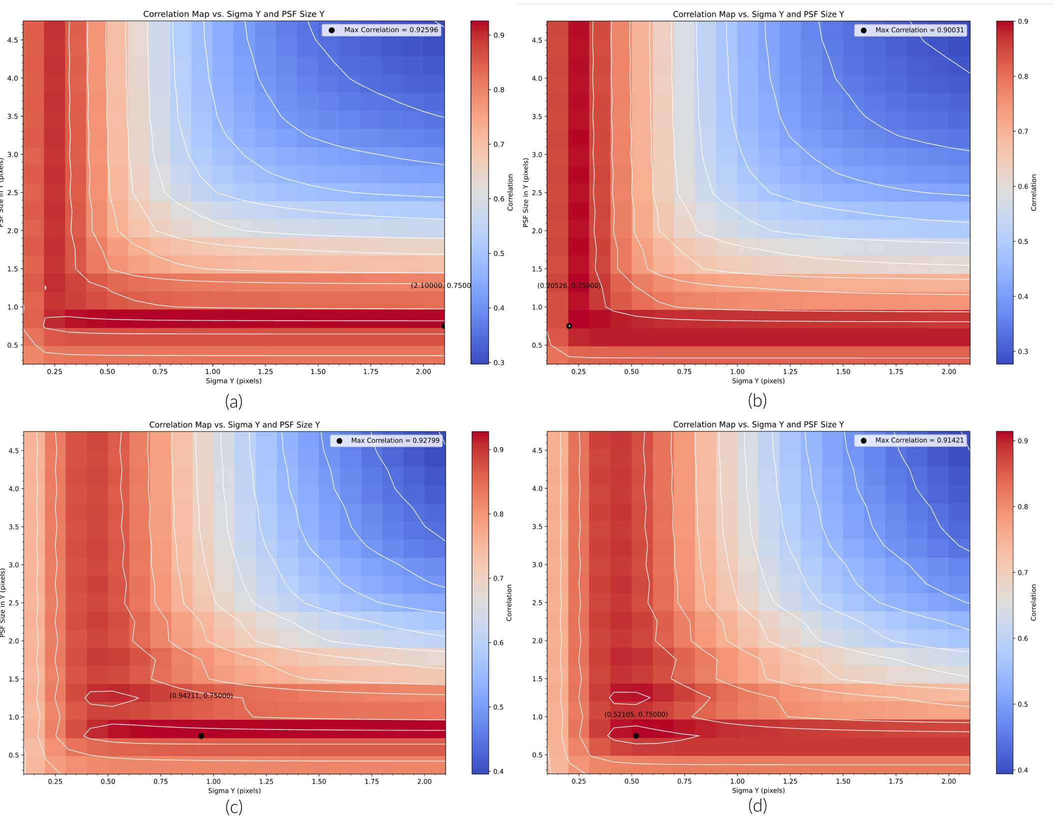
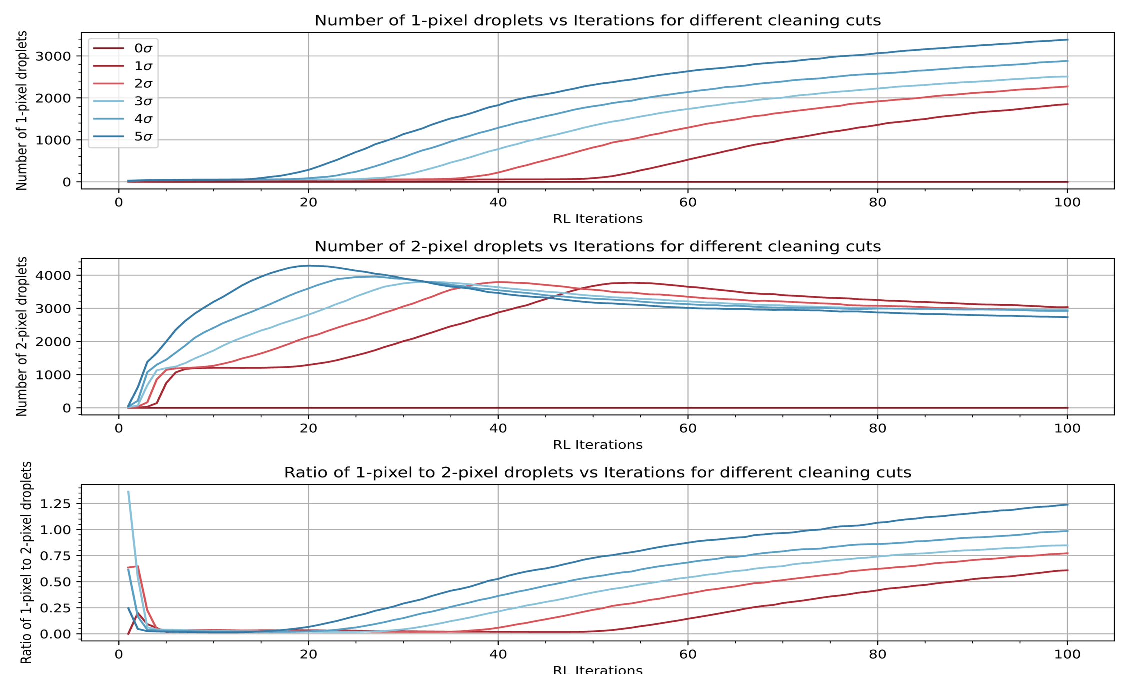


Figure 2: Correlation map with ratio a). $L_x = 3L_y$ and $\sigma_x = 4\sigma_y$ b). $L_x = 4L_y$ and $\sigma_x = 4\sigma_y$ c). $L_x = 3L_y$ and $\sigma_x = 1.61\sigma_y$ d). $L_x = 4L_y$ and $\sigma_x = 1.61\sigma_y$

OPTIMIZING RL



- We introduce a 5σ threshold cut before RL to address the lack of regularization in RL [7, 8]
- Cleaning cut applied after RL to address artifacts that may arise during RL as well as reconstruction left-overs [9]

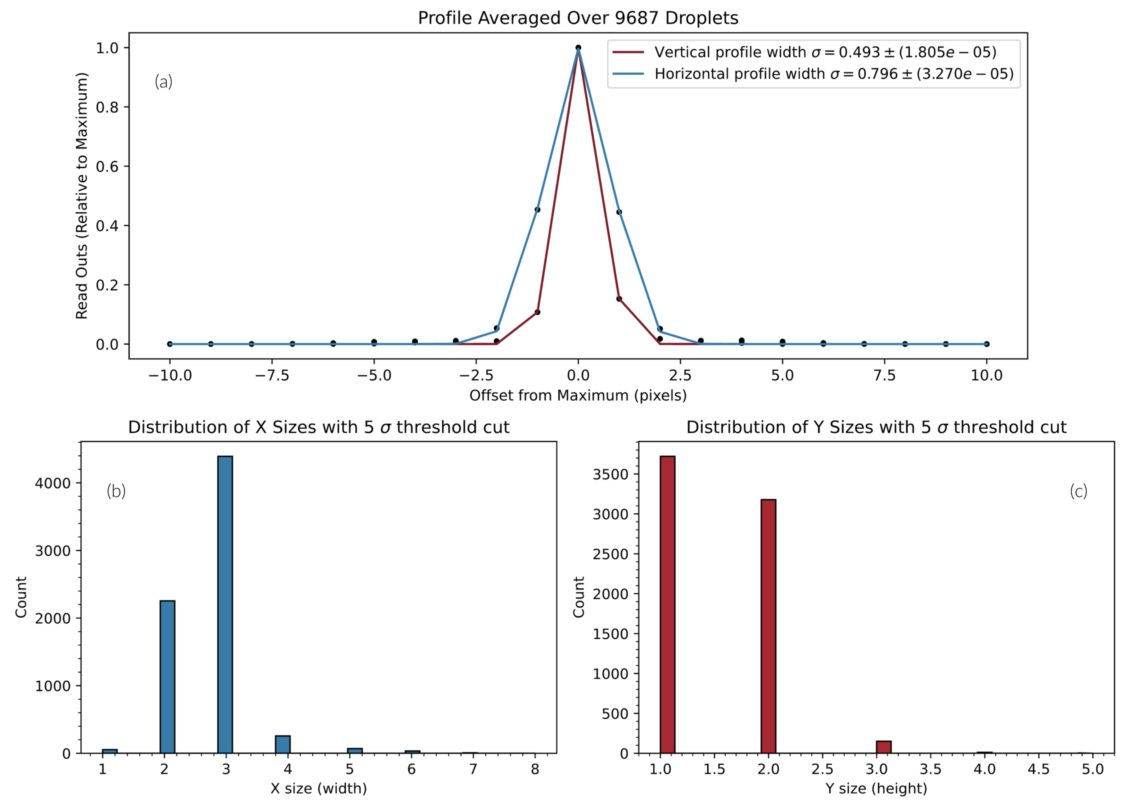
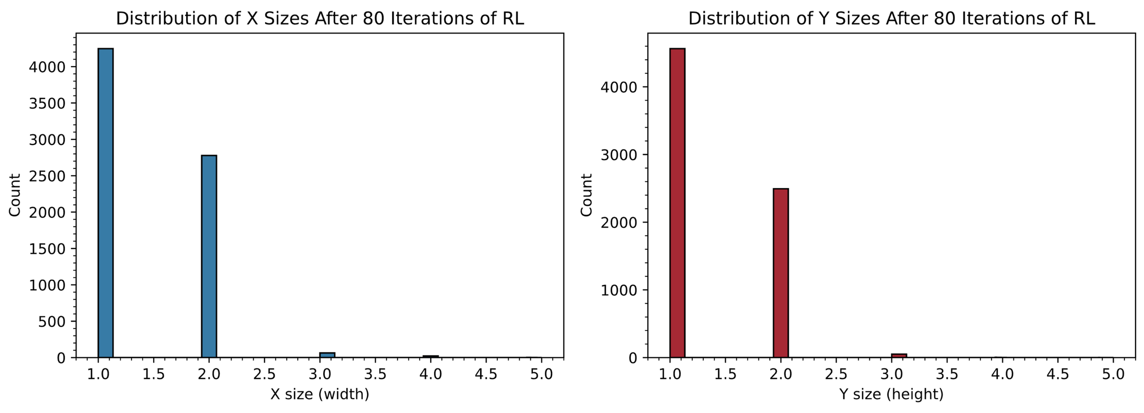
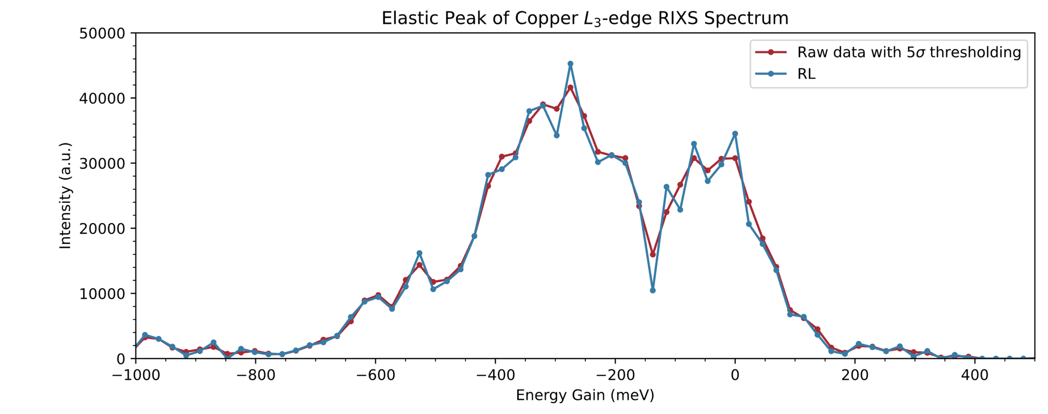


Figure 3: a). Droplet profile and fitted Gaussian. Distribution of b). horizontal and c). vertical droplet sizes of Copper L-data

RESULTS AFTER IMPLEMENTING RL

- Effective 'thinning' of droplets
- Contrast enhancement of the elastic peak
- At beamline resolution limit. To further enhance the peak, we can closedown the exist slit from 20 to 5 micron, further focus the x-ray beam along the dispersion direction from 20 to few microns, or replacing the spectrometer grating with one that has higher line density (already planned)





FUTURE DIRECTIONS

- Study on possible bias with having 5σ threshold cut
- Sub-pixel resolution PSF can be determined experimentally
- PSF-maps can address inelastic photons of different energy
- Since RL operates on the detector image, it is also applicable to XPCS, and a bias study on RL can further illuminate this potential

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