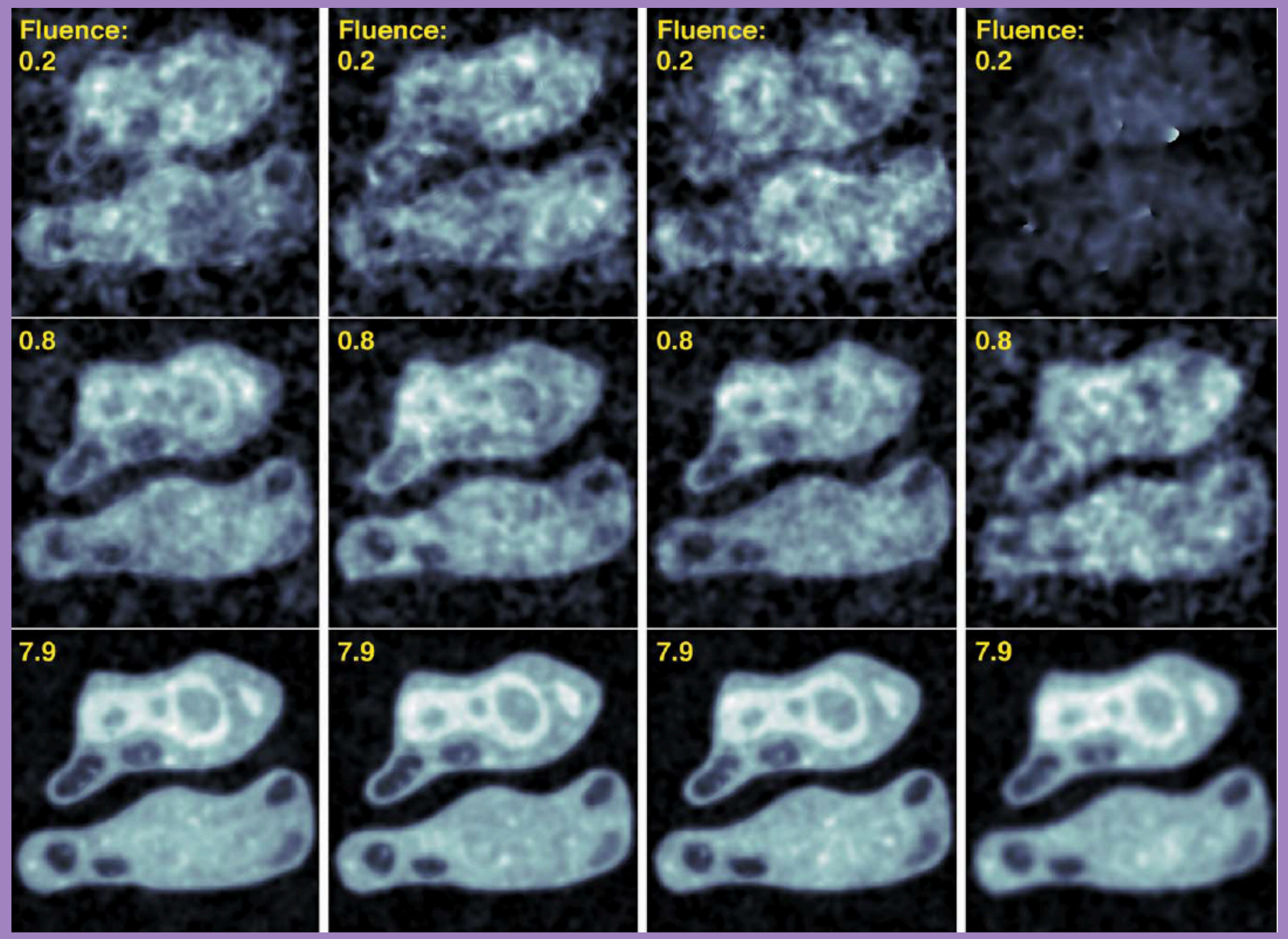
Ptychography

Compress the x-ray imaging dataset

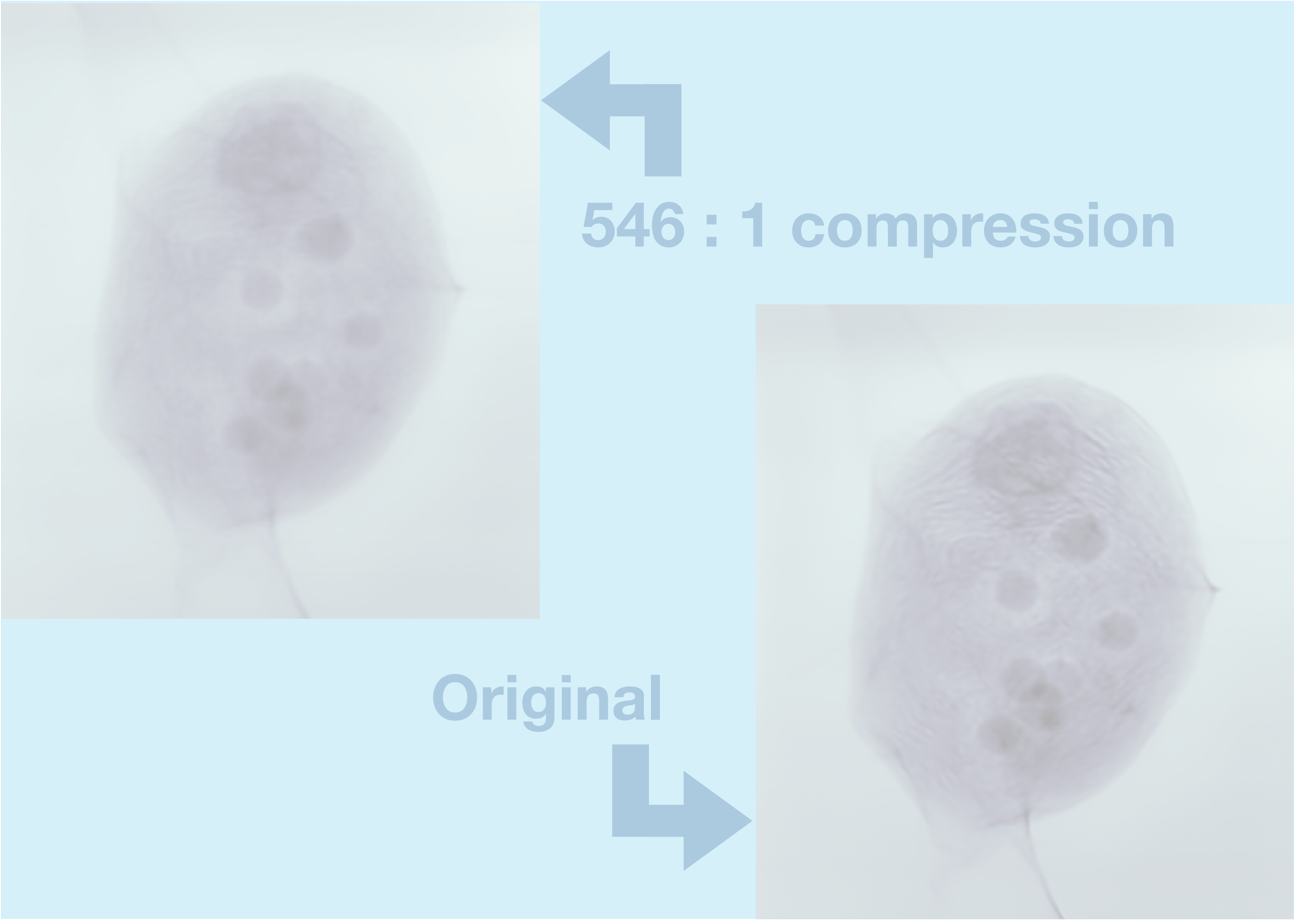
Fluorescence Tomography

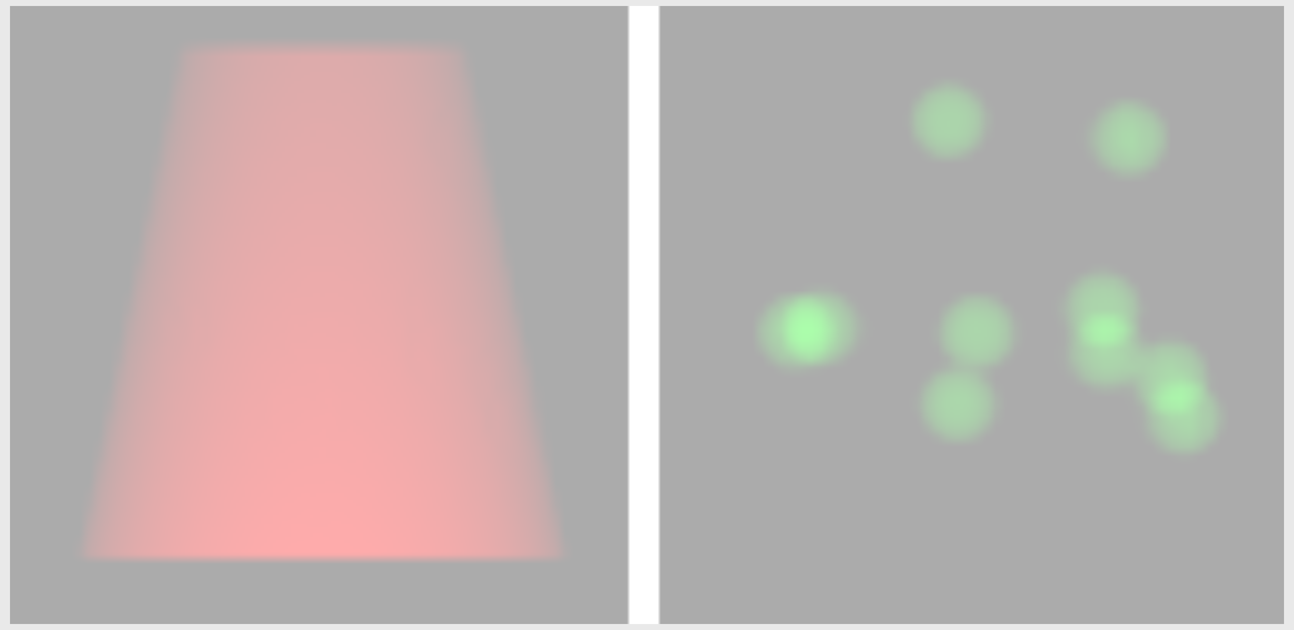
3D reconstruction of quantitative elemental map using automatic differentiation with self-absorption correction model

Compress the bit depth



Compress the dimension





Compress the dataset - How could the noise statistics “help”?

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- Save the disk space:
  many GBs of data to reconstruct few MBs of images
- Speed up the data transfer:
  faster frame rates are needed for the future
  Potential data generation rate > Data transfer rate

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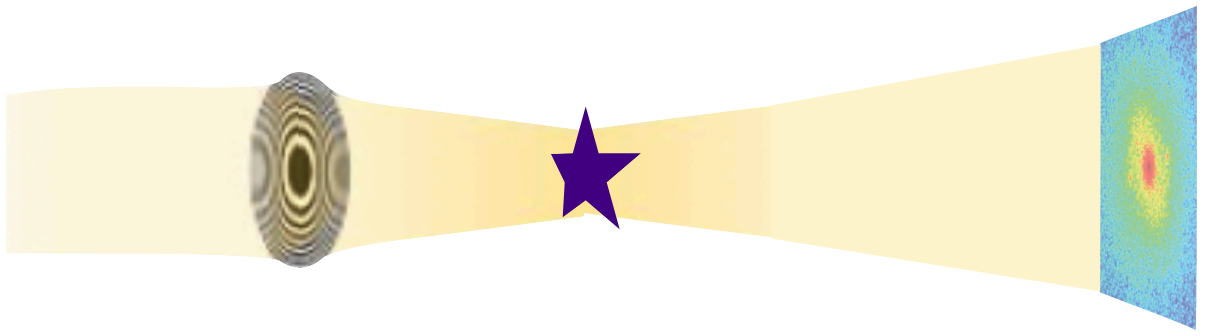
What kind of dataset?

X-ray image dataset: Ptychography

- Coherent diffraction imaging (CDI)
- Retrieve the ***object function*** of the sample from its far-field diffraction **intensity**
  - object function :

$$\begin{aligned} o(\mathbf{r}) &= \exp\left[k(i\delta-\beta)t(\mathbf{r})\right] \\ &= \underbrace{\exp\left[ik\delta t(\mathbf{r})\right]}_{\text{Phase}}\underbrace{\exp\left[-k\beta t(\mathbf{r})\right]}_{\text{Attenuation}} \end{aligned}$$



$$\psi(\mathbf{r}) = p(\mathbf{r})o(\mathbf{r}) \qquad I = |\mathcal{F}\{\psi\}|^2$$

$$\psi(\mathbf{r}) \;\not\longleftarrow\; \mathcal{F}^{-1}\{\sqrt{I}\}$$

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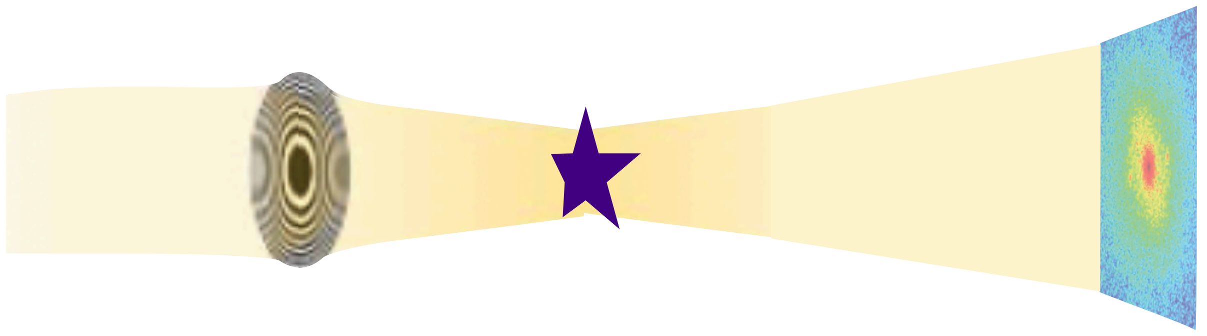
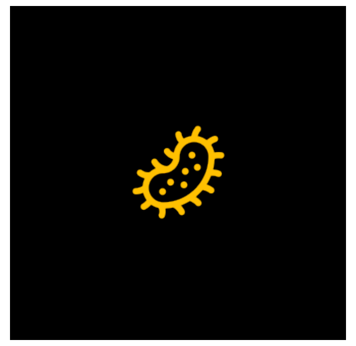


$\psi(\mathbf{r}) = p(\mathbf{r})o(\mathbf{r})$ $\quad I = |\mathcal{F}\{\psi\}|^2$

- “Small object” probe



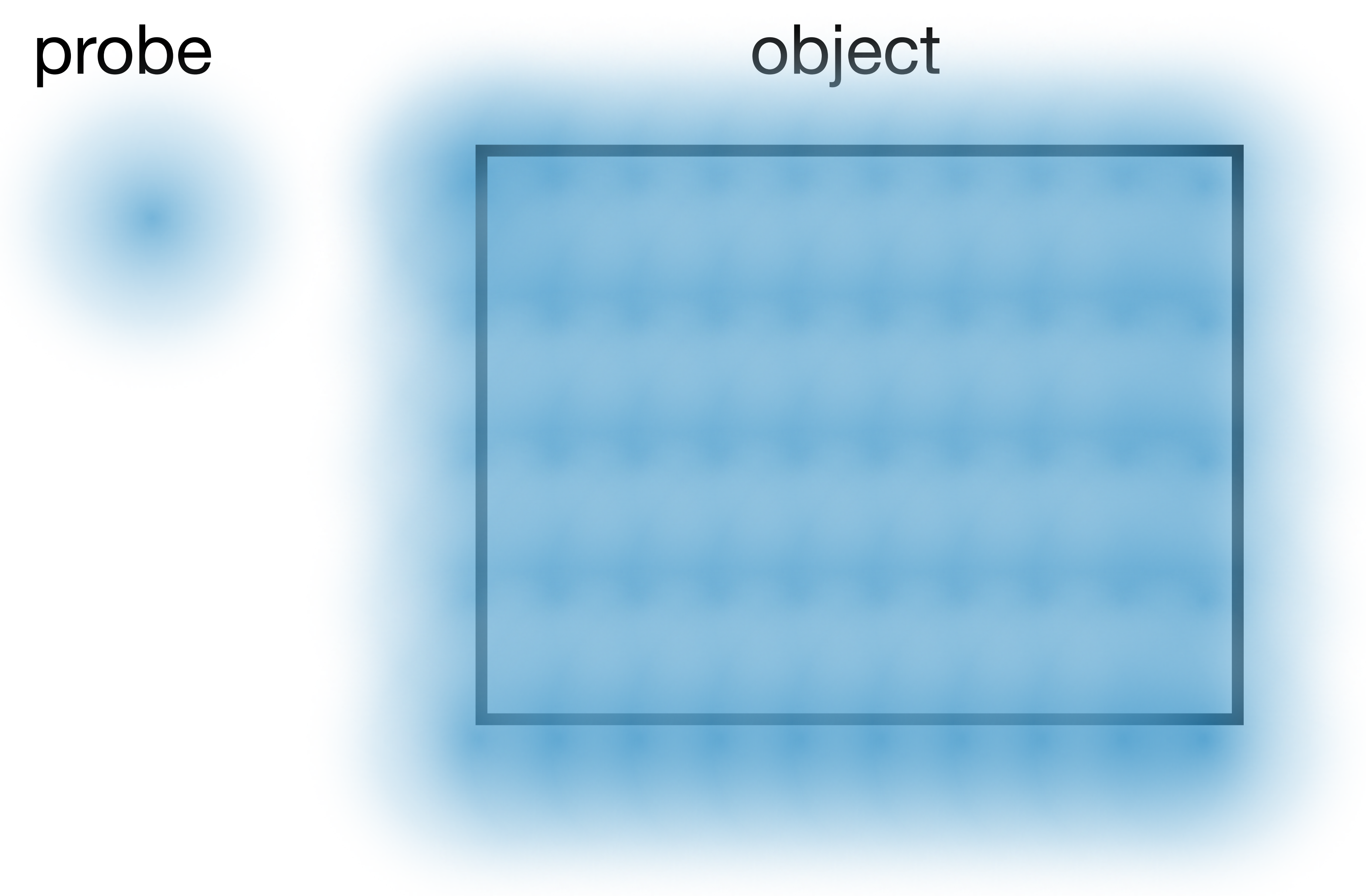
$\psi(\mathbf{r}) \not\leftarrow \mathcal{F}^{-1}\{\sqrt{I}\}$

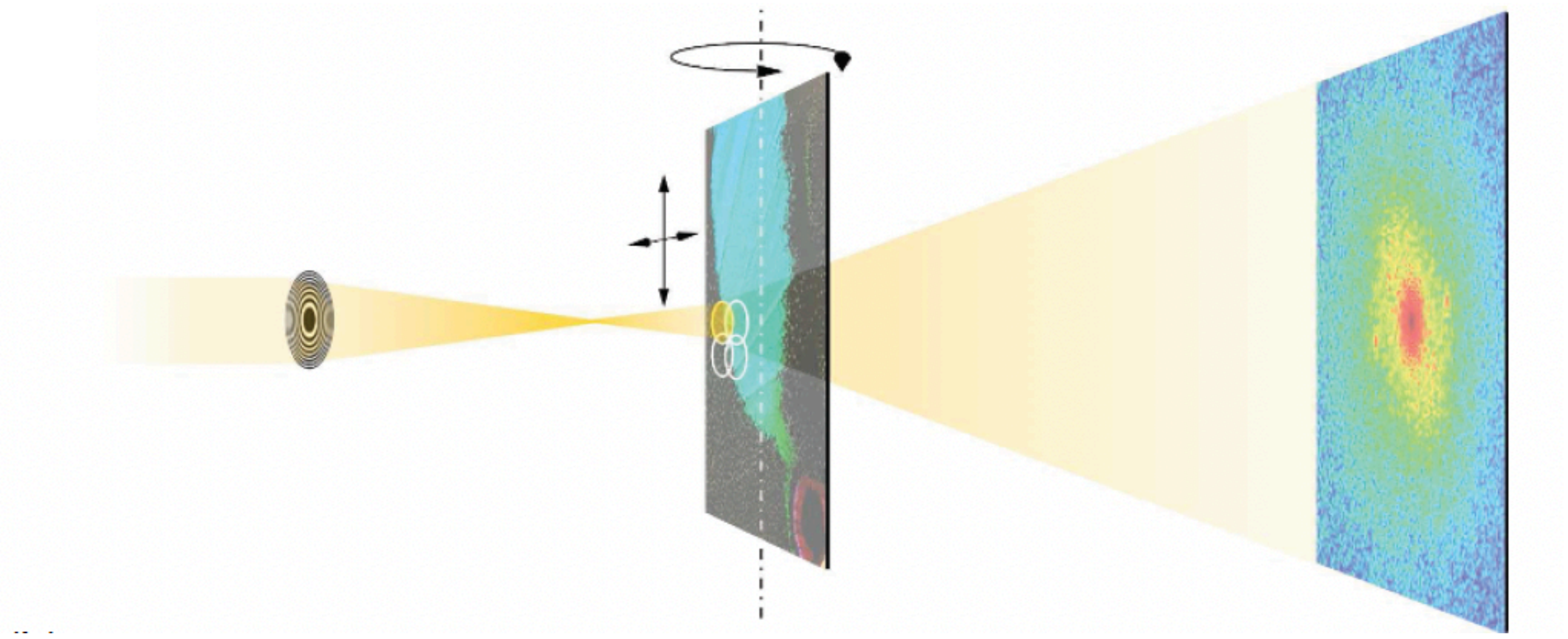
Fienup algorithm:
Iterative method of retrieving the phase

- “Large object” ?

Ptychography

Ptychography





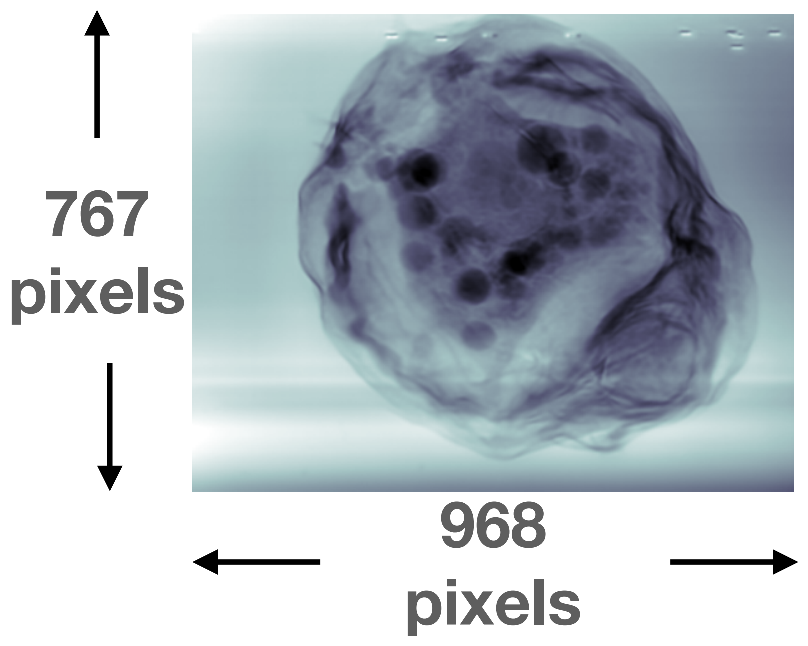
$$\psi_j = p(\mathbf{r} - \mathbf{r}_j)o(\mathbf{r}) \qquad I_j = |\mathcal{F}\{\psi_j\}|^2$$

- Use large overlapping area between probes to retrieve the object function
- Object function can be solved iteratively
- Huge data size compared to the object size to be solved.
- Example [1]:

Number of scanning positions: $201 \times 221 = 44{,}421$

Each diffraction pattern: 256^2 pixels, 16-bit data

$$\frac{\text{data size}}{\text{object size}} = \frac{5.18 \text{ GBs}}{1.4 \text{ MBs}} = 3740$$



[1] Deng, J. *et al.*, Scientific Reports, **7**(1), 445 (2017)

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How do we do this?

- Noise statistics helps
  ✓ Finite exposure time -> Stochastic noise (Poisson distribution)

  x Thermal noise in a detector
  x Optics imperfections
  x Other instrumentation noise

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Our approach:

- Poisson distribution

$$P(x; N) = \frac{N^x e^{-N}}{x!}$$

$$\text{mean} \;\; = N$$
$$\text{standard deviation } \sigma = \sqrt{N}$$

- Convert the measured photon counts N into N':

$$|N' - N| \leq \sigma$$

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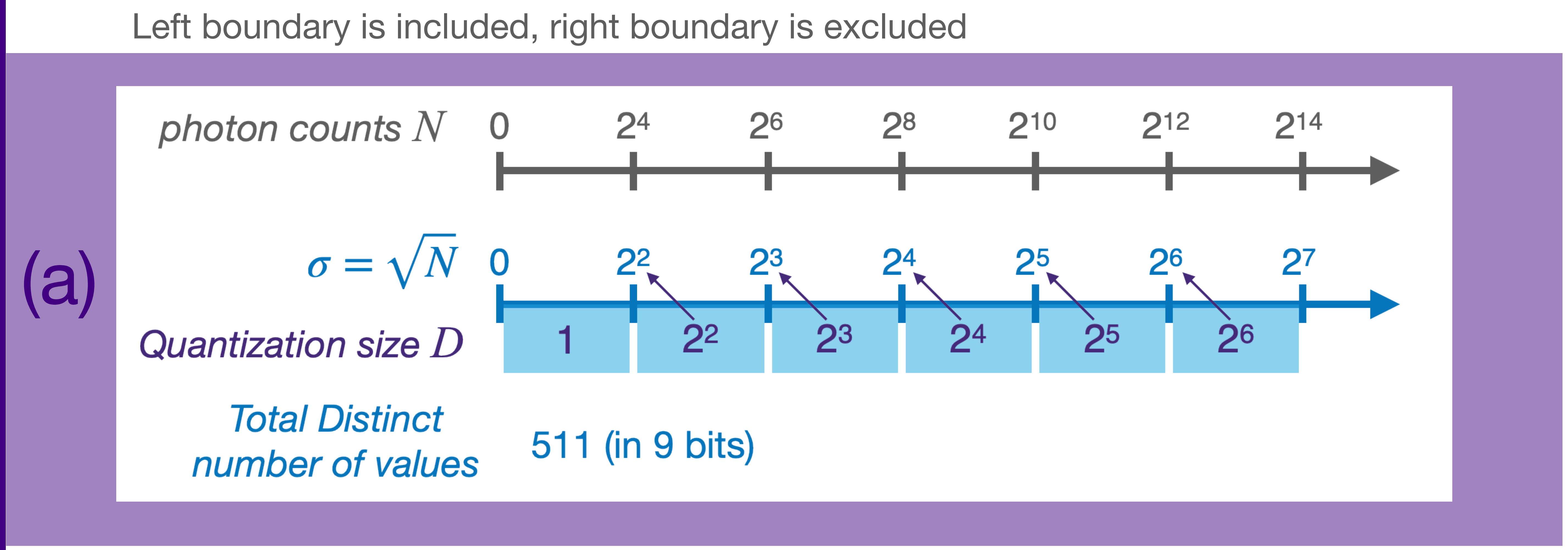

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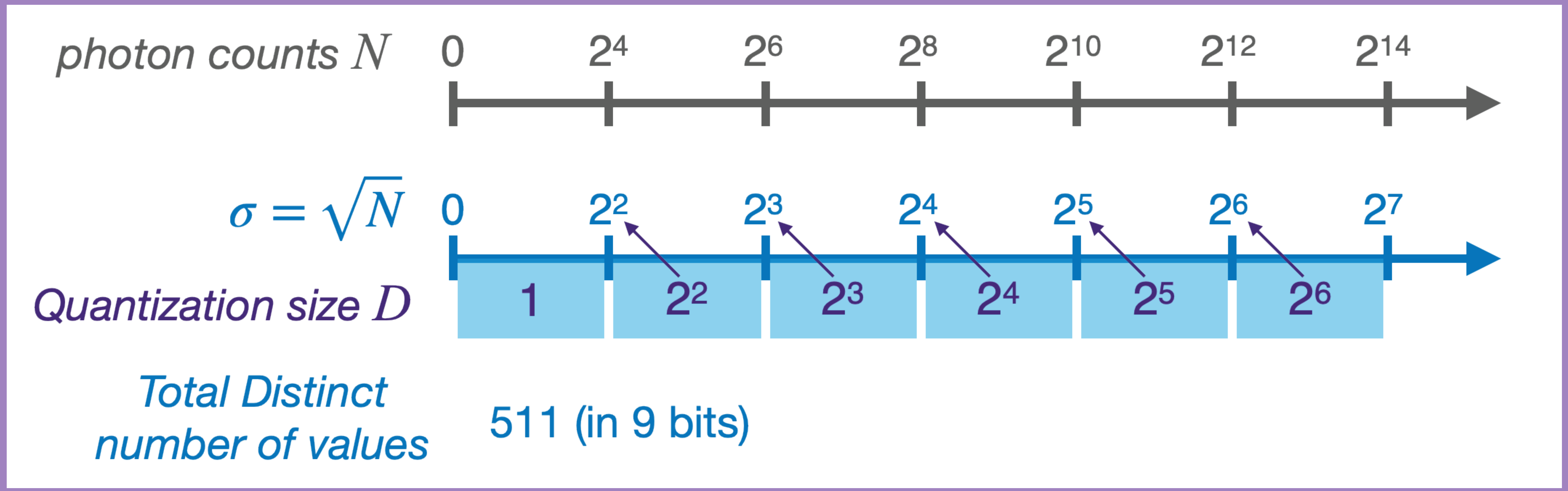
Left boundary is included, right boundary is excluded

(a)



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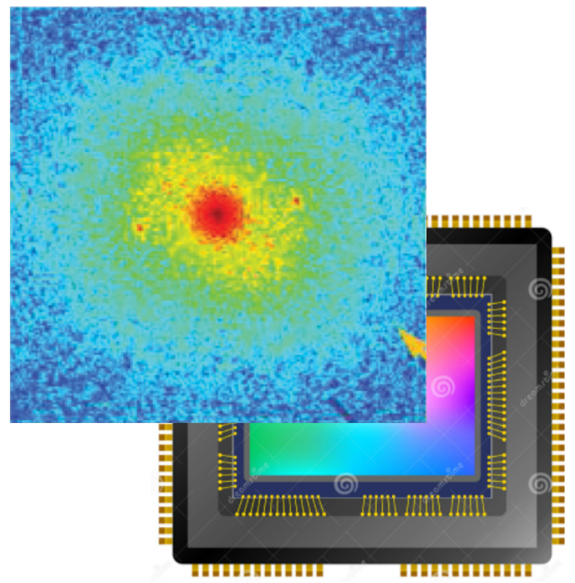
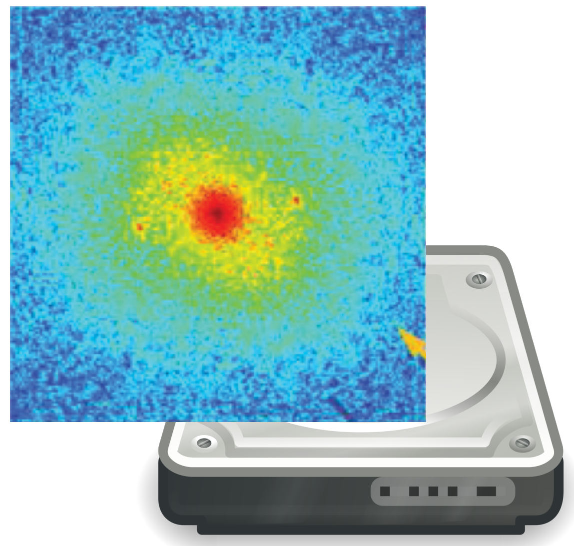


$N = 0 \text{ to } 2^{14} - 1$

D_r and F_r are both 2[int]
Division and addition are easy to be implemented on binary data

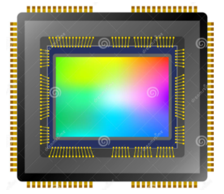


N'

Reconstruction

Encoding

$$M = \text{floor}(\frac{N}{D_r}, 1) + F_r$$



$M = 0 \text{ to } 2^9 - 1$

Decoding

$$N' = (M - F_r)D_r$$

Numerical optimization-based reconstruction

Unknown model parameters → Construct a forward model → Define loss function → Optimization

Ptychography

Data $\hat{y}(\mathbf{r})$

$p(\mathbf{r}-\mathbf{r}_p)$

$o(\mathbf{r})$

Forward model

$|\mathscr{F}\{p(\mathbf{r}-\mathbf{r}_p)\, o(\mathbf{r})\}|^2$

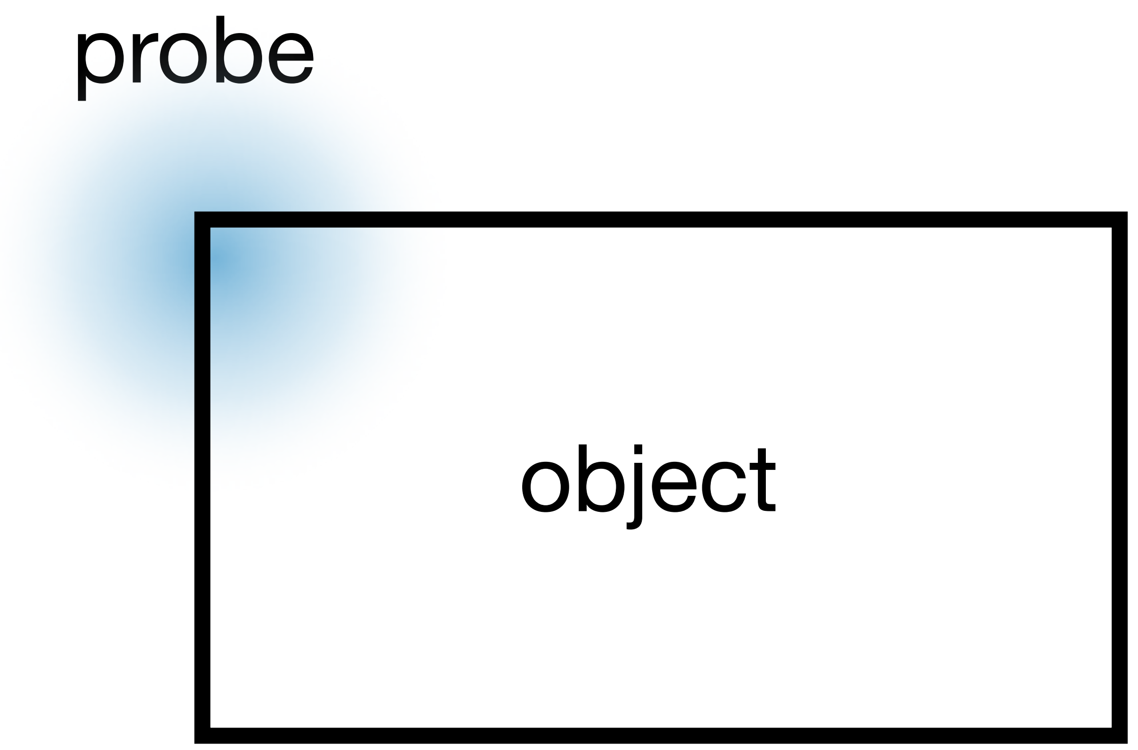
$y(\mathbf{r})$

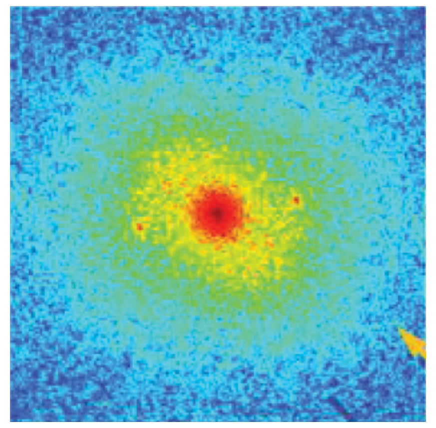
$L(\mathbf{r})$

e.g., gradient descent

$$p^{k+1}(\mathbf{r}-\mathbf{r}_p) = p^k(\mathbf{r}-\mathbf{r}_p) - \eta \frac{\partial L}{\partial p^k(\mathbf{r}-\mathbf{r}_p)}$$

$$o^{k+1}(\mathbf{r}) = o^k(\mathbf{r}) - \eta \frac{\partial L}{\partial o^k(\mathbf{r})}$$





Numerical optimization-based reconstruction

Unknown model parameters → Construct a forward model → Define loss function → Optimization

PyTorch

Automatic differentiation

Ptychography

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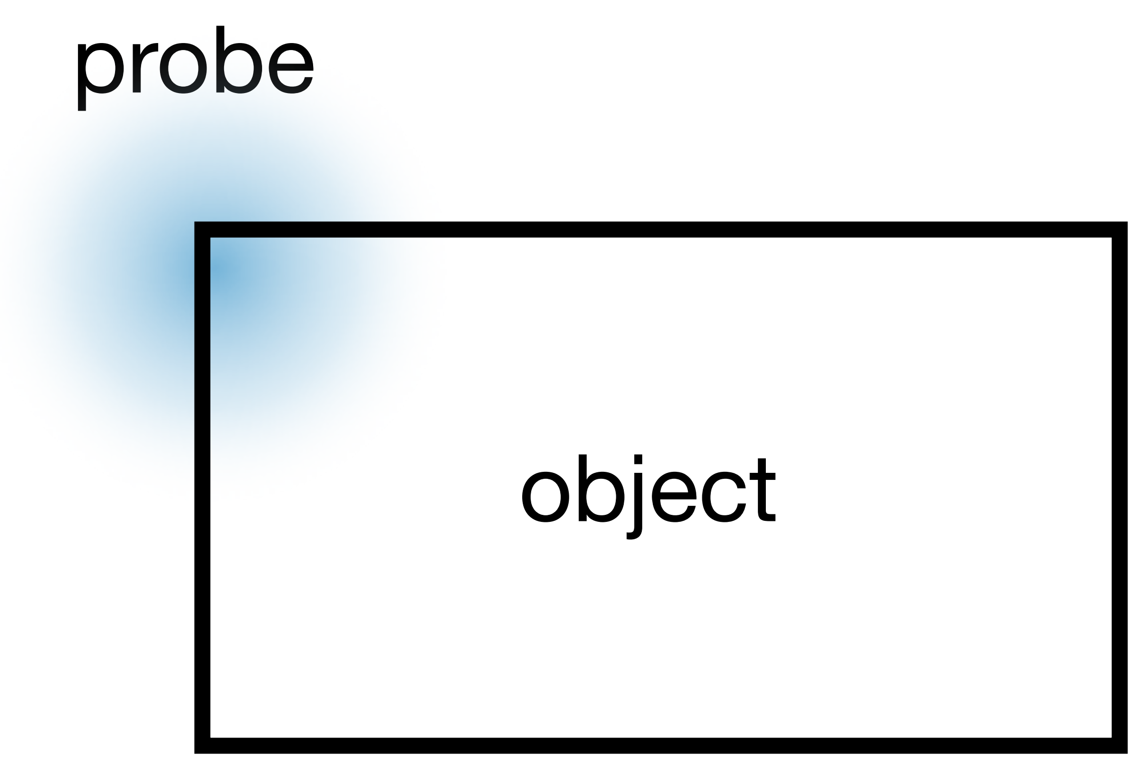

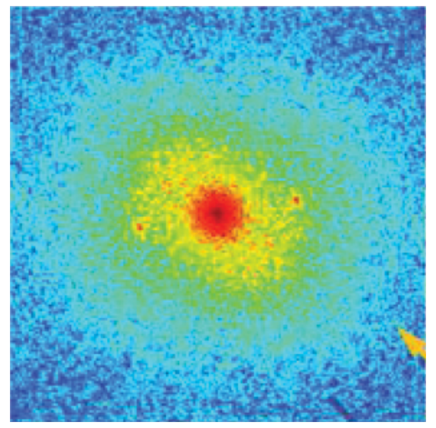

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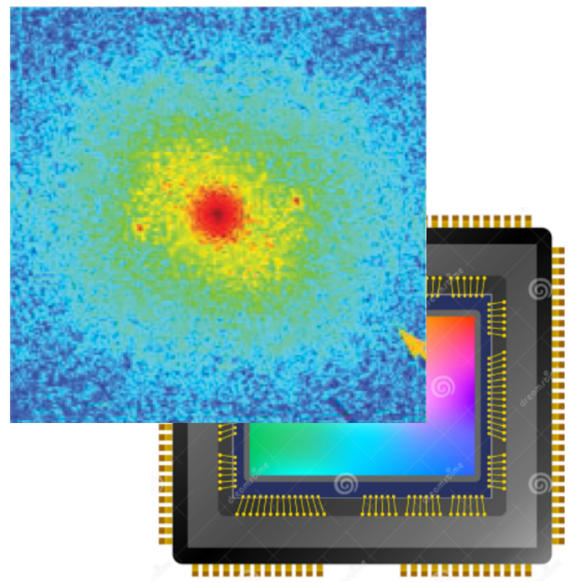
(a)

photon counts N	0	2^4	2^6	2^8	2^{10}	2^{12}	2^{14}
$\sigma = \sqrt{N}$	0	2^2	2^3	2^4	2^5	2^6	2^7
Quantization size D	1	2^2	2^3	2^4	2^5	2^6	
Total Distinct number of values	511 (in 9 bits)						

PyTorch

Adorym : Automatic Differentiation-based Object Reconstruction with DynaMical Scattering

Du, M. *et al.,* Optics Express, **29**(7), 10000 (2021).



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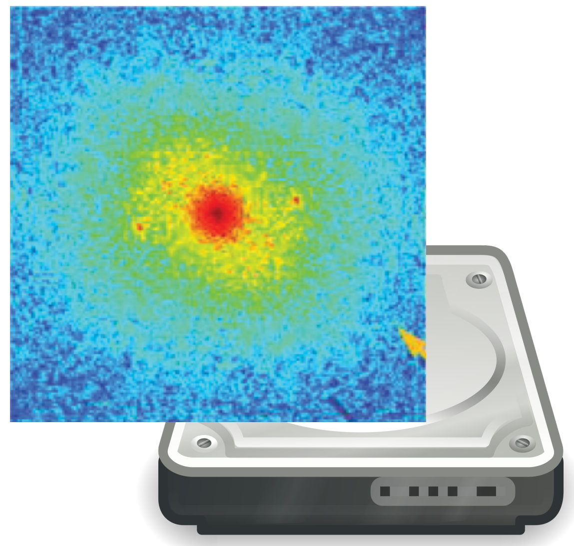

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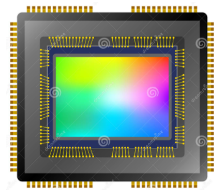

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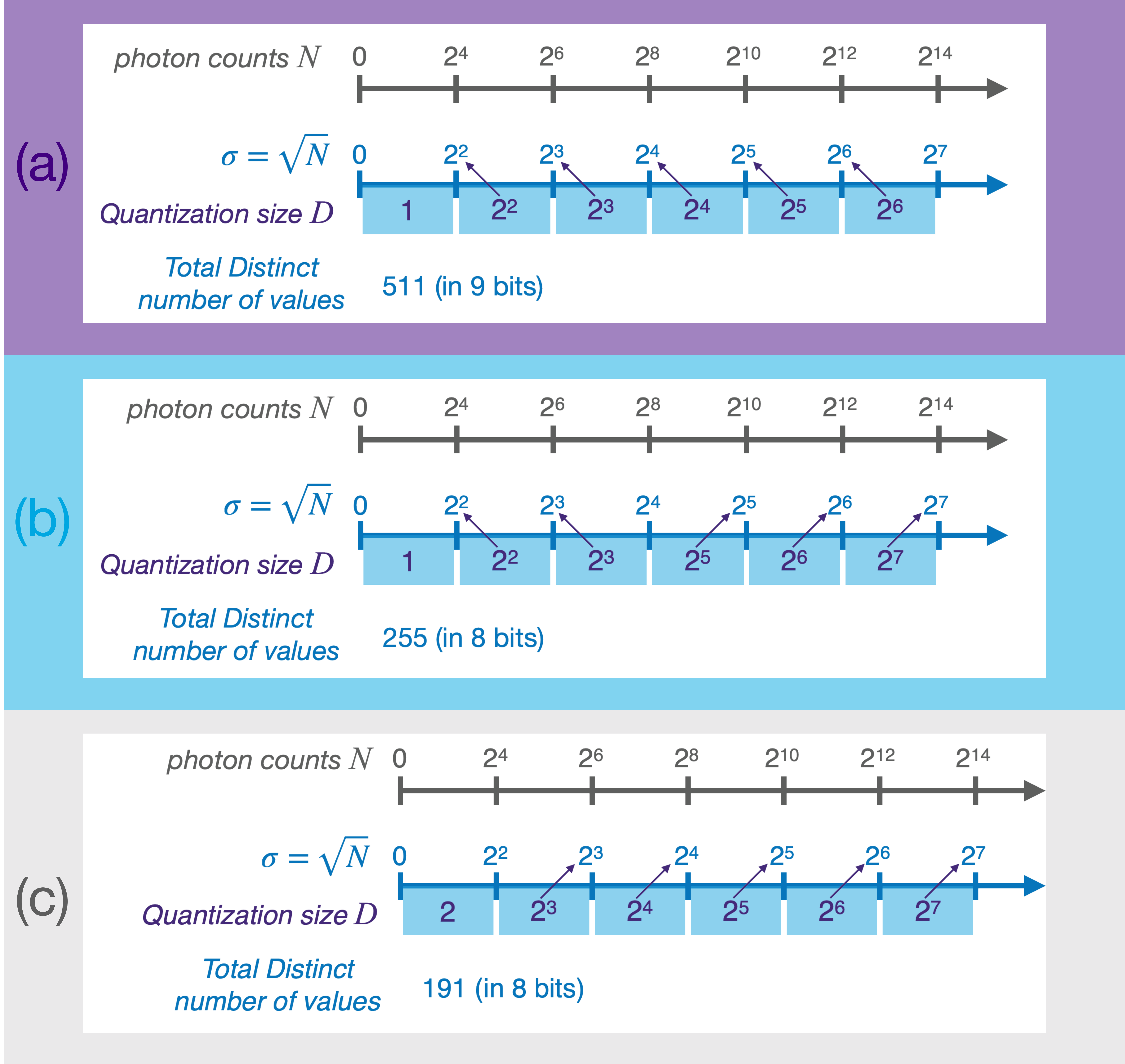
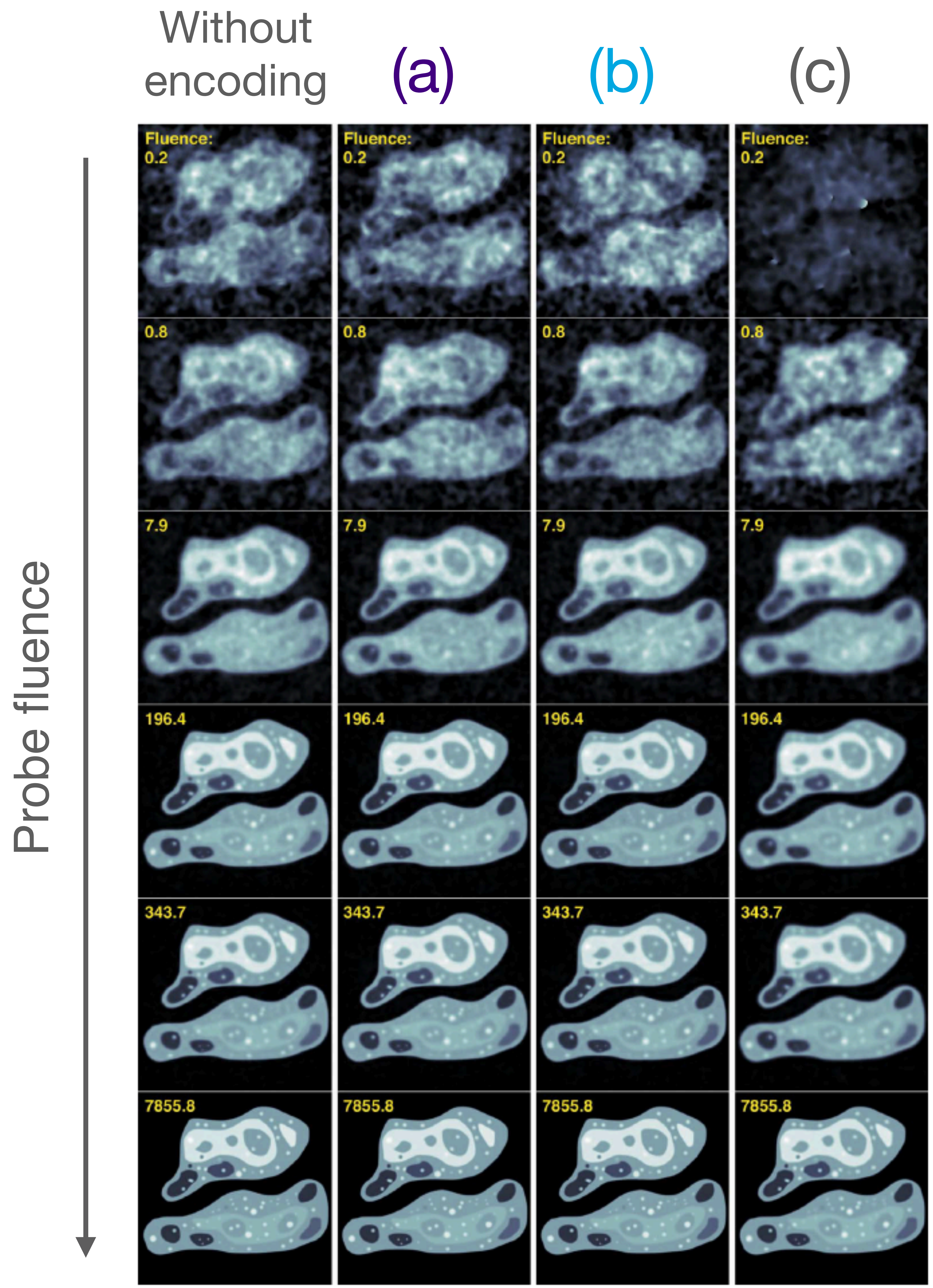
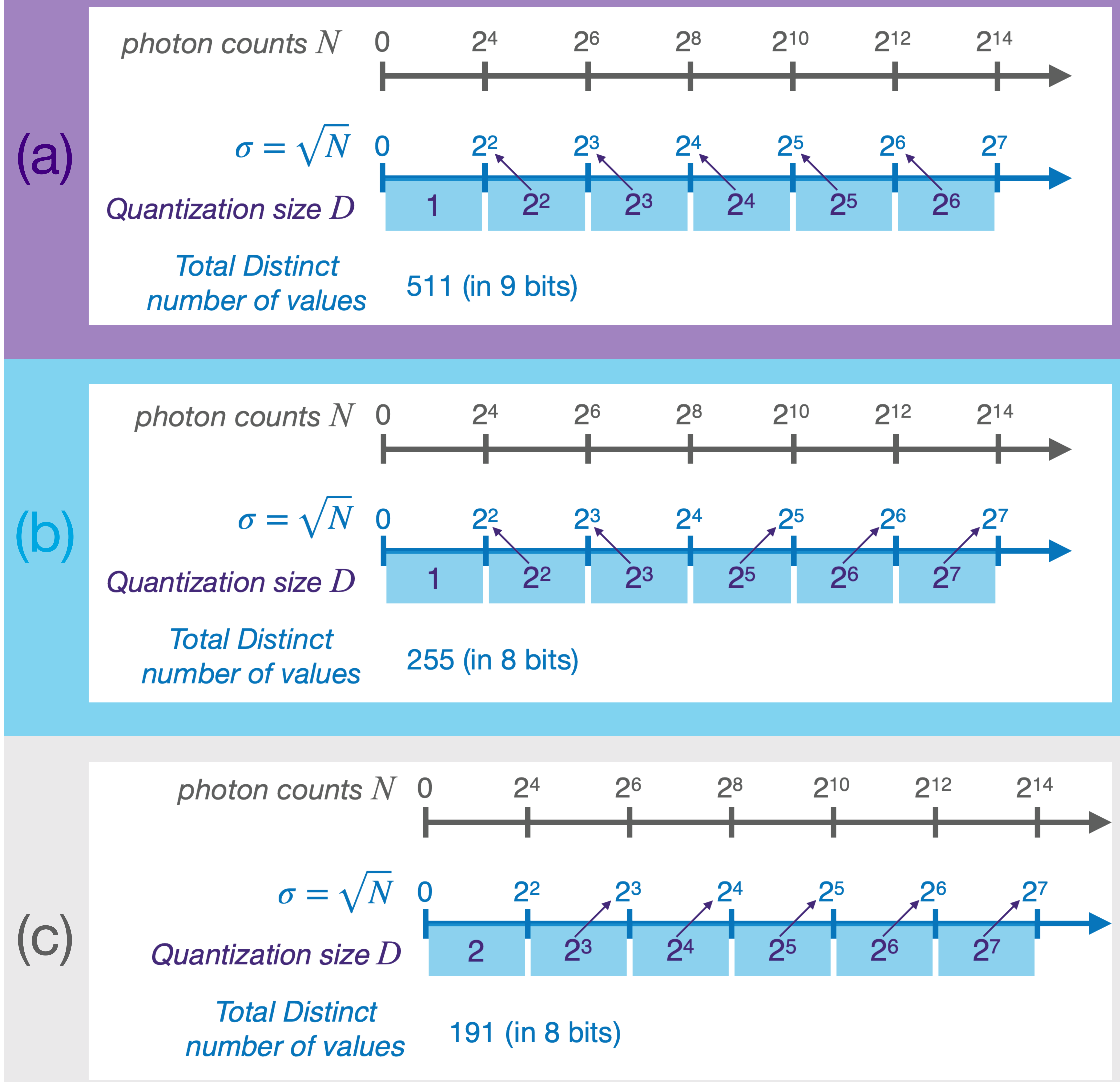
What do we achieve?

- compress the data bit depth from 14 bits to 9 or 8 bits without sacrificing the resolution



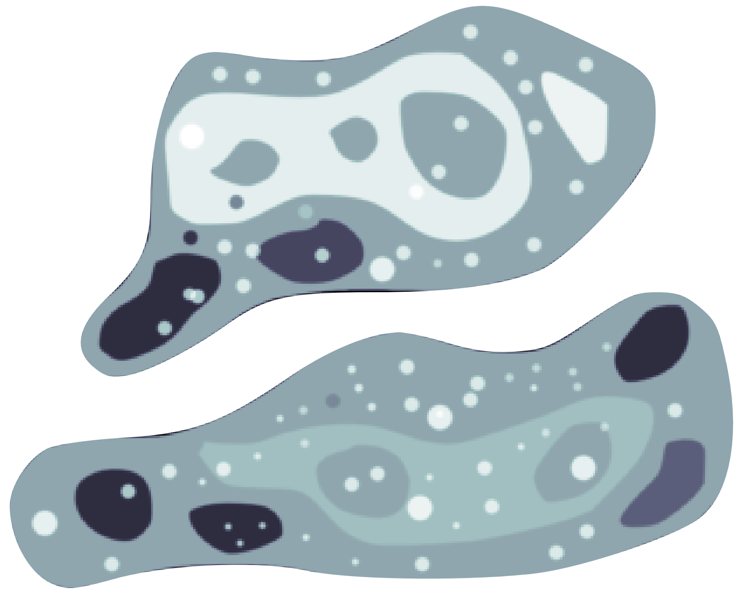

Without encoding
(a)
(b)
(c)
Probe fluence
Fluence: 0.2
0.8
7.9
196.4
343.7
7855.8


(a)
photon counts N
0 2^4 2^6 2^8 2^{10} 2^{12} 2^{14}
$\sigma = \sqrt{N}$
0 2^2 2^3 2^4 2^5 2^6 2^7
Quantization size D
1 2^2 2^3 2^4 2^5 2^6
Total Distinct number of values
511 (in 9 bits)
(b)
photon counts N
0 2^4 2^6 2^8 2^{10} 2^{12} 2^{14}
$\sigma = \sqrt{N}$
0 2^2 2^3 2^4 2^5 2^6 2^7
Quantization size D
1 2^2 2^3 2^5 2^6 2^7
Total Distinct number of values
255 (in 8 bits)
(c)
photon counts N
0 2^4 2^6 2^8 2^{10} 2^{12} 2^{14}
$\sigma = \sqrt{N}$
0 2^2 2^3 2^4 2^5 2^6 2^7
Quantization size D
2 2^3 2^4 2^5 2^6 2^7
Total Distinct number of values
191 (in 8 bits)

Metric for reconstructed images - Within-support mean-squared error

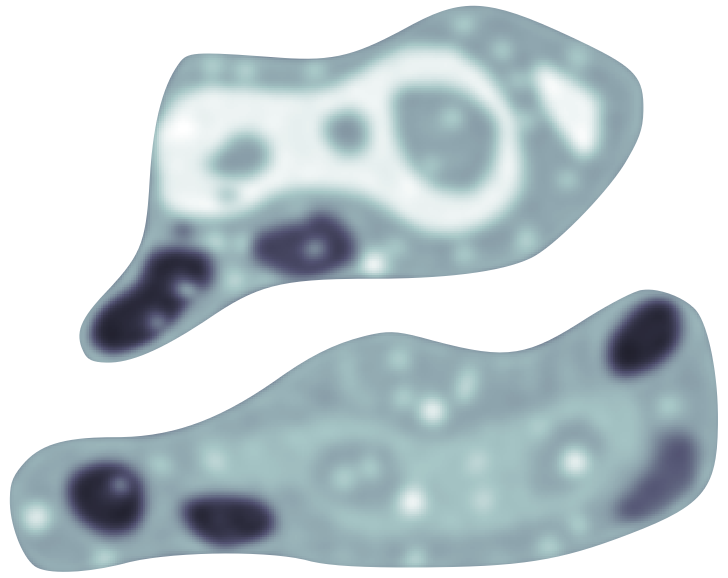
Ground truth

Within-Support

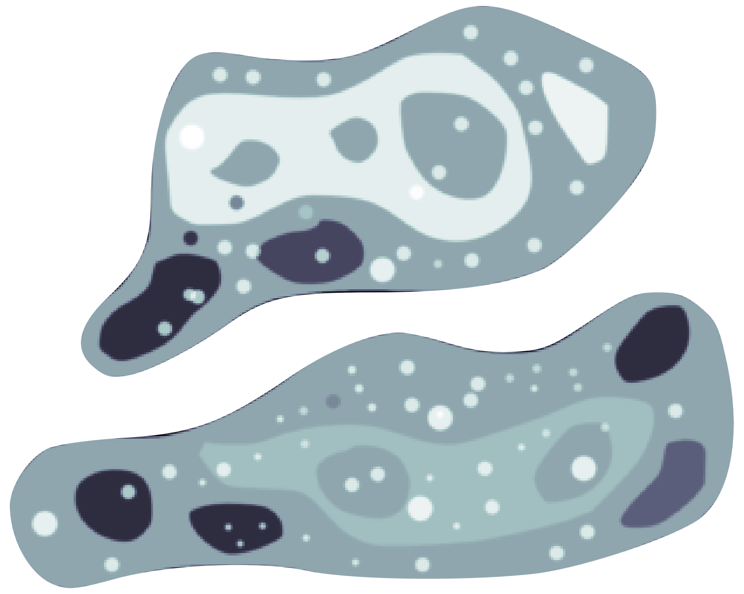


- Within-support mean-squared error (SMSE)

Σ (



-



$)^2$

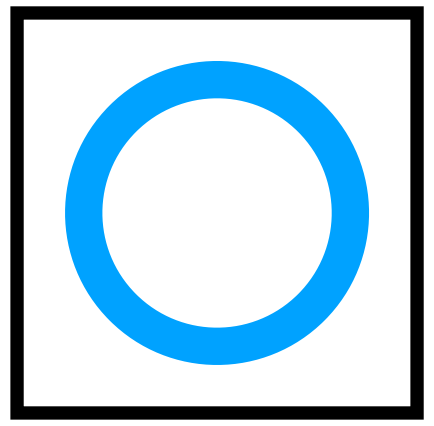
SMSE = ―――――――――――――――――――――――――――――――

number of pixels within the support

Metric for resolution: Fourier ring correlation (FRC) half-bit threshold

$F_1(\mathbf{u}) = \mathscr{F}\{$  $\}$

$F_1(\mathbf{u} = u_i)$

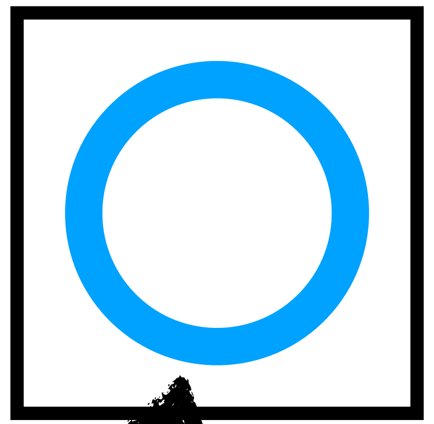


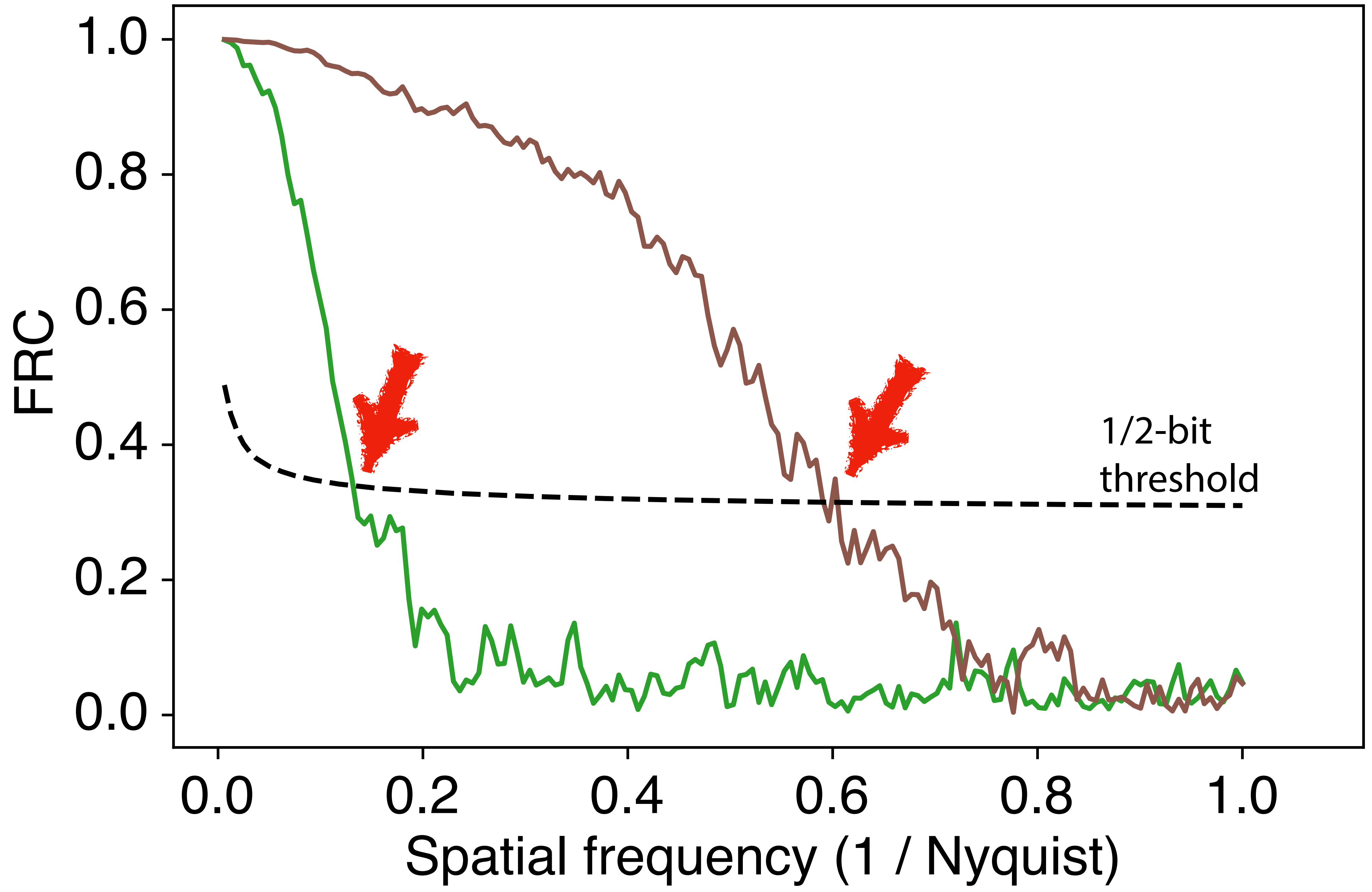
$$\mathrm{FRC}_{1,2}(u_i) = \frac{\sum_{|\boldsymbol{u}|=u_i} F_1(\boldsymbol{u}) \cdot F_2(\boldsymbol{u})^\dagger}{\sqrt{\sum_{|\boldsymbol{u}|=u_i} F_1^2(\boldsymbol{u}) \cdot \sum_{|\boldsymbol{u}|=u_i} F_2^2(\boldsymbol{u})}}$$

Same object, different noise instances

$F_2(\mathbf{u}) = \mathscr{F}\{$  $\}$

$F_2(\mathbf{u} = u_i)$



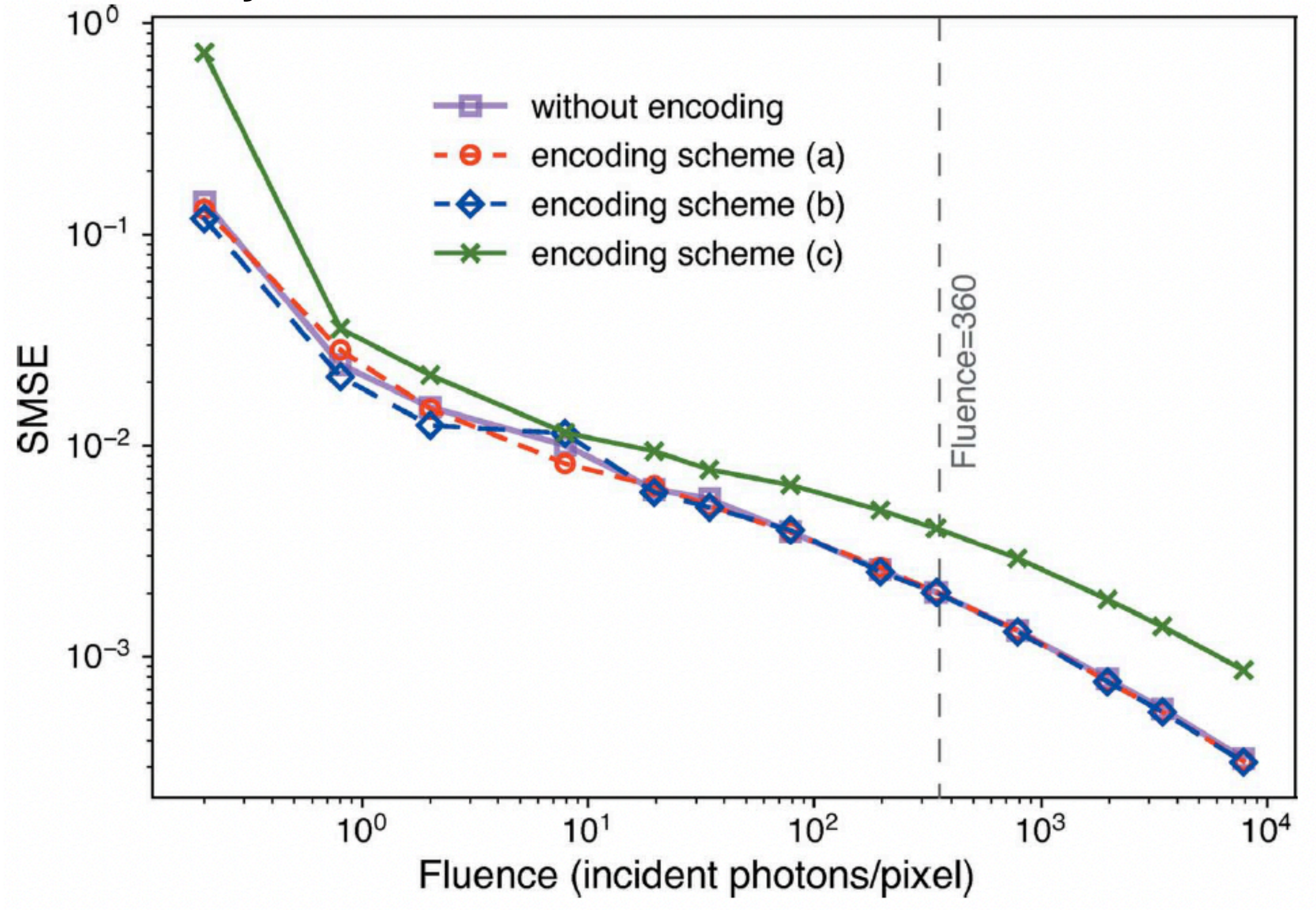


Mask in Fourier space
(on the far-field diffraction plane)

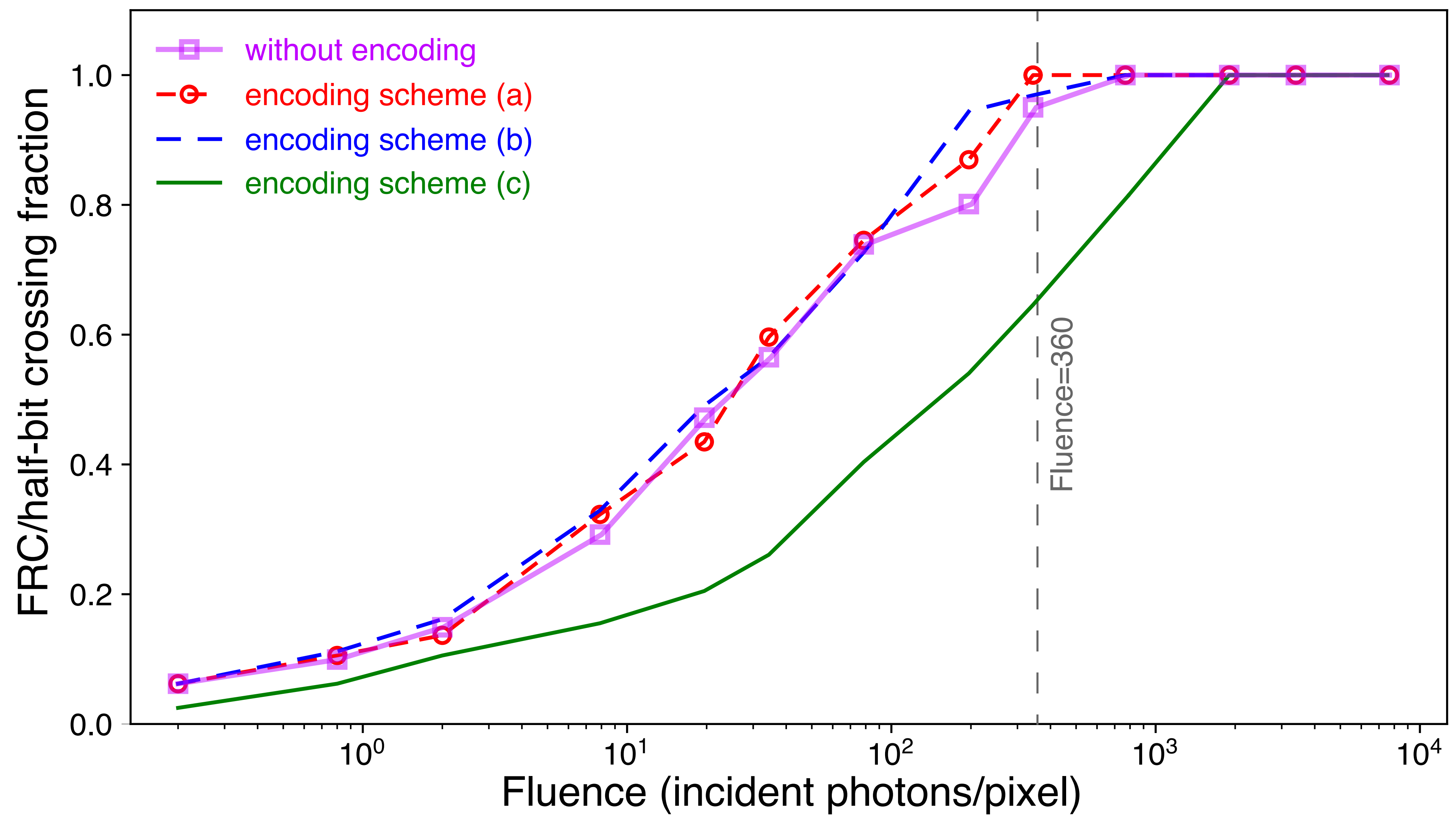
Object should correlate; noise should not

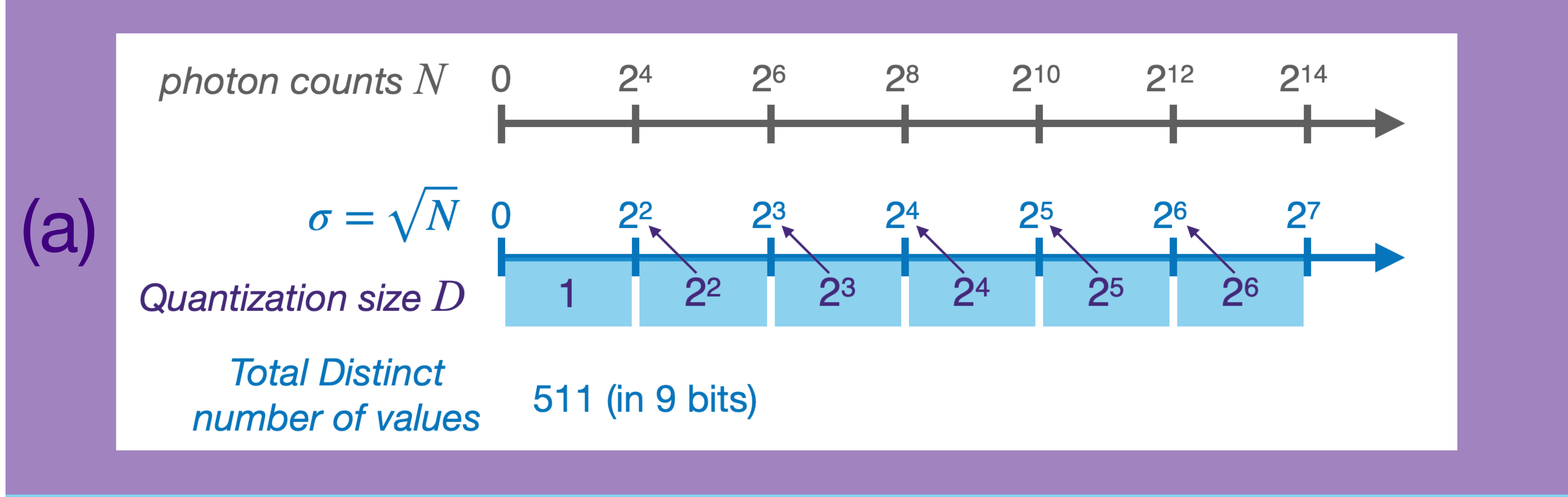
$$\text{Nyquist} = u_{\max} = \frac{1}{2\Delta_p}$$

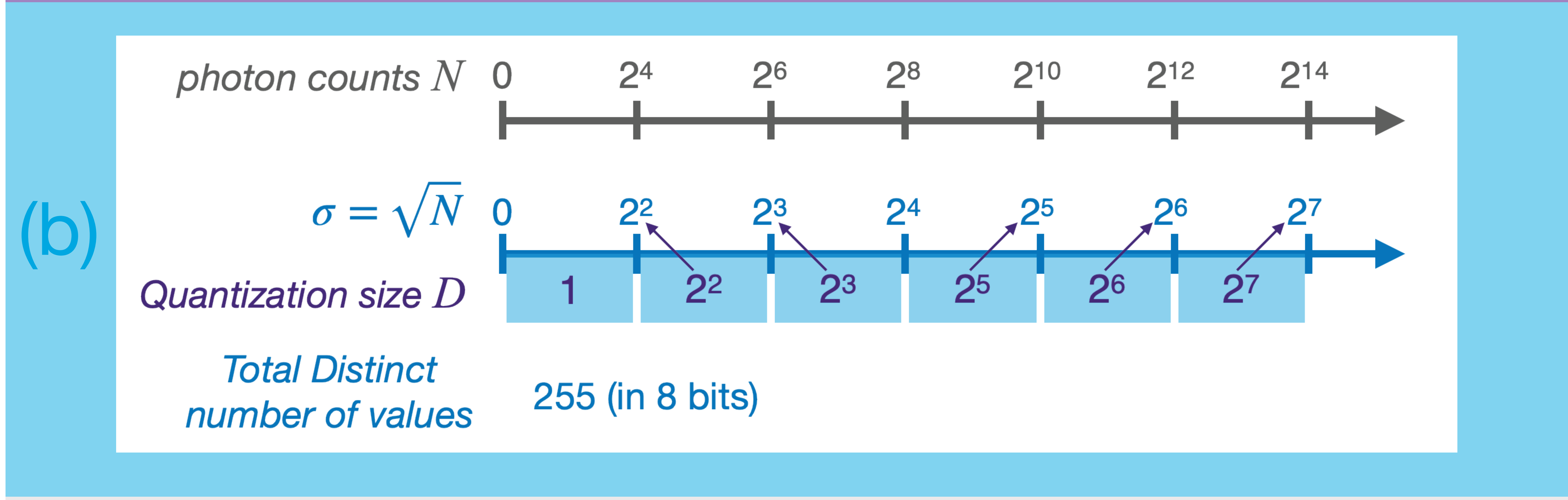
Object correctness

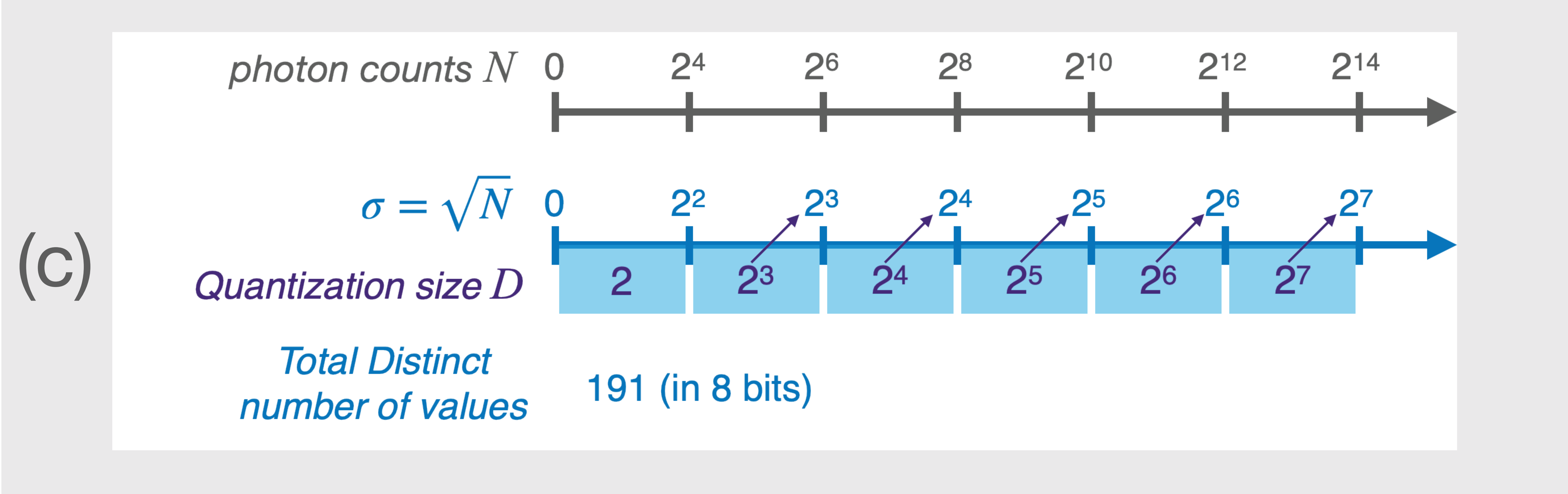


Diffraction correlation



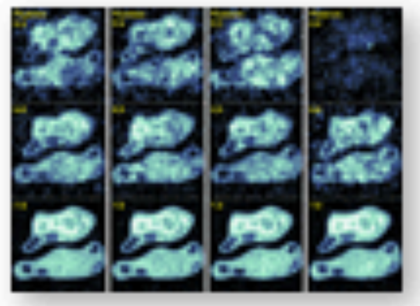






RESEARCH PAPERS

J. Synchrotron Rad. (2021). **28**, 292-300
https://doi.org/10.1107/S1600577520013326



Fast digital lossy compression for X-ray ptychographic data

P. Huang, M. Du, M. Hammer, A. Miceli and C. Jacobsen

Increases in X-ray brightness from synchrotron light sources lead to a requirement for higher
photon counting. However, transfer of the full uncompressed data will begin to constrain dete
that is easy to implement in a HPAD's application-specific integrated circuit (ASIC) is describe
employed coherent imaging method, is examined. Using adaptive encoding quantization, it is
information) using only 8 or 9 bits for data transfer, with negligible effect on the reconstructe

Keywords: X-ray ptychography; pixel array detectors; lossy compression.

Journal of Instrumentation

Strategies for on-chip digital data compression for X-ray pixel detectors

M. Hammer[1], K. Yoshii[1] and A. Miceli[1]

Published 25 January 2021 •

Journal of Instrumentation, Volume 16, January 2021

Citation M. Hammer *et al* 2021 *JINST* **16** P01025

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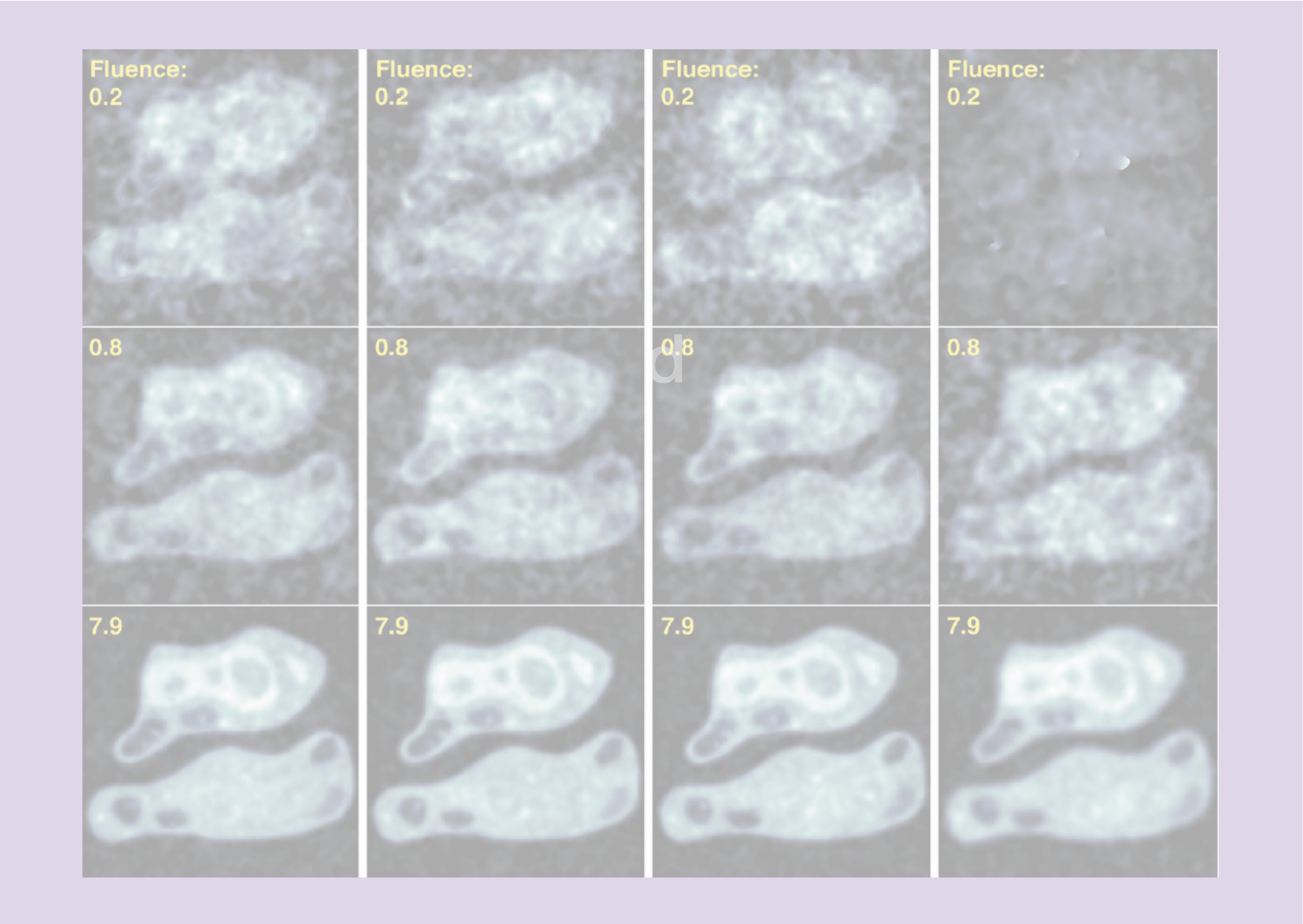
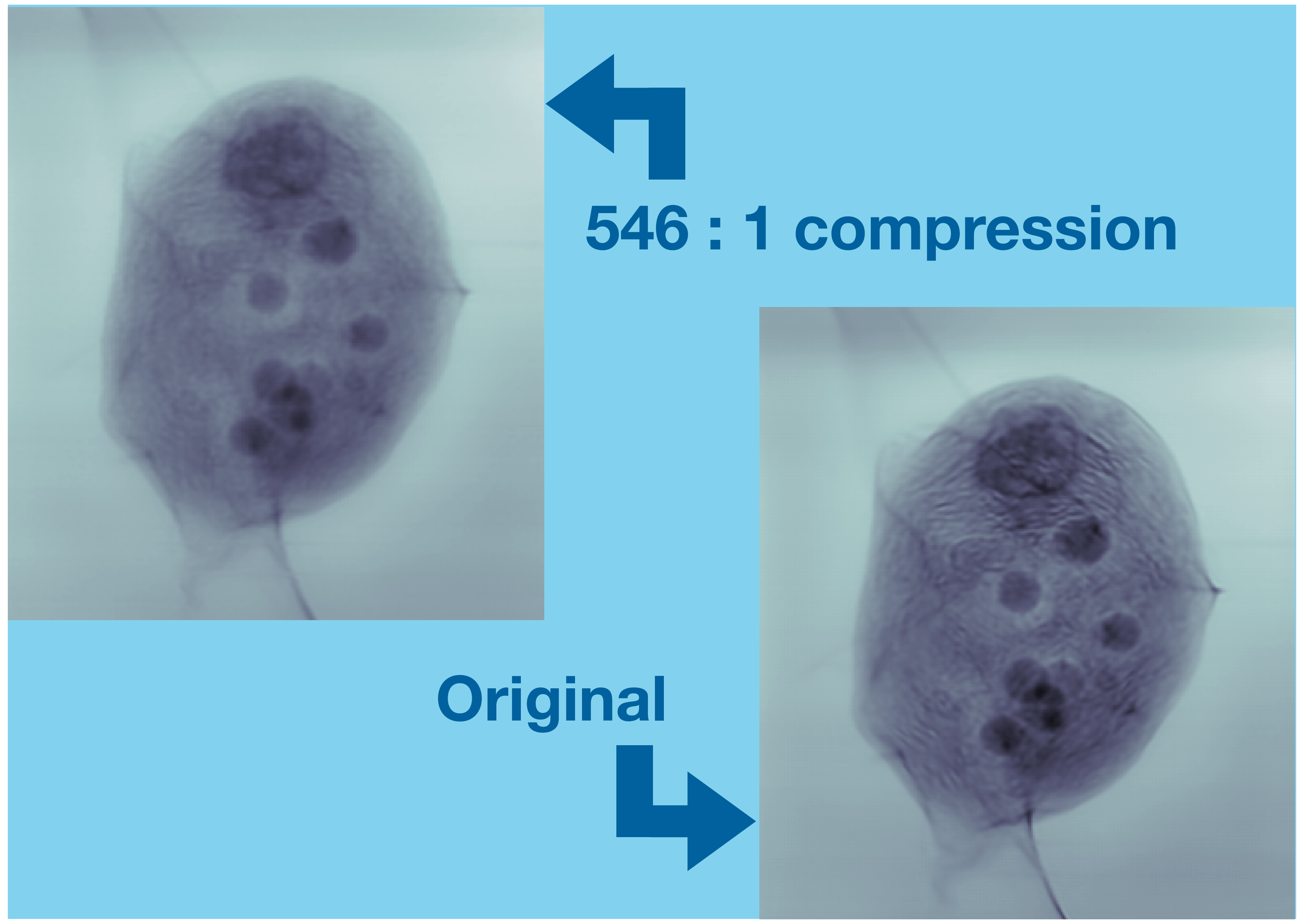
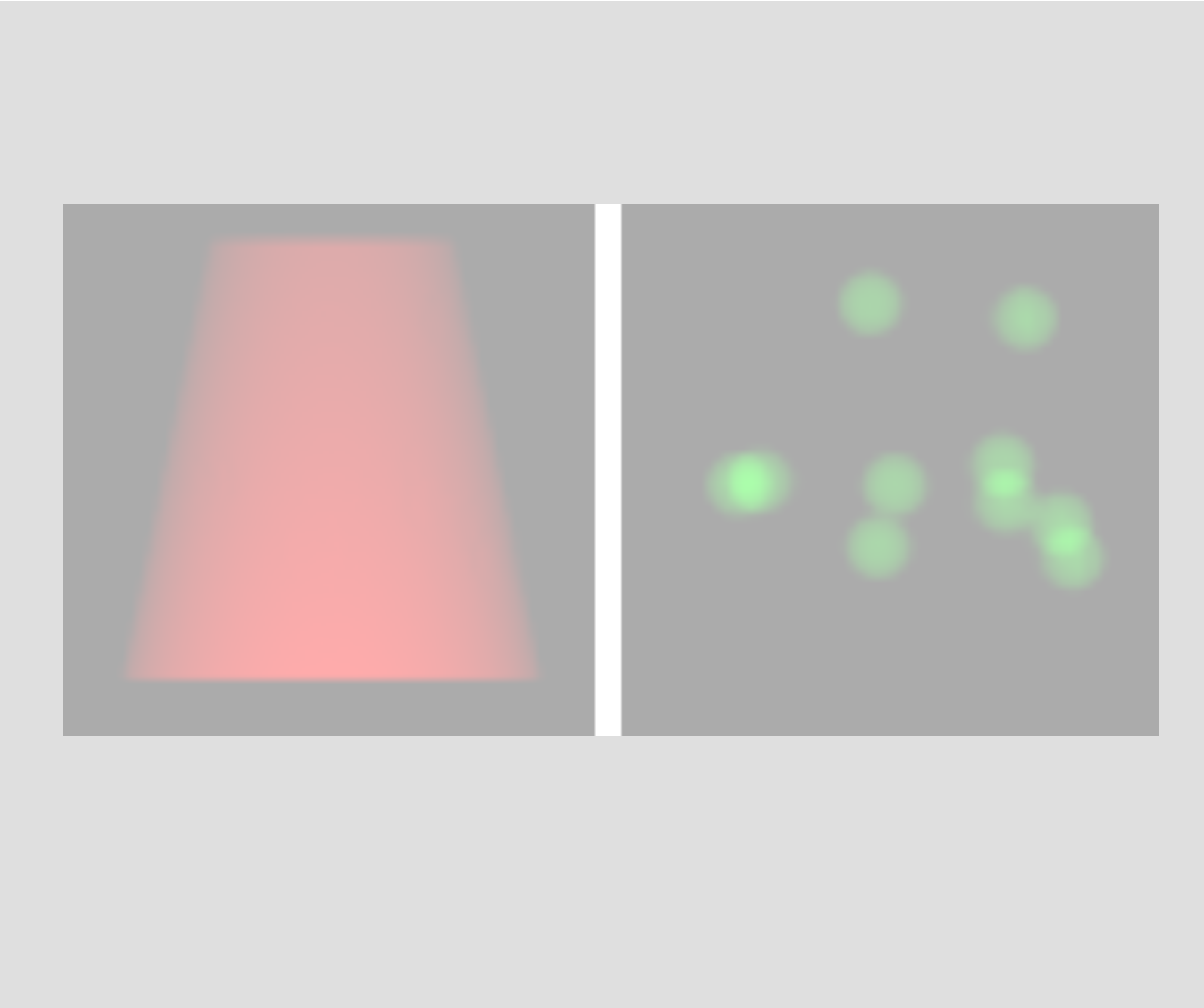


Compress the dimension



with self-absorption correction model



Compress the dataset - dimension reduction

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How do we do this?

- Principal component analysis (PCA)
  - Using PCA but requiring the entire dataset

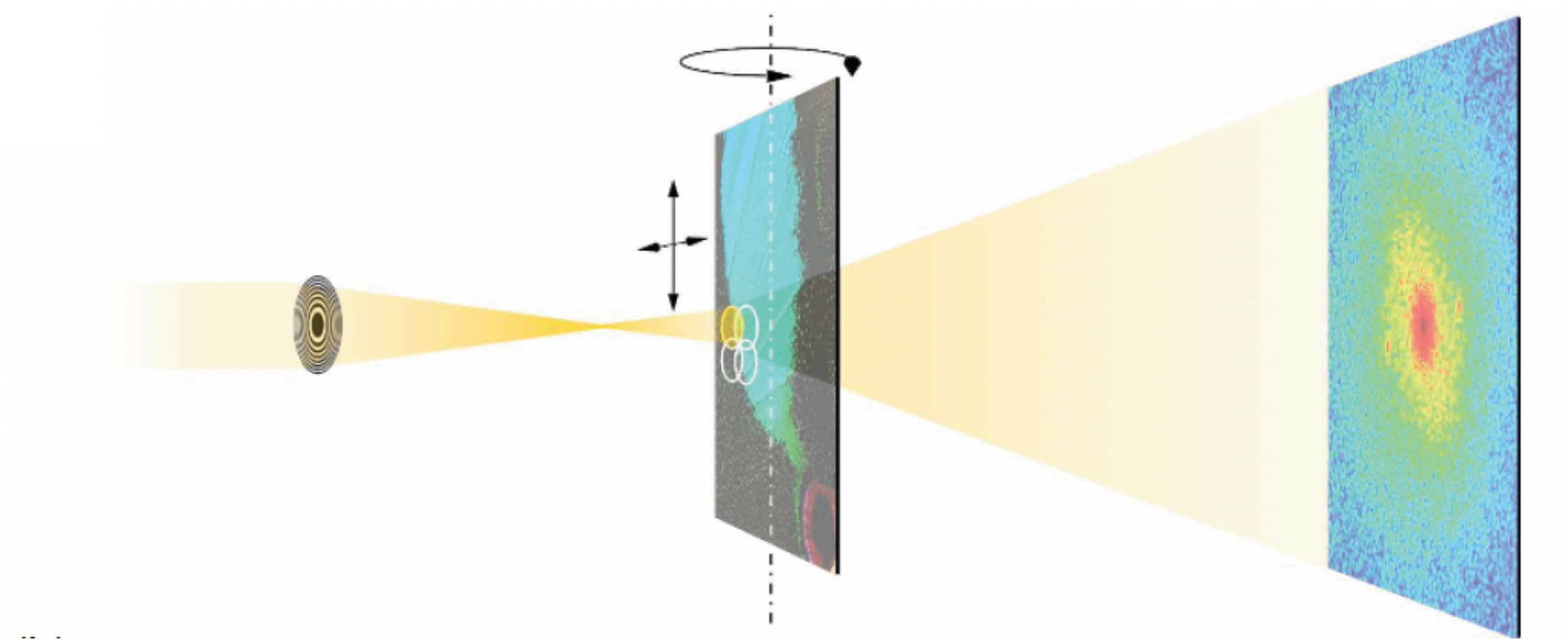
Lars Loetgering*, Max Rose, David Treffer, Ivan A. Vartanyants, Axel Rosenhahn and Thomas Wilhein

Data compression strategies for ptychographic diffraction imaging

Loetgering *et al.*, Advanced Optical Technologies, **6**(6), 475 (2017)

Ptychography

Far-field diffraction pattern

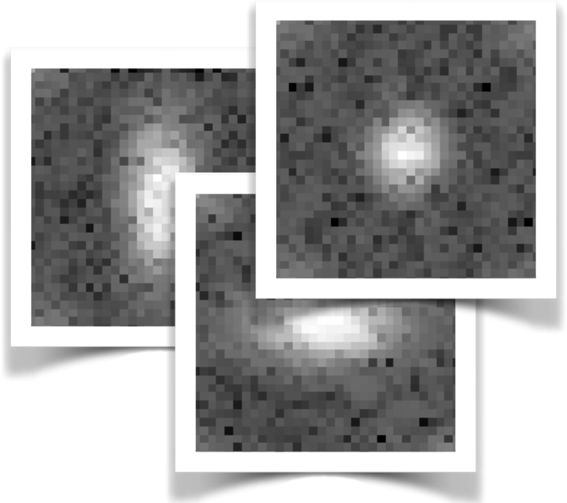


$$\psi_j = p(\mathbf{r} - \mathbf{r}_j)o(\mathbf{r}) \qquad I_j = |\mathcal{F}\{\psi_j\}|^2$$

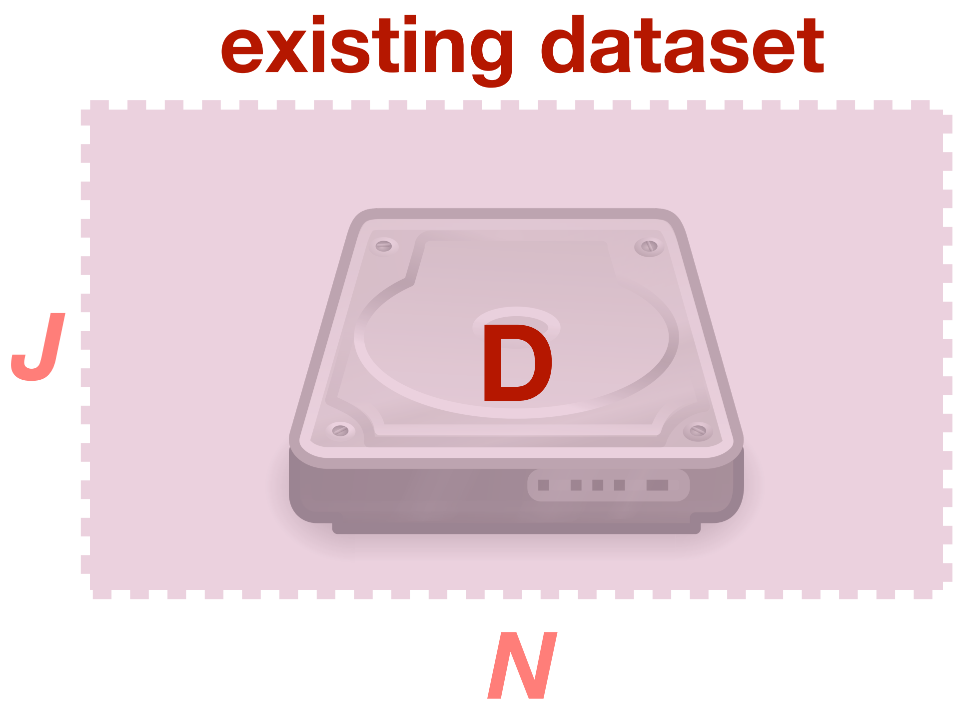
PCA

“eigen” features

“eigen” patterns



Principal component analysis (PCA)



J : # of probe positions
N : # of pixels in 1 diffraction pattern (DP)

$$\mathbf{D} = \begin{bmatrix} d_{11} & d_{12} & \cdots & d_{1N} \\ d_{21} & d_{22} & \cdots & d_{2N} \\ \vdots & \vdots & & \\ d_{J1} & d_{J2} & \cdots & d_{JN} \end{bmatrix} \begin{matrix} \rightarrow \mathrm{DP}_1 \\ \rightarrow \mathrm{DP}_2 \\ \\ \rightarrow \mathrm{DP}_J \end{matrix}$$

$$\mathrm{cov}[\mathbf{D}, \mathbf{D}] = \begin{bmatrix} \mathrm{var}(\mathrm{DP}_1) & & \mathrm{cov}(\mathrm{DP}_i, \mathrm{DP}_j) \\ & \mathrm{var}(\mathrm{DP}_2) & \\ & \ddots & \\ \mathrm{cov}(\mathrm{DP}_i, \mathrm{DP}_j) & & \mathrm{var}(\mathrm{DP}_J) \end{bmatrix}$$

eigenvectors: principal axes

eigenvalues: variances of distribution along new axes

$$\mathbf{D}_{J\times N} = \mathbf{P}_{J\times J}\mathbf{R}_{J\times N}$$

$\mathbf{P}_{J\times J}$: sorted principal axes by their corresponding eigenvalues

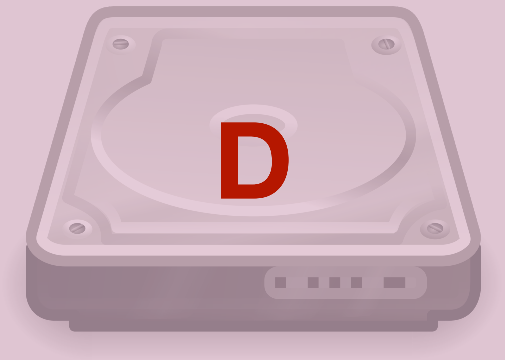
$\mathbf{R}_{J\times N}$: principal components

Our new idea: compress the data *on the detector*

Applying PCA on an existing dataset

J : # of probe positions
N : # of pixels in 1 diffraction pattern (DP)

existing dataset

J  *N*

$$\mathbf{D}_{J\times N} = \mathbf{P}_{J\times J}\mathbf{R}_{J\times N}$$

$\mathbf{P}_{J\times J}$: principal axes

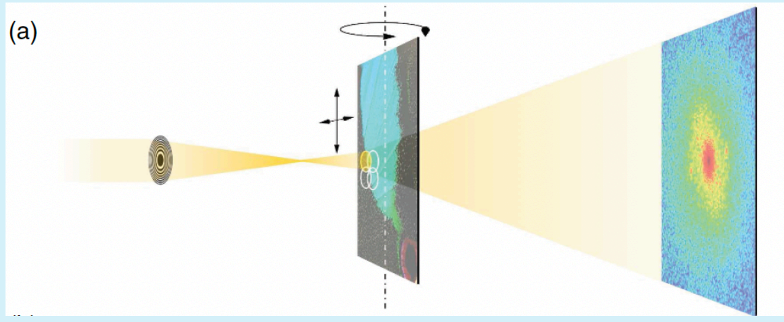
$\mathbf{R}_{J\times N}$: principal components

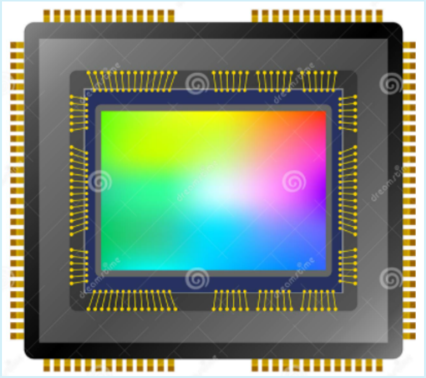
$\mathbf{R}_{S'\times N}$ $(S' < J)$

encoding matrix

S' **R** *N*

New data acquisition compress DP

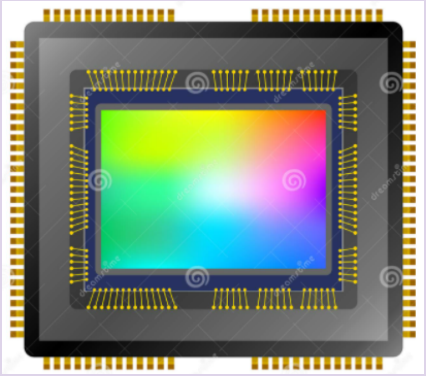




P' principal axes ($1 \times S'$) = **D'** 1 diffraction pattern ($1 \times N$) × **R⁻¹** inv. encoding matrix ($N \times S'$)

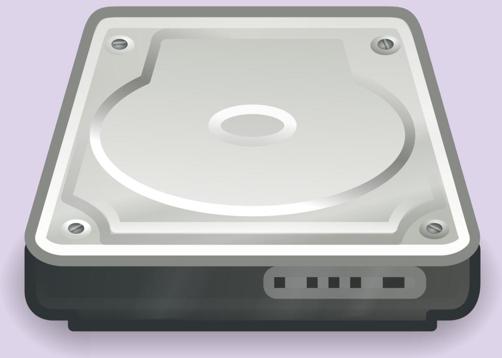
$$\mathbf{P'}_{1\times S'} = \mathbf{D'}_{1\times N}\mathbf{R}^{-1}_{N\times S'}$$

Transfer the compressed data



. . .

Less data transfer faster

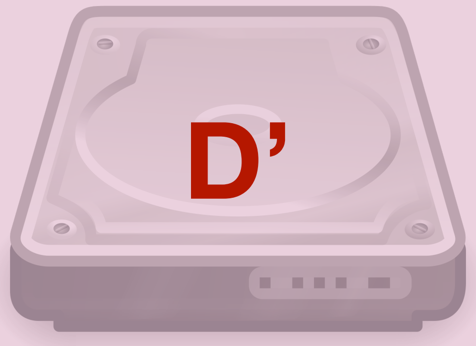


principal axes

J **P'** *S'*

Recover the dataset

recovered dataset

J  *N*

= *J* **P'** principal axes *S'* × *S'* **R** encoding matrix *N*

Compress the dataset - dimension reduction

Why do we need to compress the data?

- Save the disk space:
  many GBs of data to reconstruct few MBs of images
- Speed up the data transfer:
  faster frame rates are needed for the future
  Potential data generation rate > Data transfer rate

What are the existing data compression methods?

- Currently often no compression
- Compression done after experiments:
  Requires access to the entire dataset

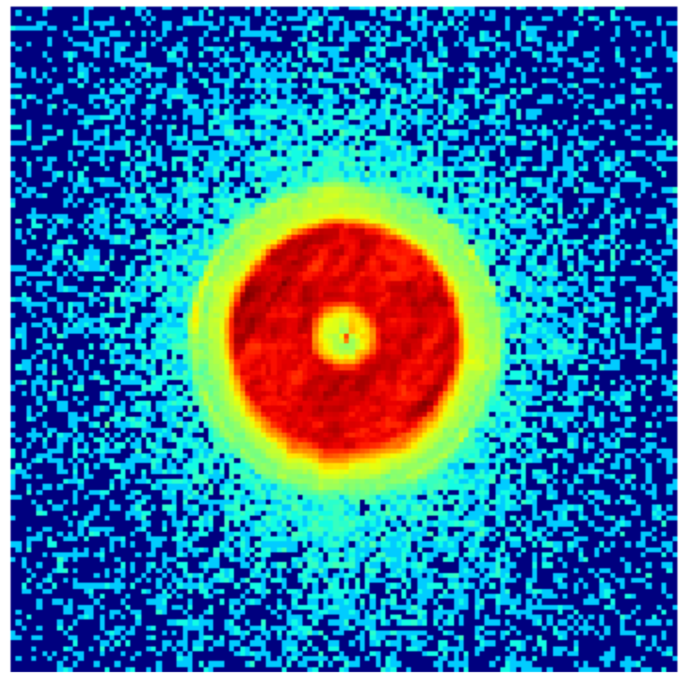
How do we do this?

- Principal component analysis (PCA)
  - Using PCA but requiring the entire dataset

  ✓ On the circuit of the camera:
  Use the pre-loaded principal components
  to compress diffraction patterns

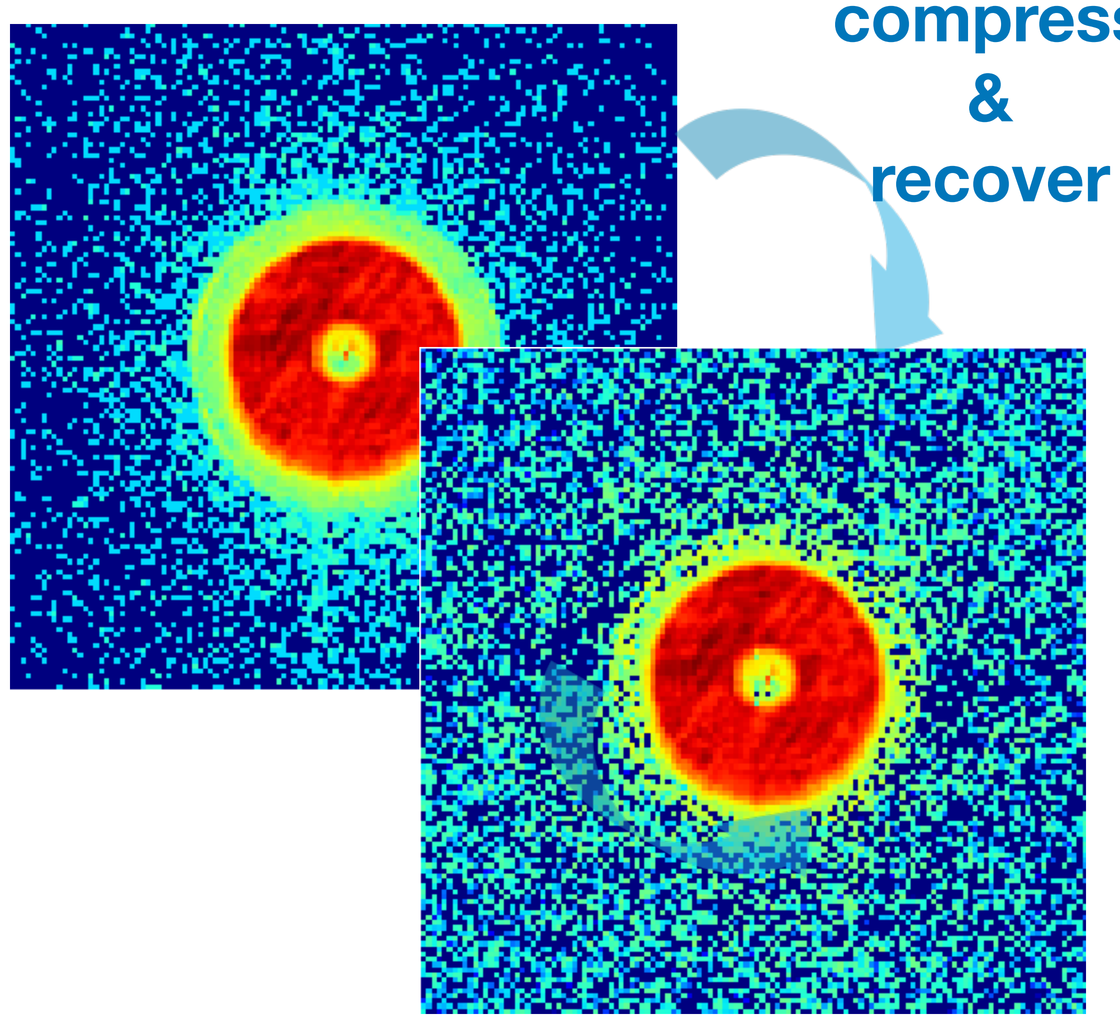
compression ratio $C_{\text{det}} = \dfrac{N}{S'}$

Existing dataset:
the 1st dataset



PCA
Load R^{-1} to a detector

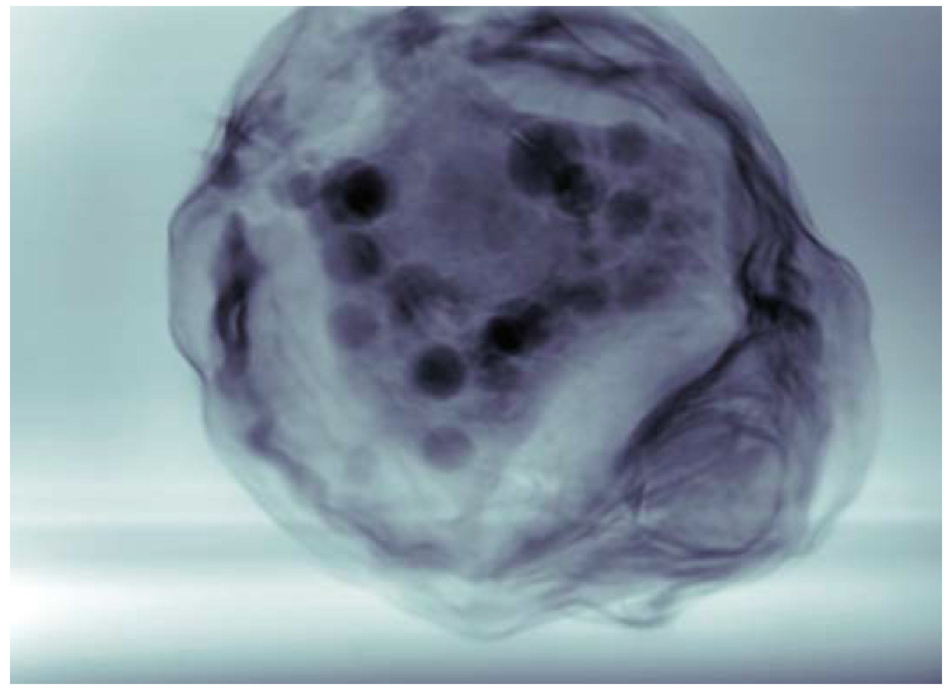
New acquisition:
the 2nd dataset



compress
&
recover

Reconstruction

Reconstructed
from the 1st dataset



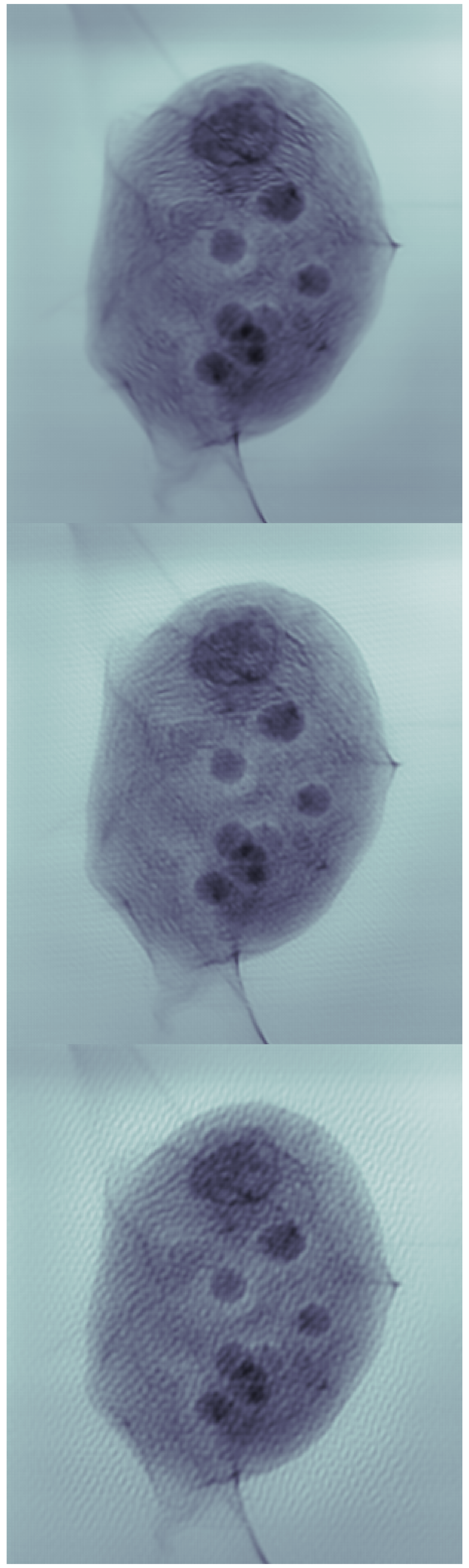
Reconstructed from
the recovered 2nd dataset

compression
ratio

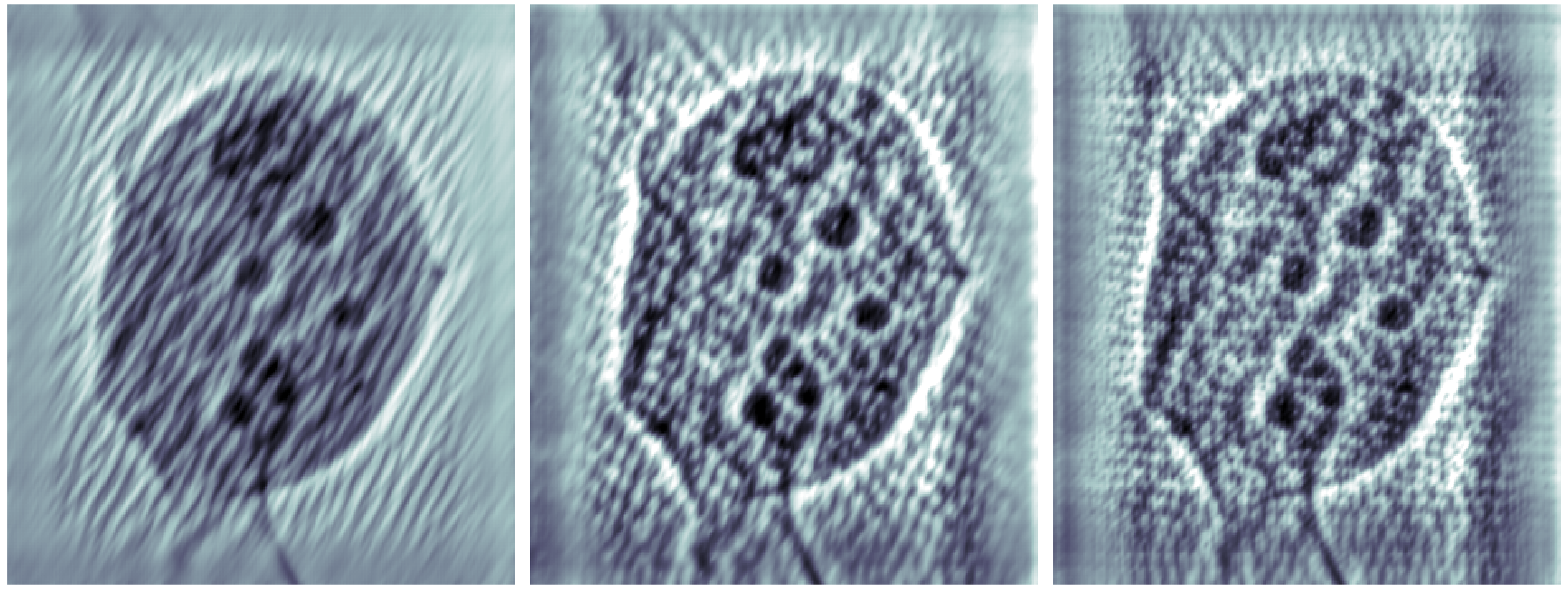
1 : 1

6 : 1

10 : 1



Imperfect reconstruction:
Encoded noise
Slightly different probe functions



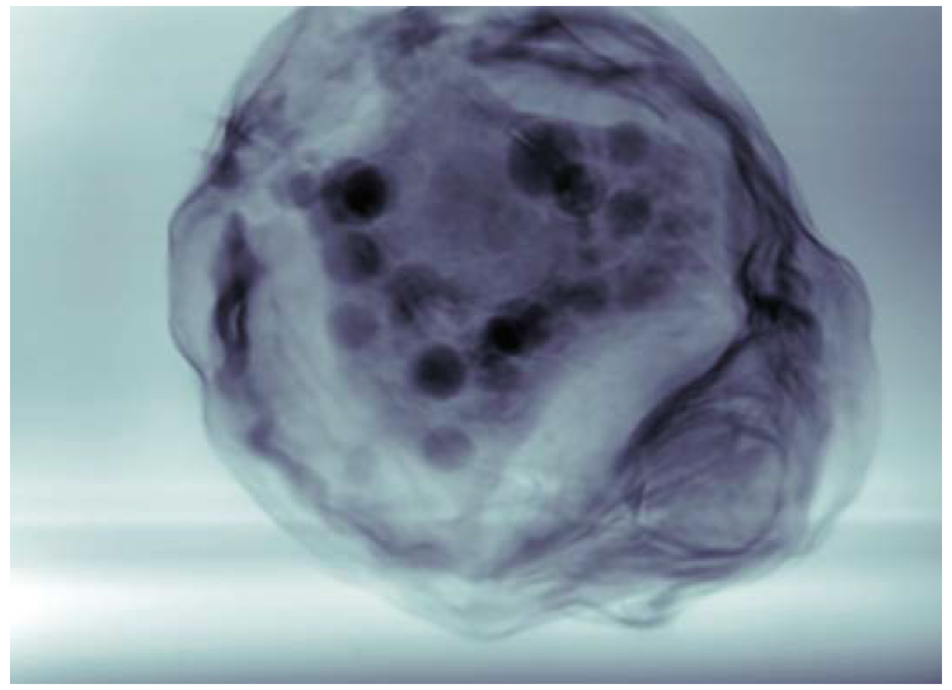
compression ratio

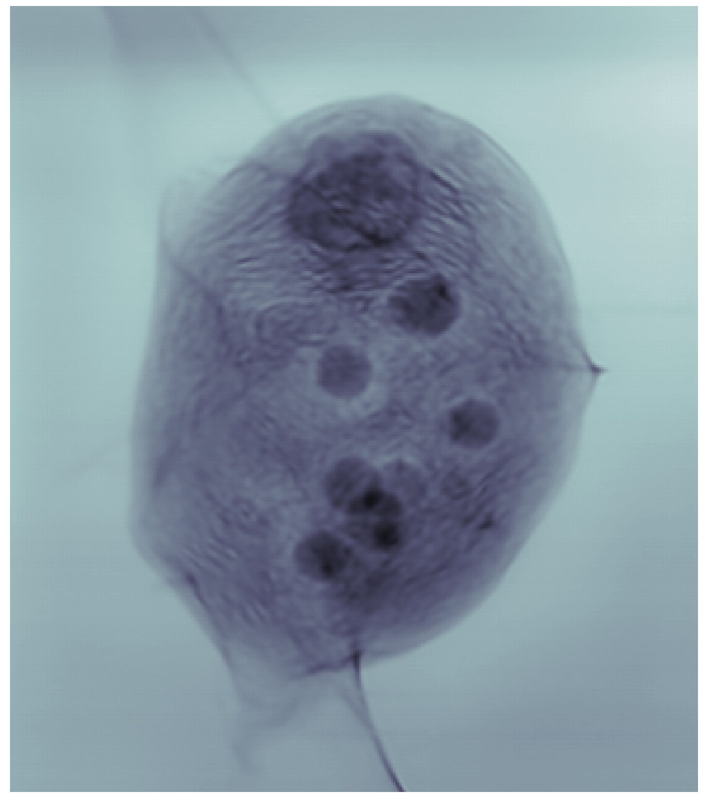
16 : 1 **55 : 1** **164 : 1**

Source of the artifacts:

(1) Different probe functions were used in these two experiments

(2) Noise was present in the encoding data





Another new idea: encoding using noise-free training object

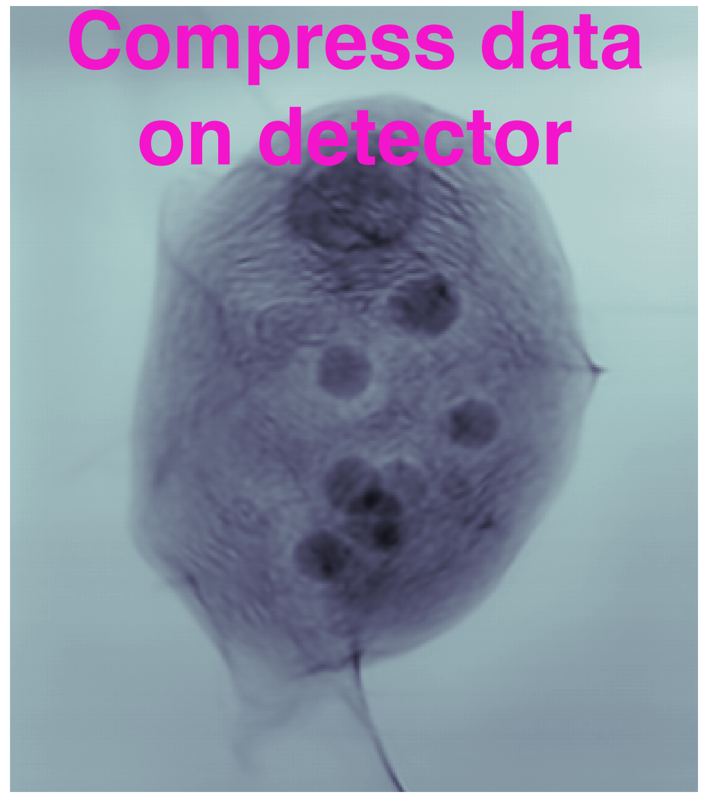
Training Object

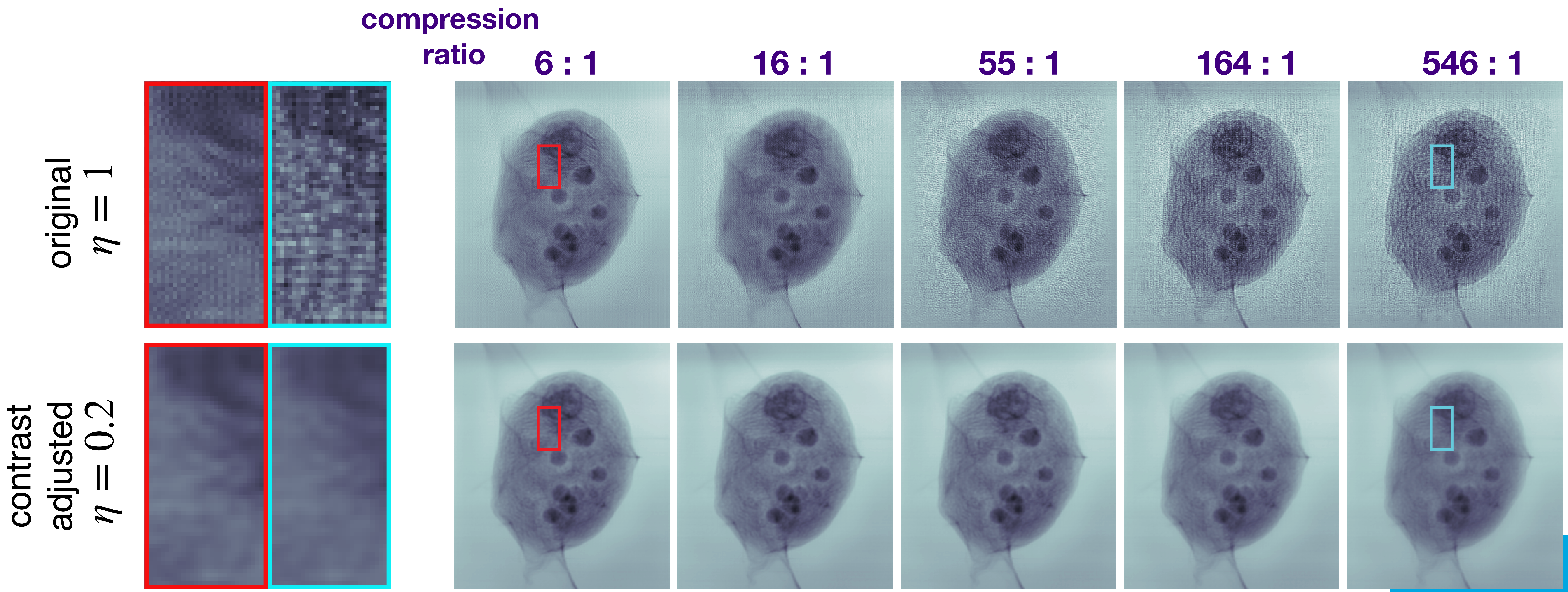
$\times \eta$

+ **Generate noise-free simulated data**

Experimentally-determined probe function

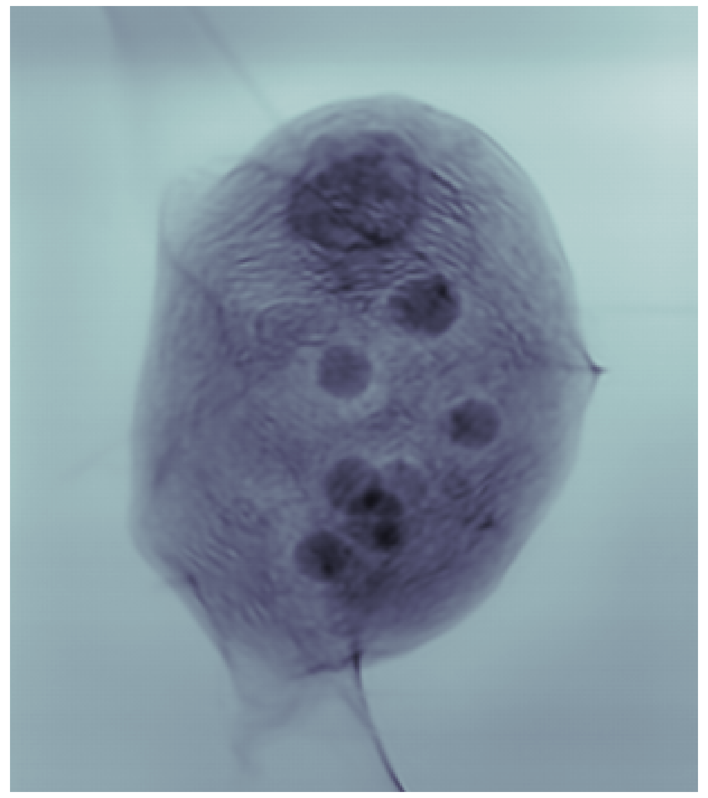
→ **Calculate eigenimages** →



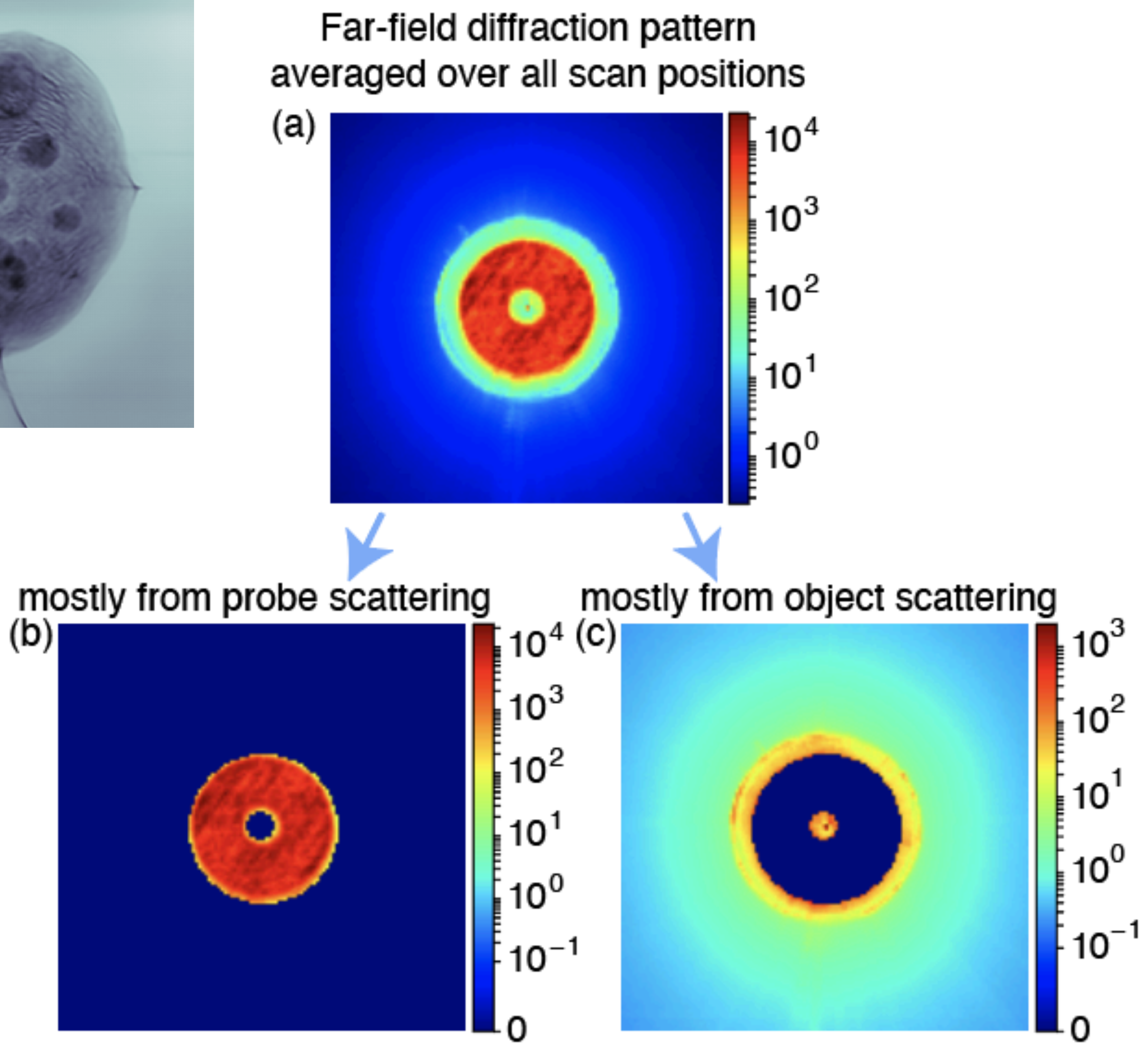


Even better: contrast-matched training object

Sample

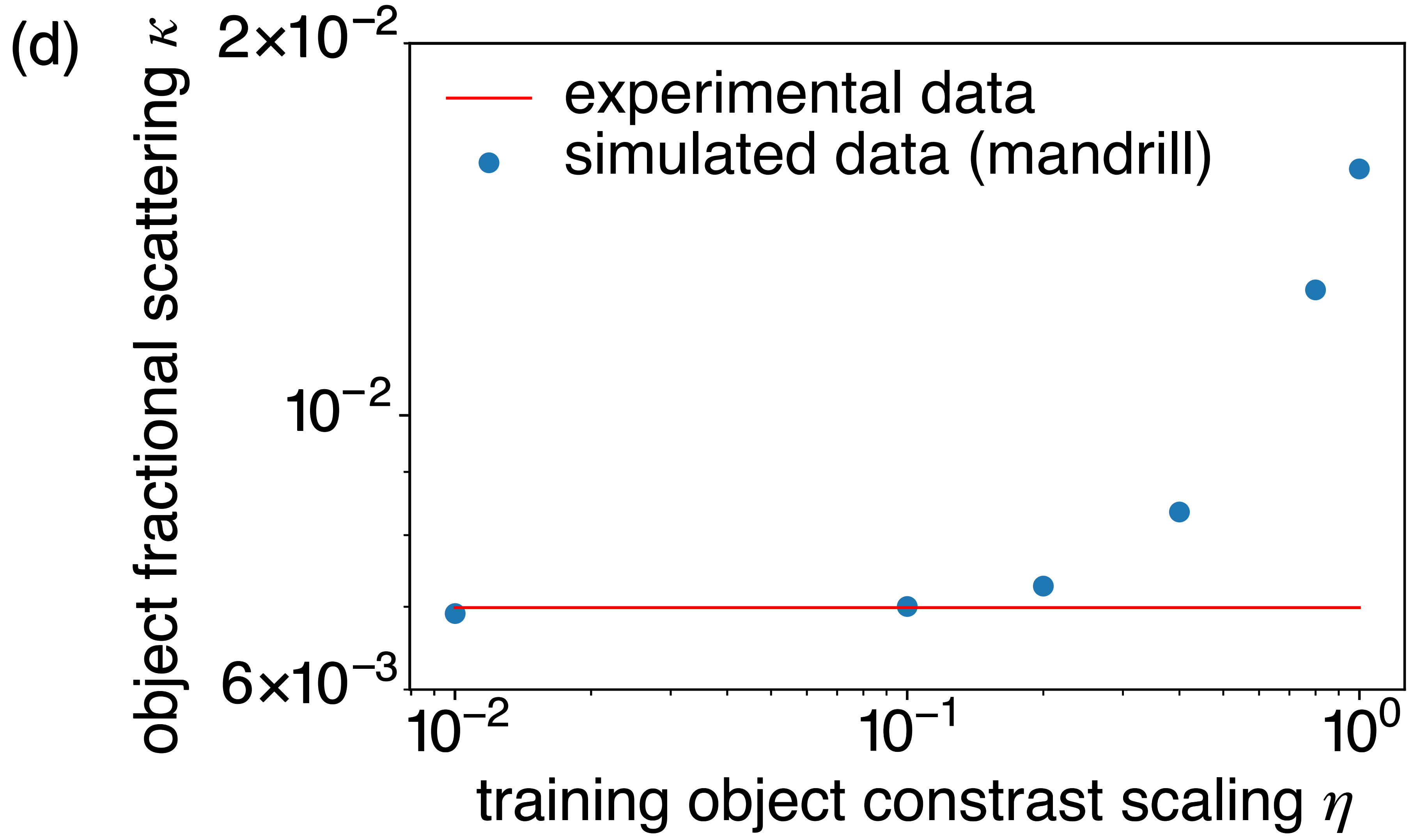


Experimental data



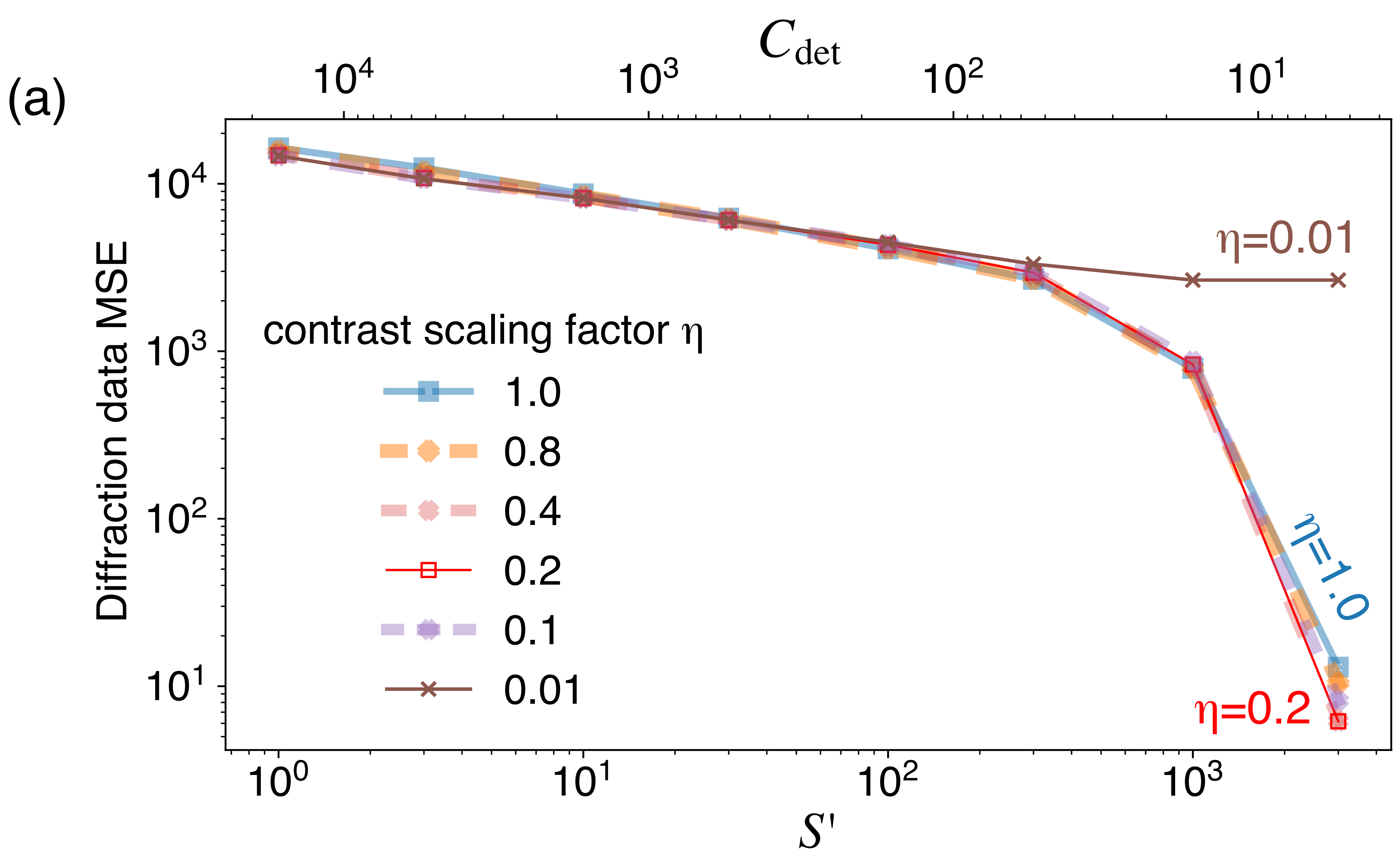
Training Object

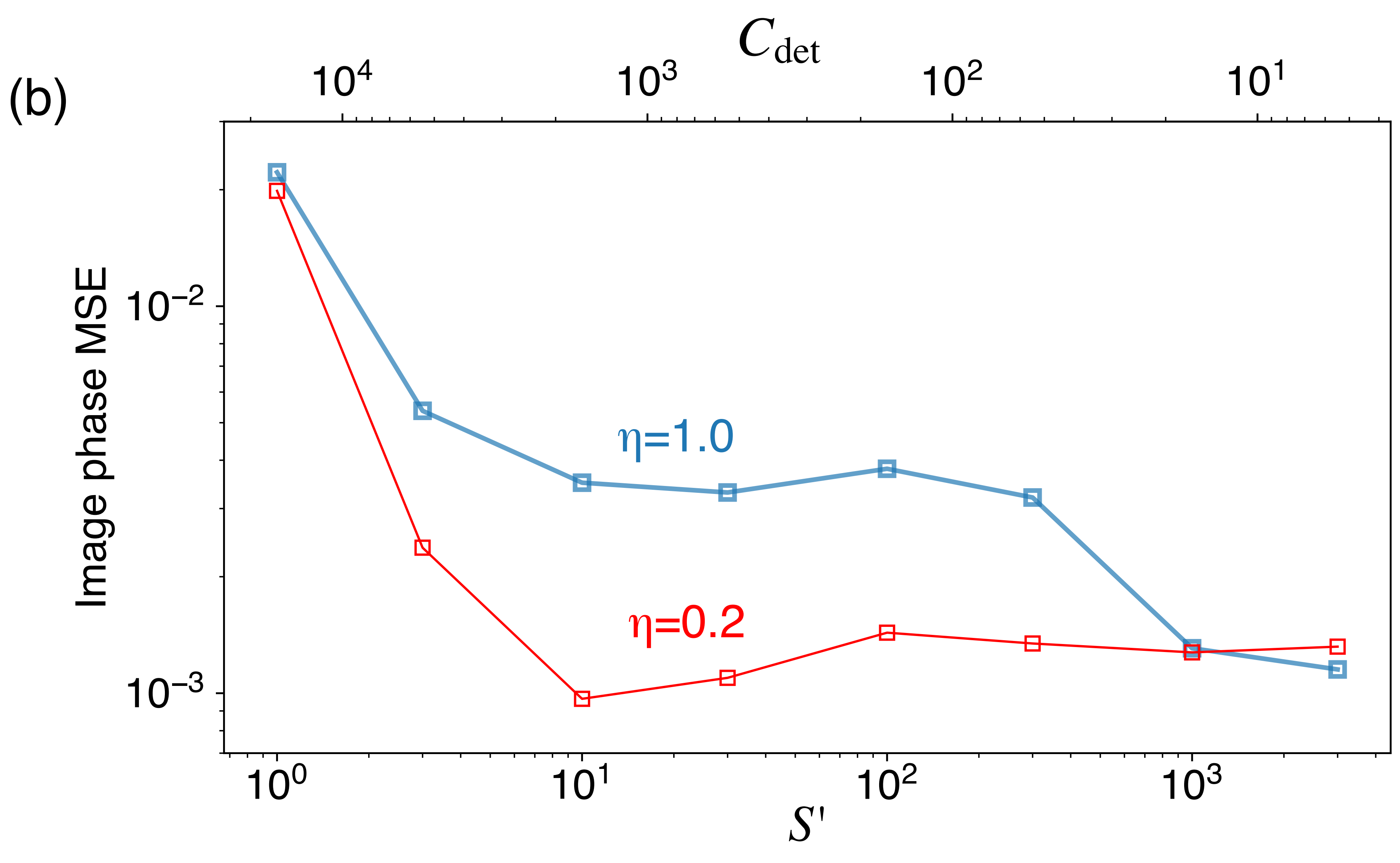
$\times \eta$



Object fractional scattering $\kappa = \dfrac{\text{object scattering}}{\text{probe scattering}}$

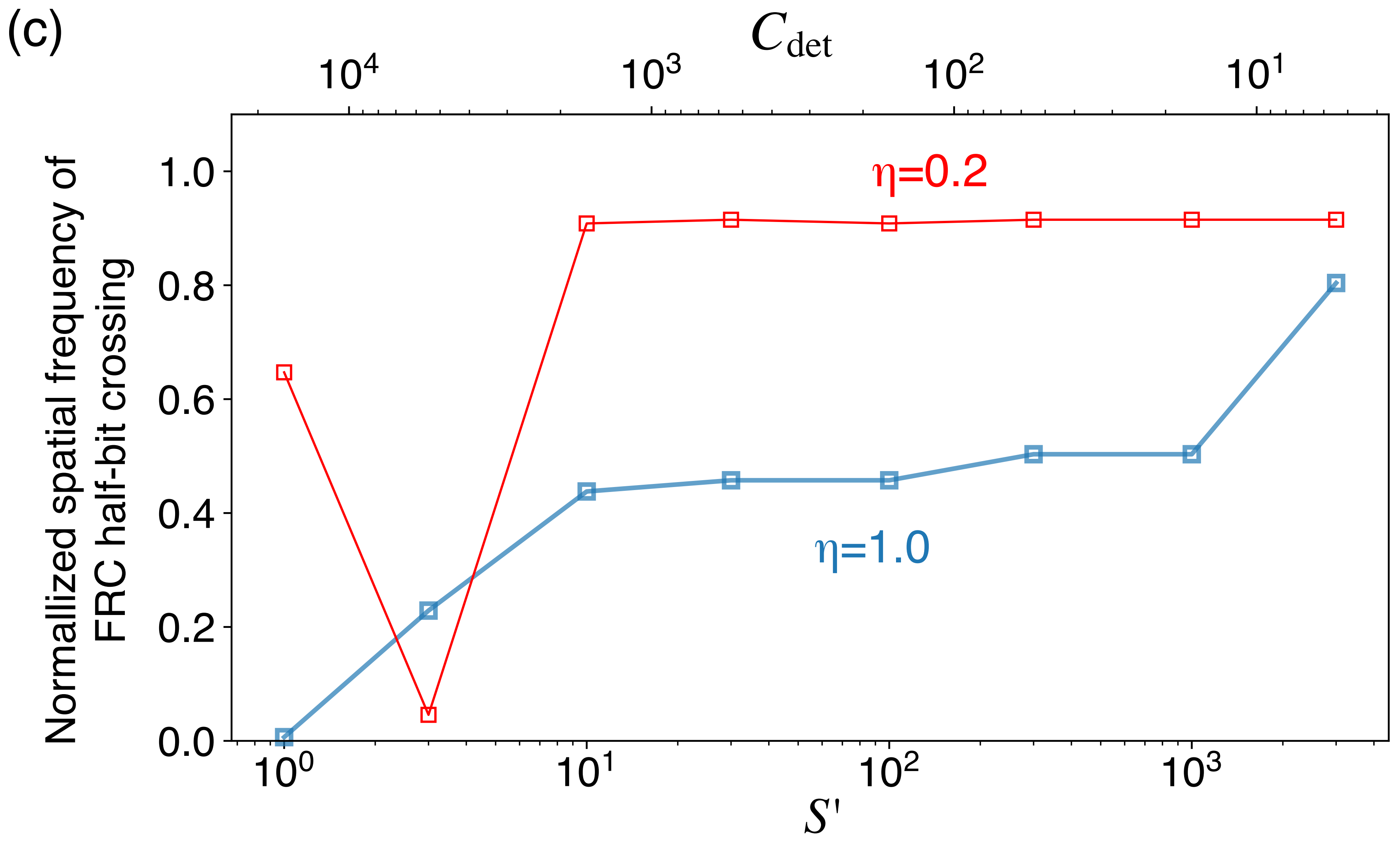
Metric for fidelity: Diffraction data MSE & Image phase MSE

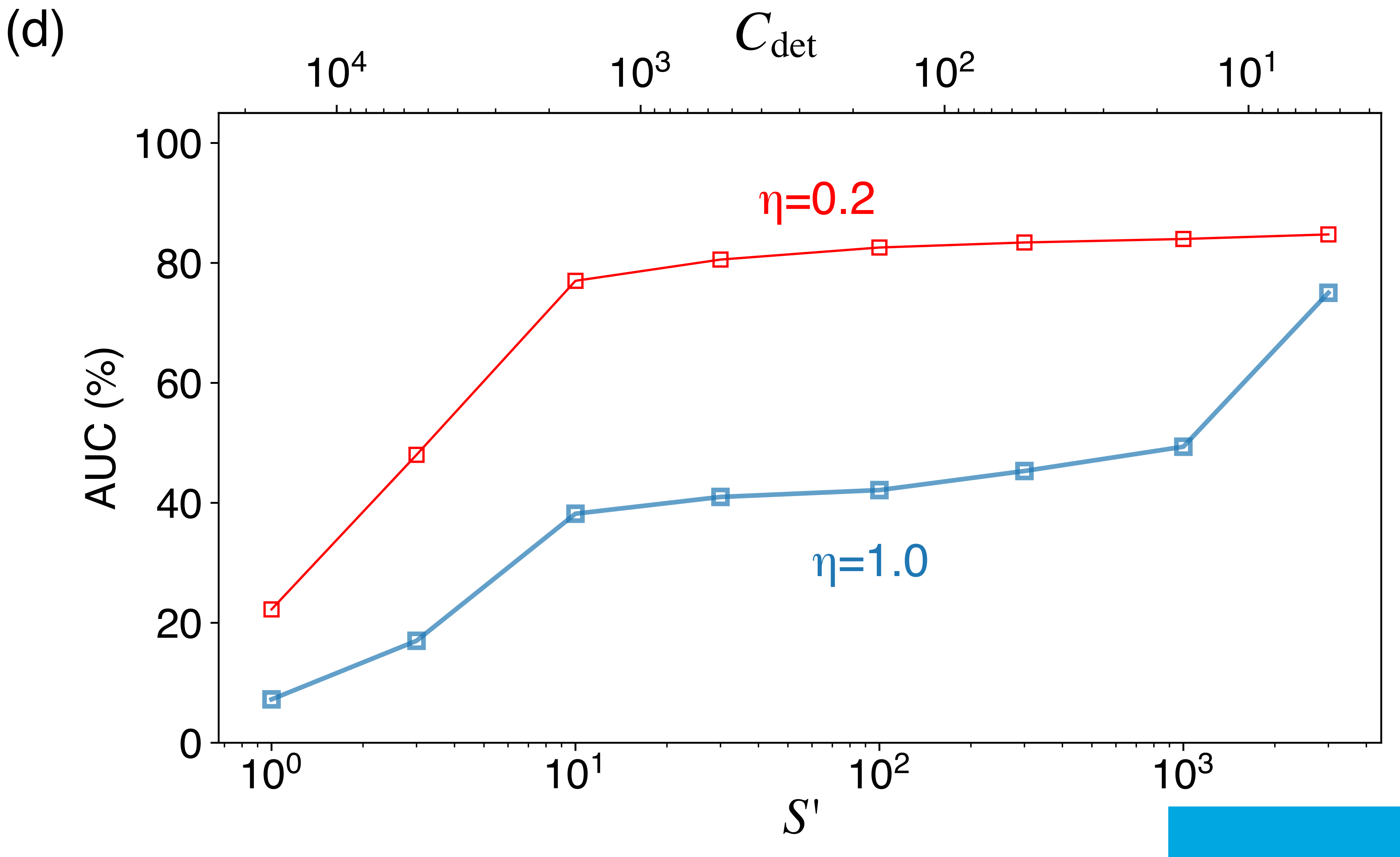




Metric for resolution: Fourier ring correlation (FRC) half-bit threshold

Compression up to ~1000x works!





Matrix factorization approaches to lossy compression of ptychography data

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