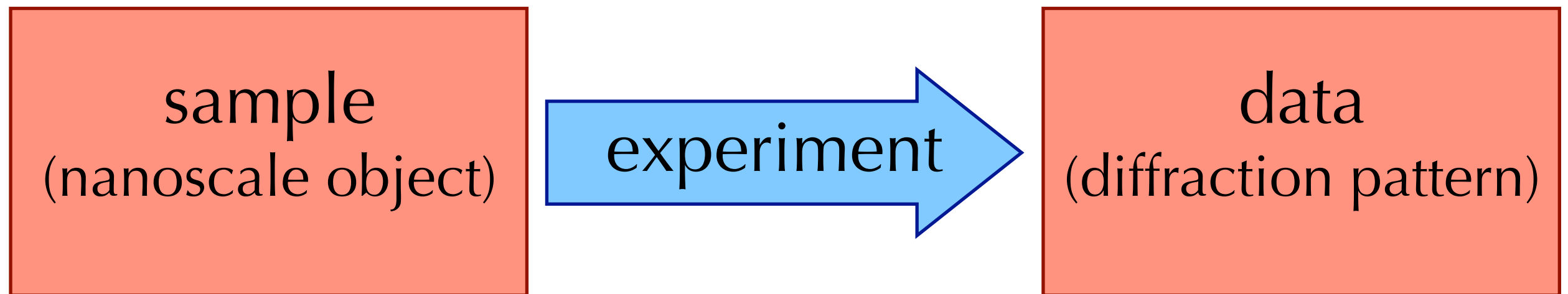


# Diffraction imaging in the presence of noise

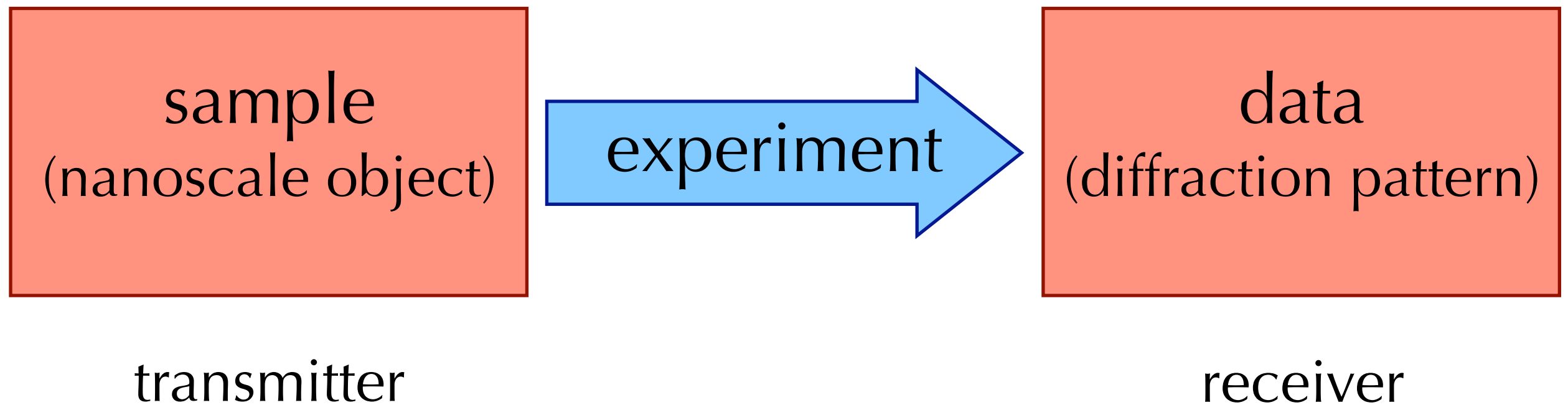
Veit Elser  
Cornell

X-ray Science in the 21<sup>st</sup> Century  
KITP, Santa Barbara

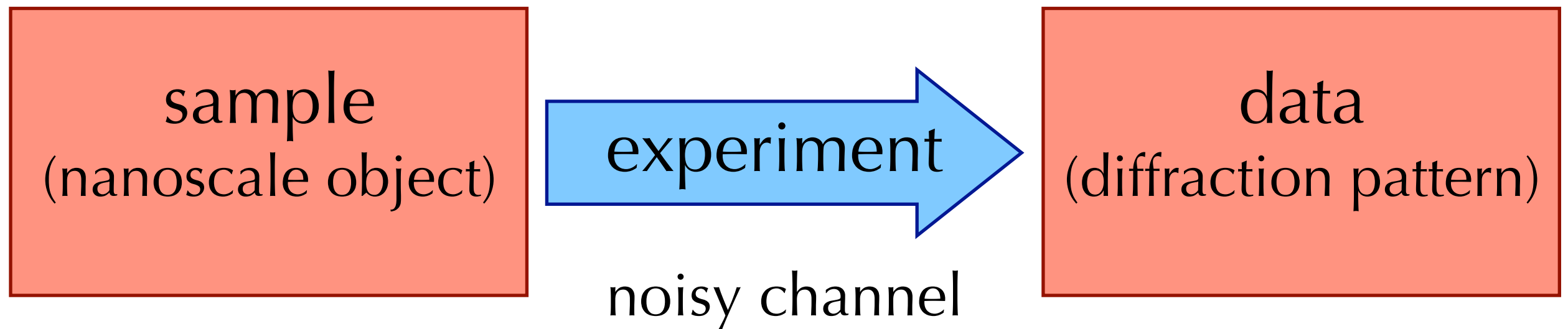
# Experiment as a noisy communication channel



# Experiment as a noisy communication channel



# Experiment as a noisy communication channel



transmitter



receiver

# `channel capacity' of experiments



C.E. Shannon

`channel capacity' of experiments

$H(s)$  = entropy of the sample



C.E. Shannon

# `channel capacity' of experiments

$H(s)$  = entropy of the sample

$H(s|d)$  = conditional entropy of  
the sample given the data



C.E. Shannon

# `channel capacity' of experiments

$H(s)$  = entropy of the sample

$H(s|d)$  = conditional entropy of  
the sample given the data



C.E. Shannon

$I(s,d)$  = information capacity of the experiment  
=  $H(s) - H(s|d)$   
(mutual information)



**experimentalists:**

increase the channel capacity

**theorists:**

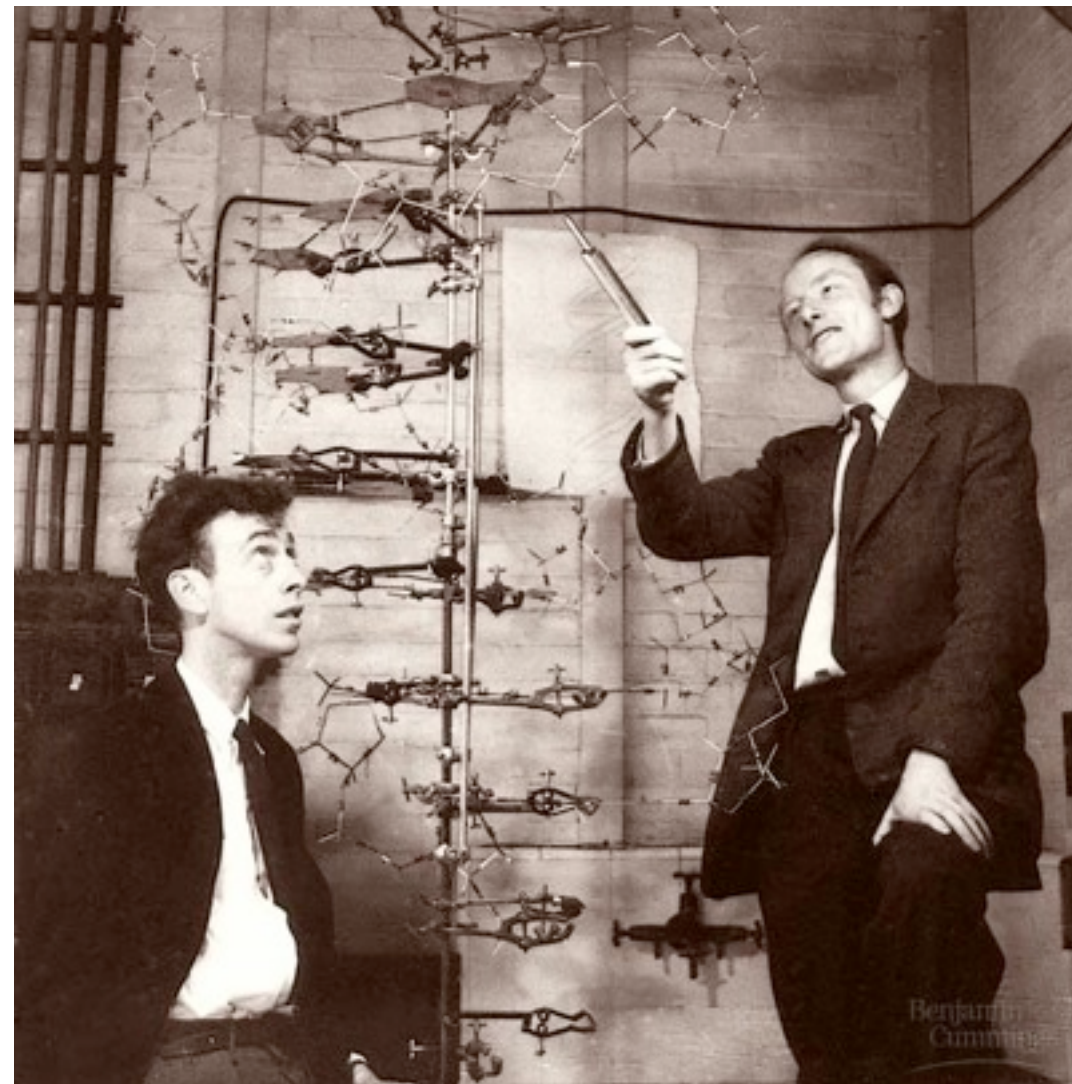
decode the data



Franklin

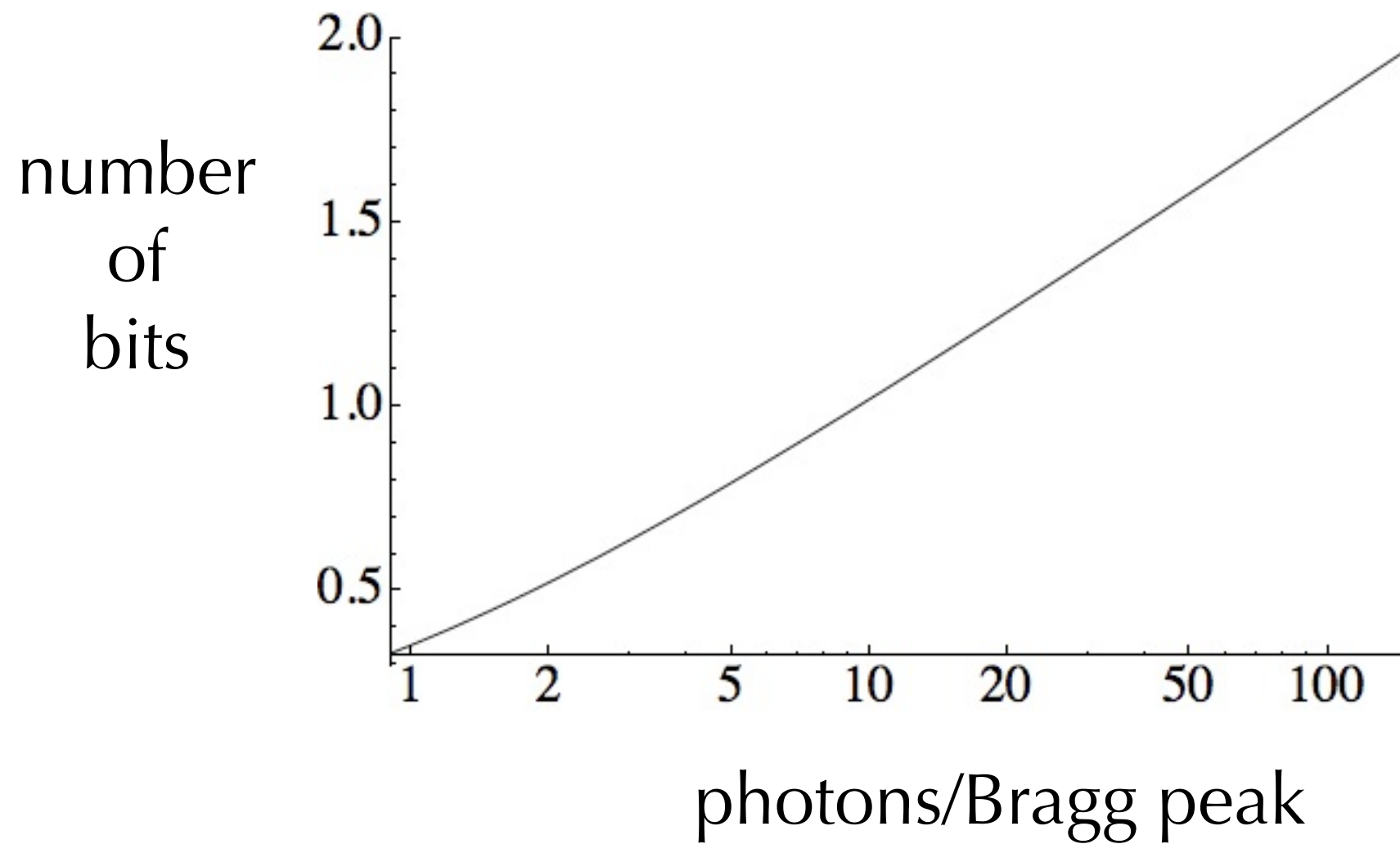
**experimentalists:**  
increase the channel capacity

**theorists:**  
decode the data

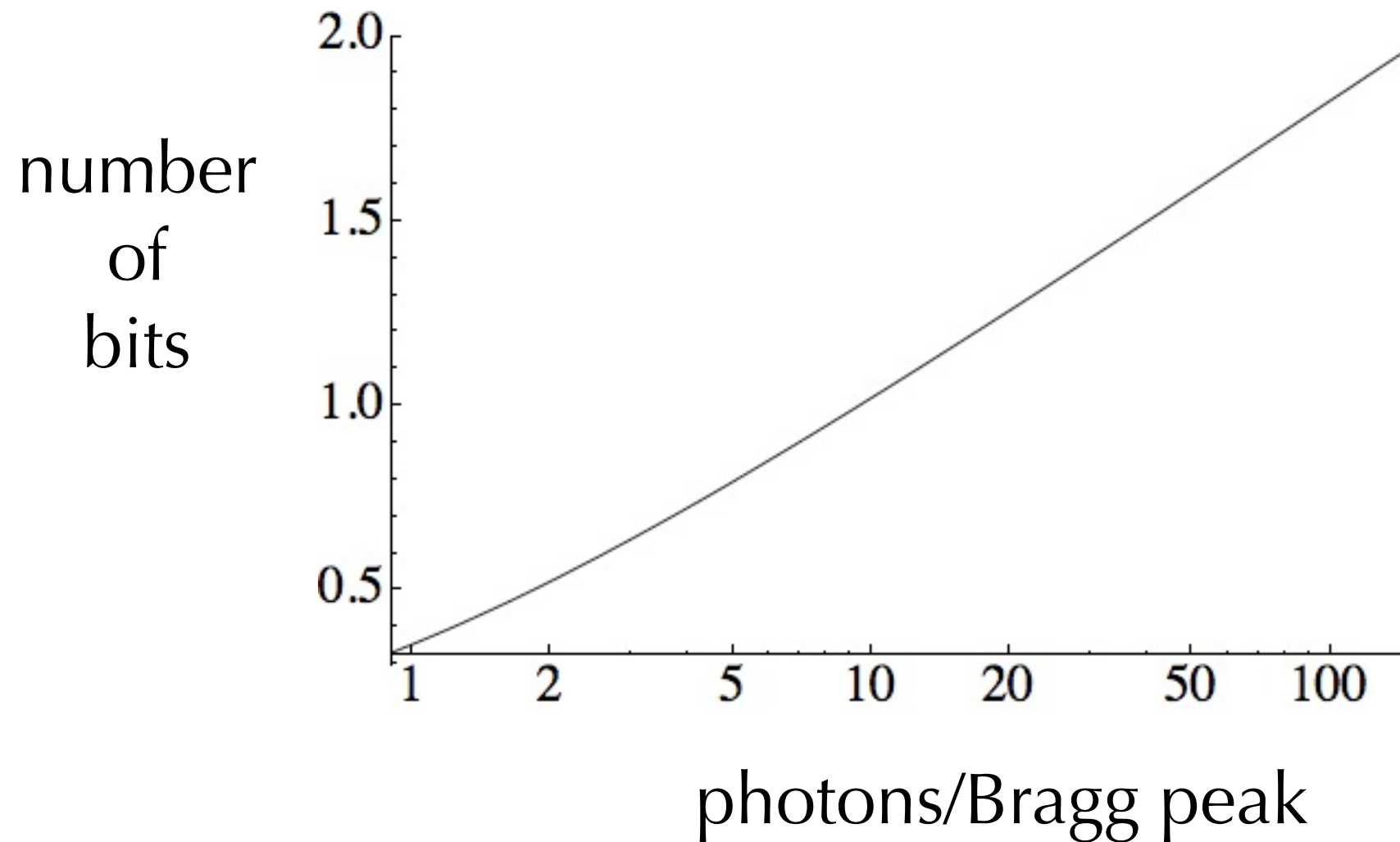


Crick & Watson

# example: information in a Bragg peak

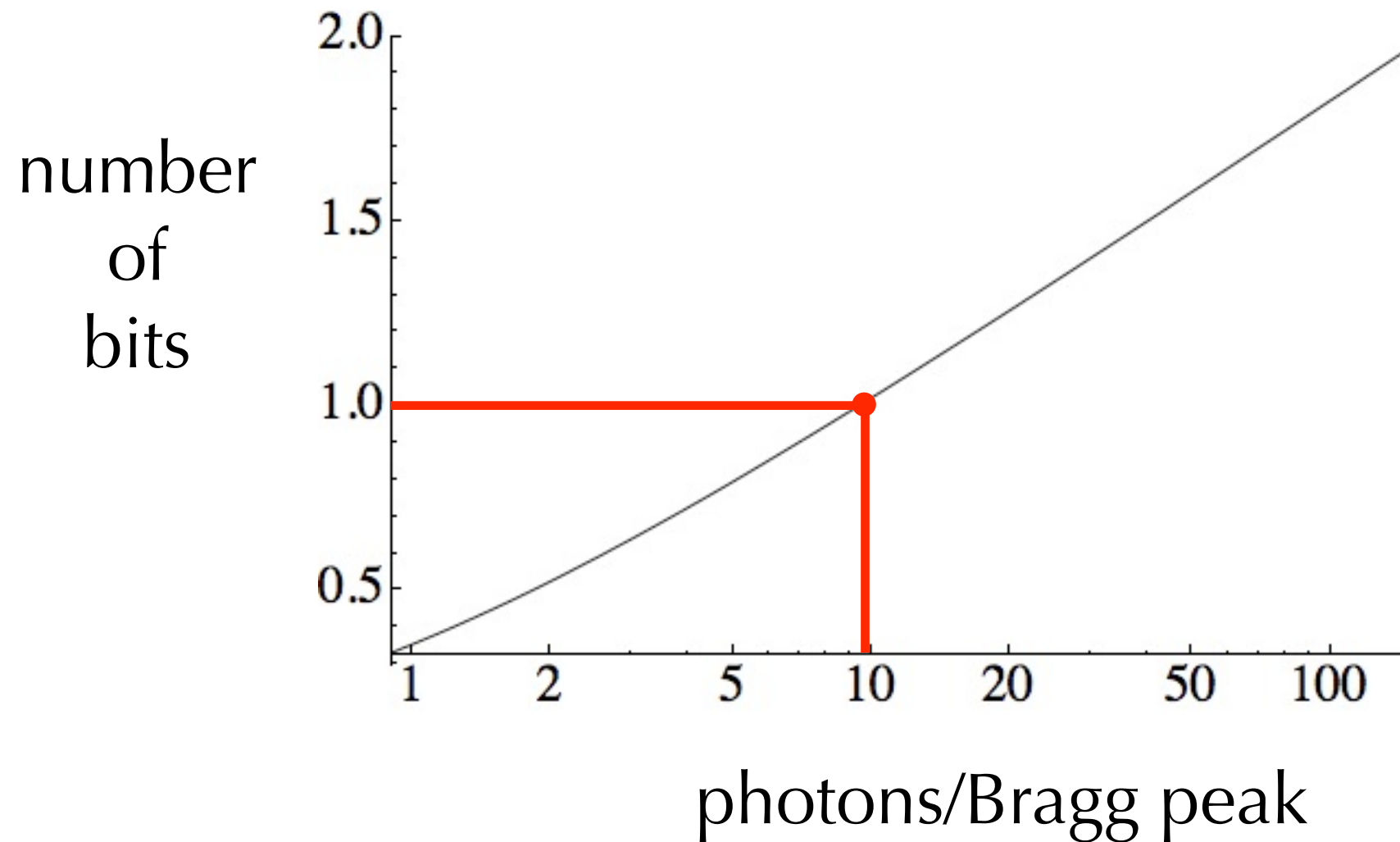


# example: information in a Bragg peak

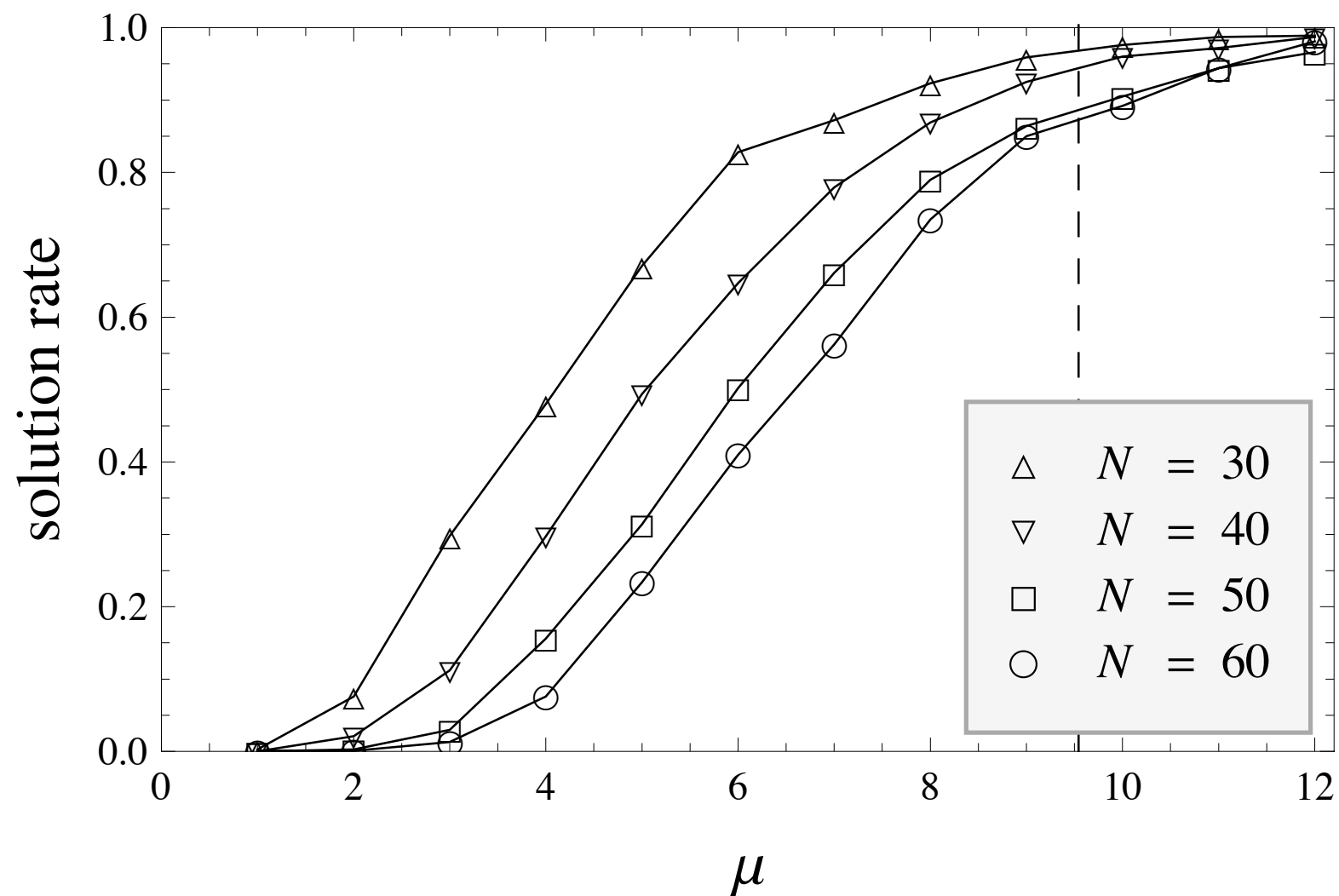


$$I(\mu) = \left(\mu + \frac{1}{2}\right) \log_2 (2\mu + 1) - \frac{\gamma\mu}{\log 2} - \frac{1}{2} \sum_{k=2}^{\infty} \frac{\log_2 k}{\left(1 + \frac{1}{2\mu}\right)^k}$$

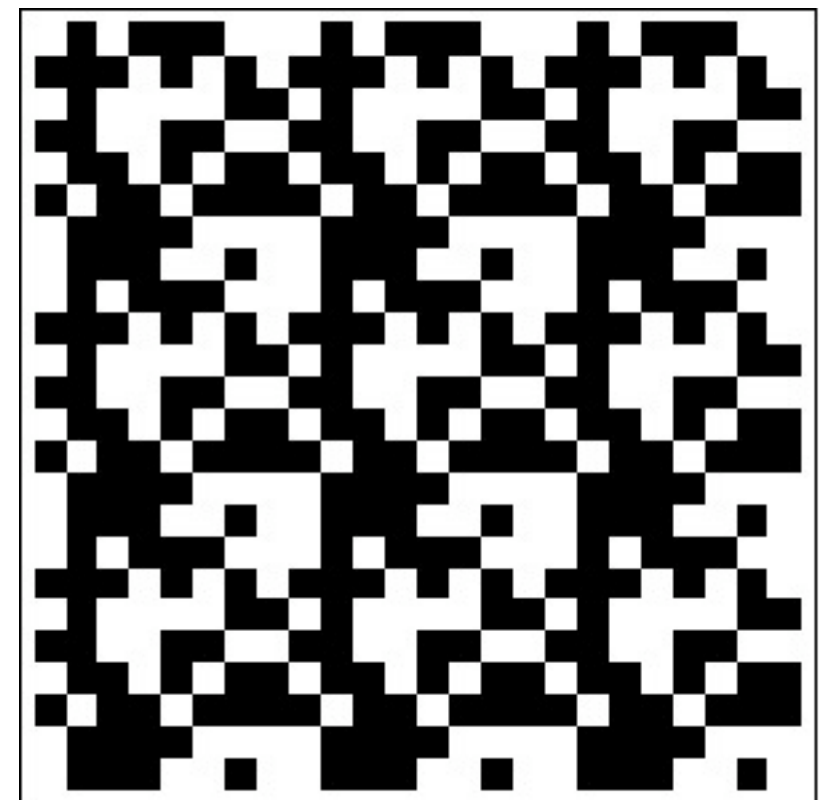
# example: information in a Bragg peak



$$I(\mu) = \left(\mu + \frac{1}{2}\right) \log_2 (2\mu + 1) - \frac{\gamma\mu}{\log 2} - \frac{1}{2} \sum_{k=2}^{\infty} \frac{\log_2 k}{\left(1 + \frac{1}{2\mu}\right)^k}$$



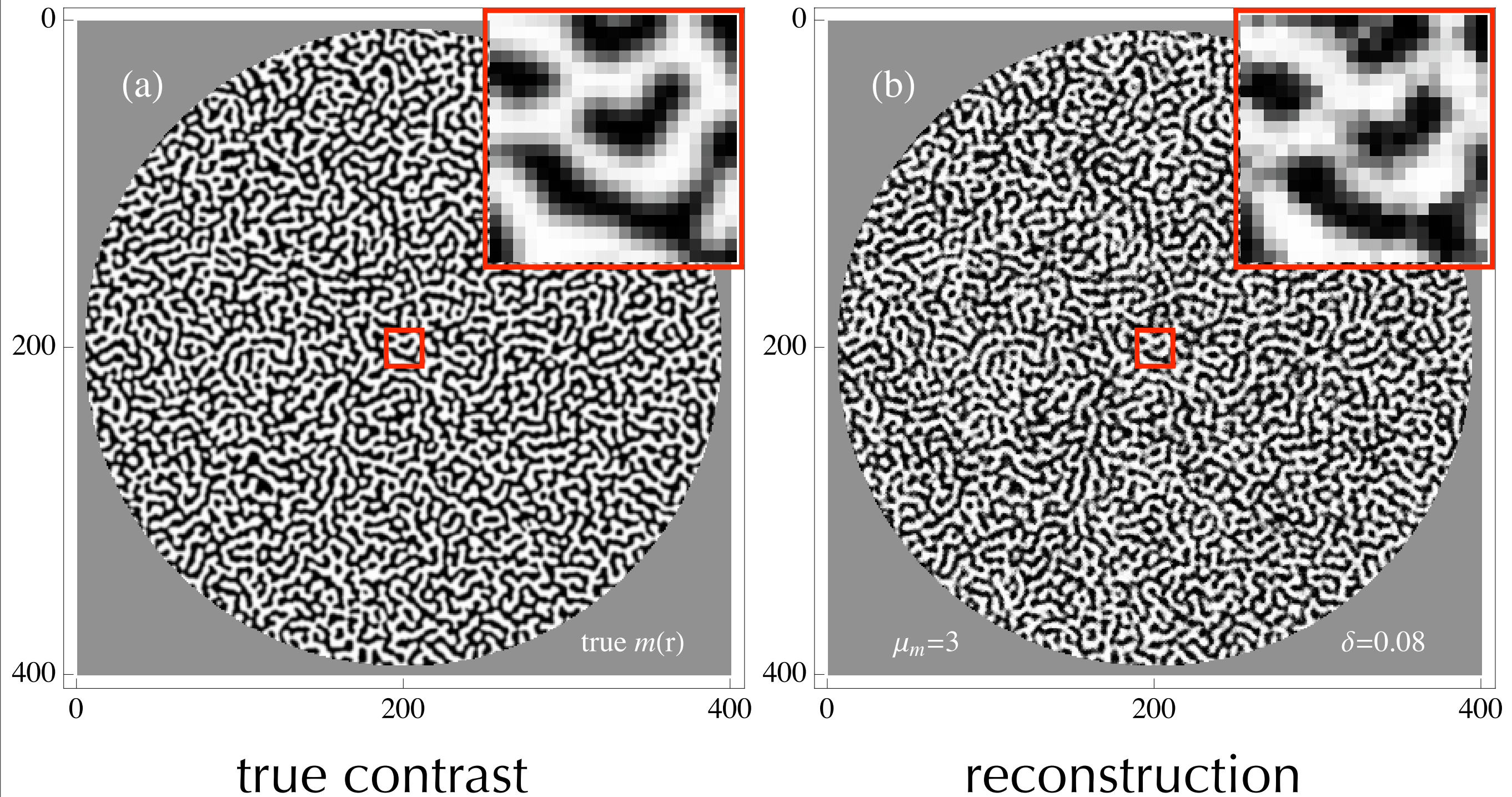
Elser & Eisbitt, NJP (2010)



decoding:  
 difference map algorithm with  
 binary value constraint

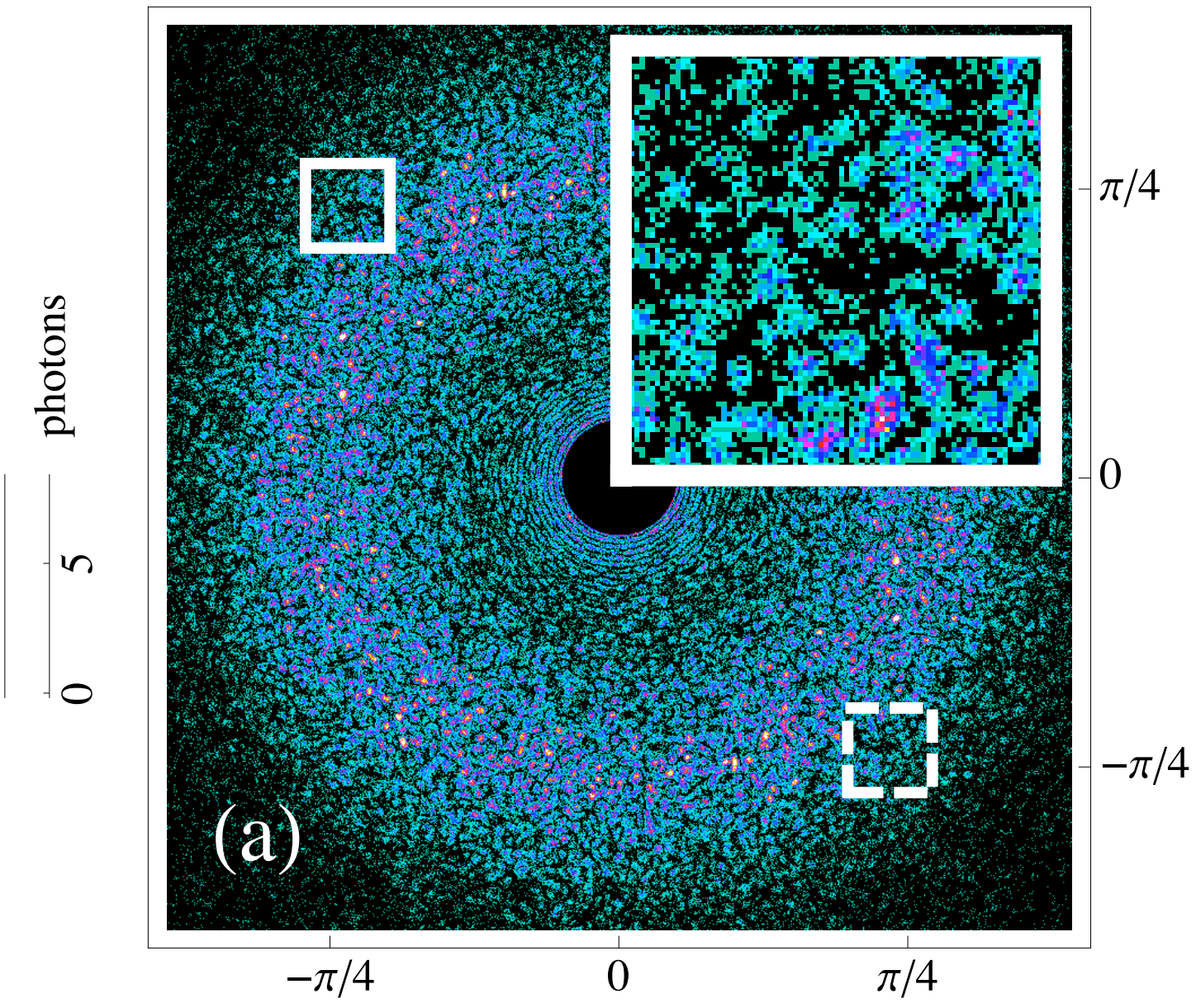
LDPC decoding: Yedidia, Wang & Draper, Physics of Algorithms (2009)

# diffractive imaging of magnetic domains

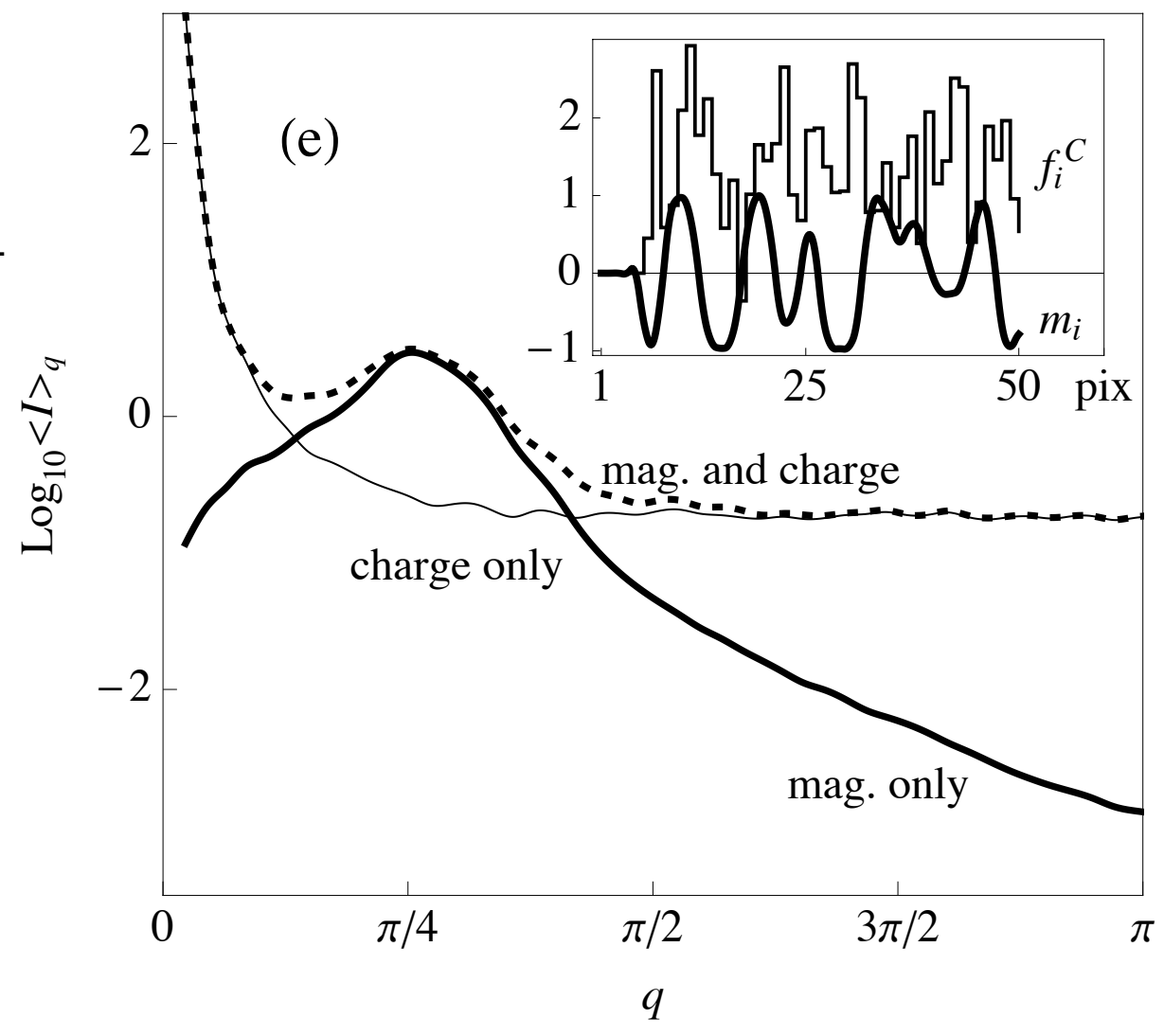


Loh, Eisebitt, Flewett & Elser (2010)

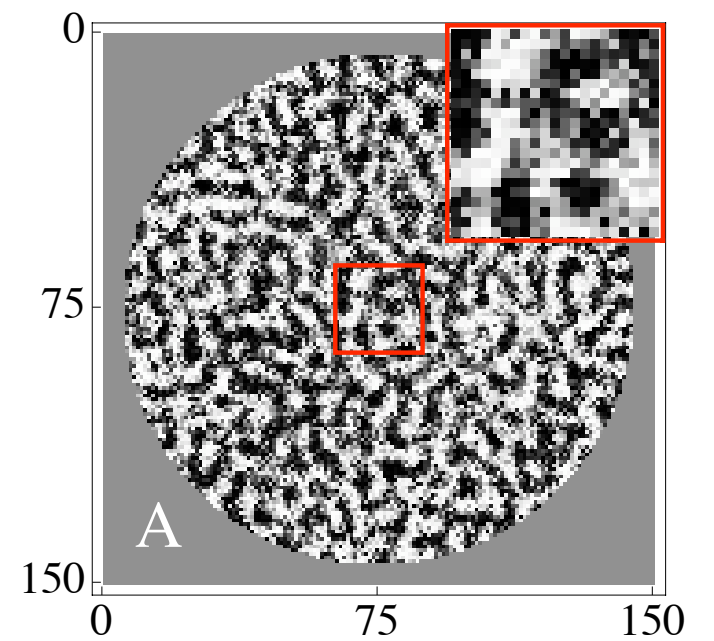
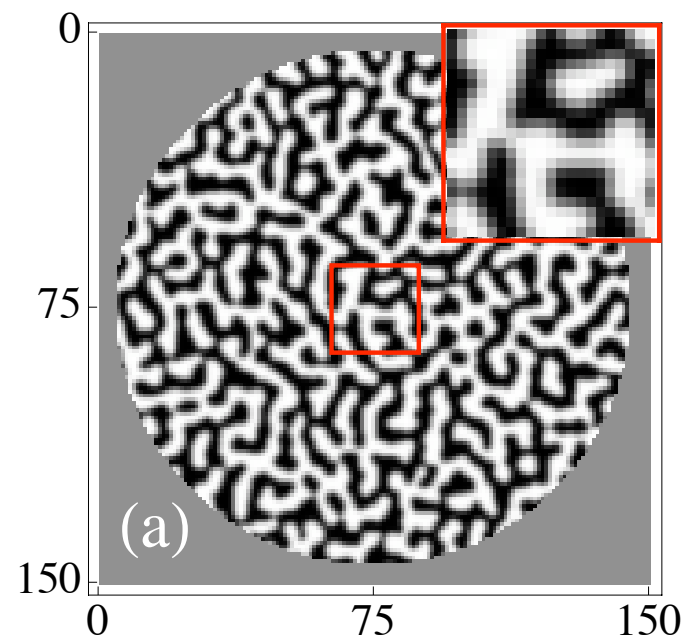
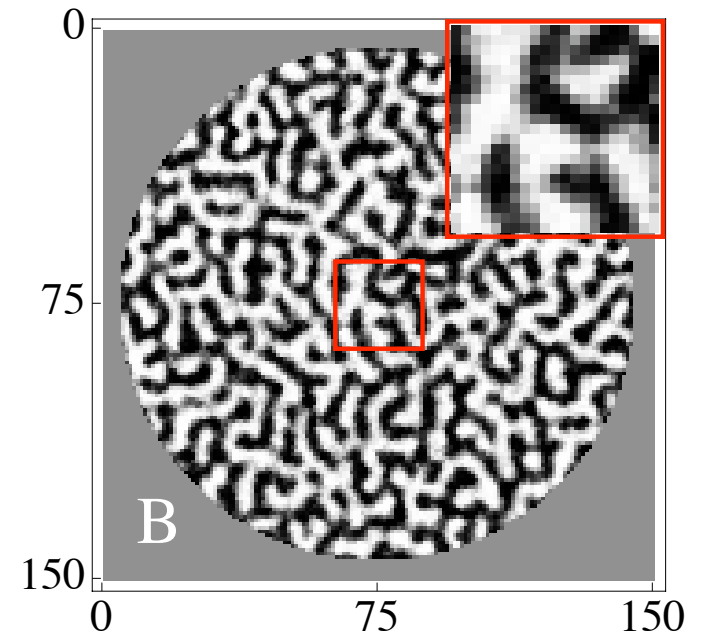
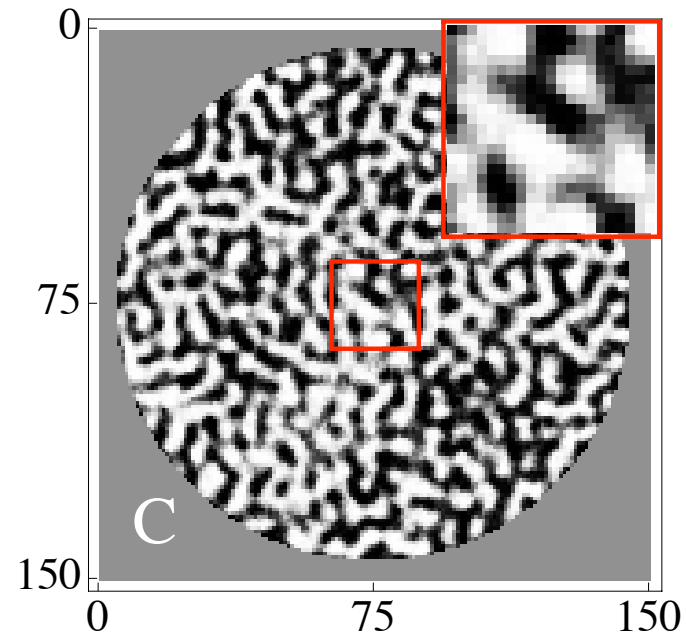
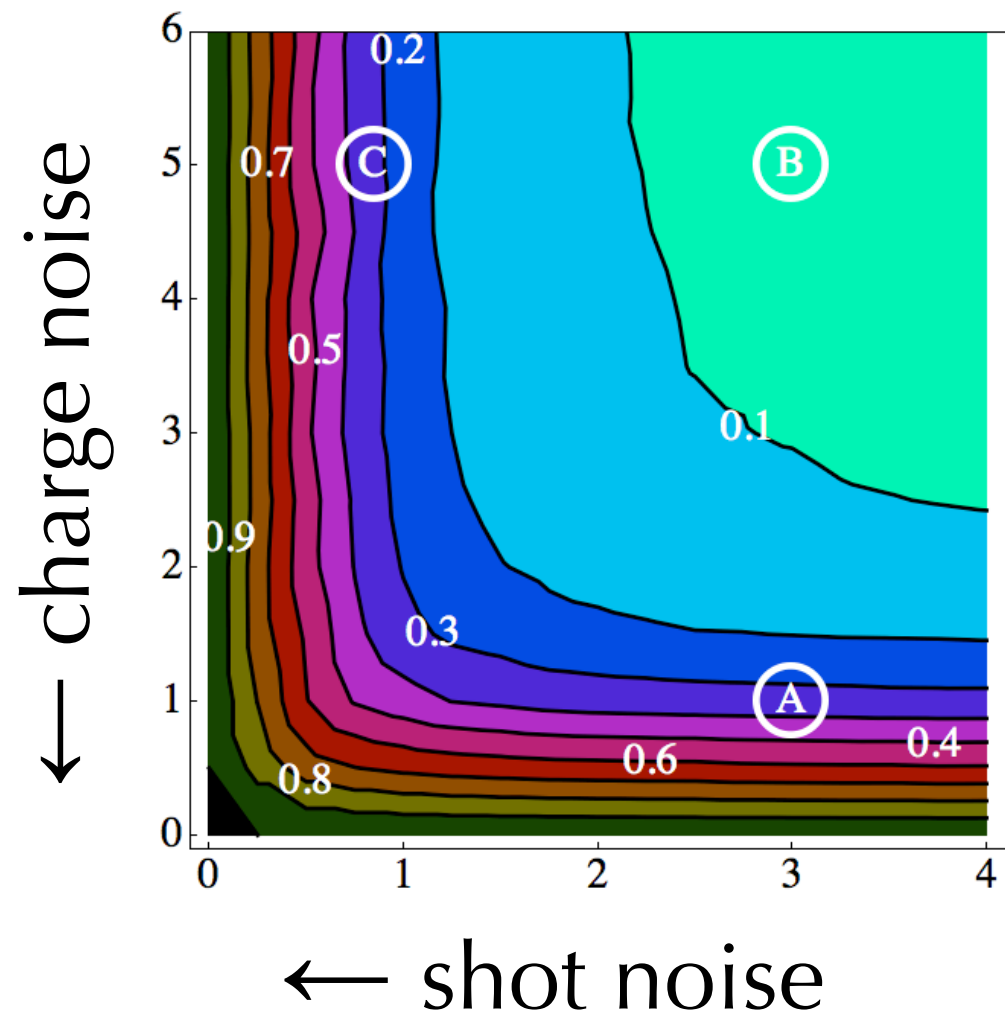




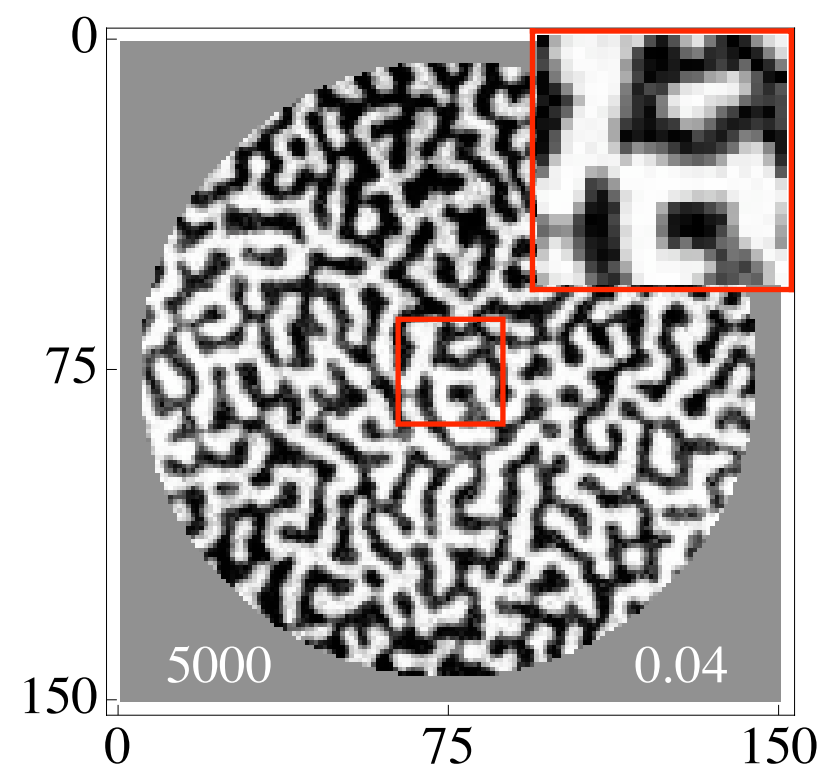
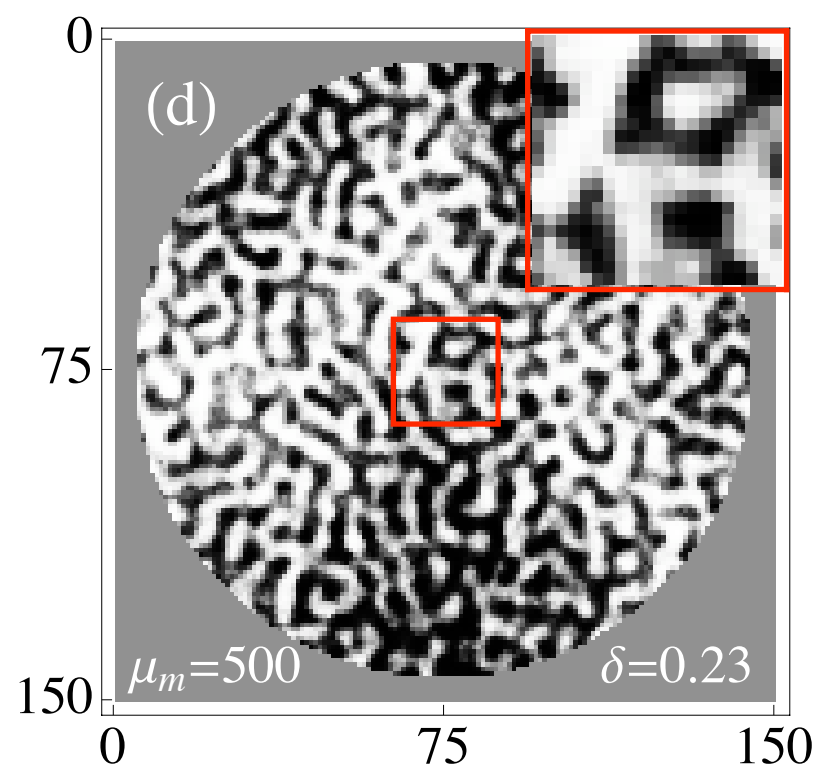
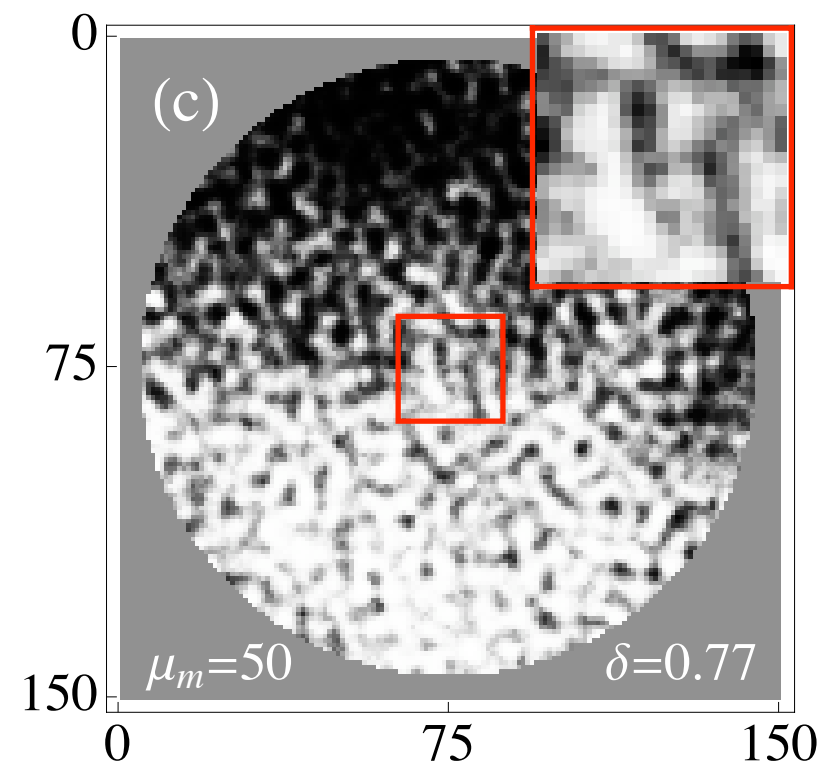
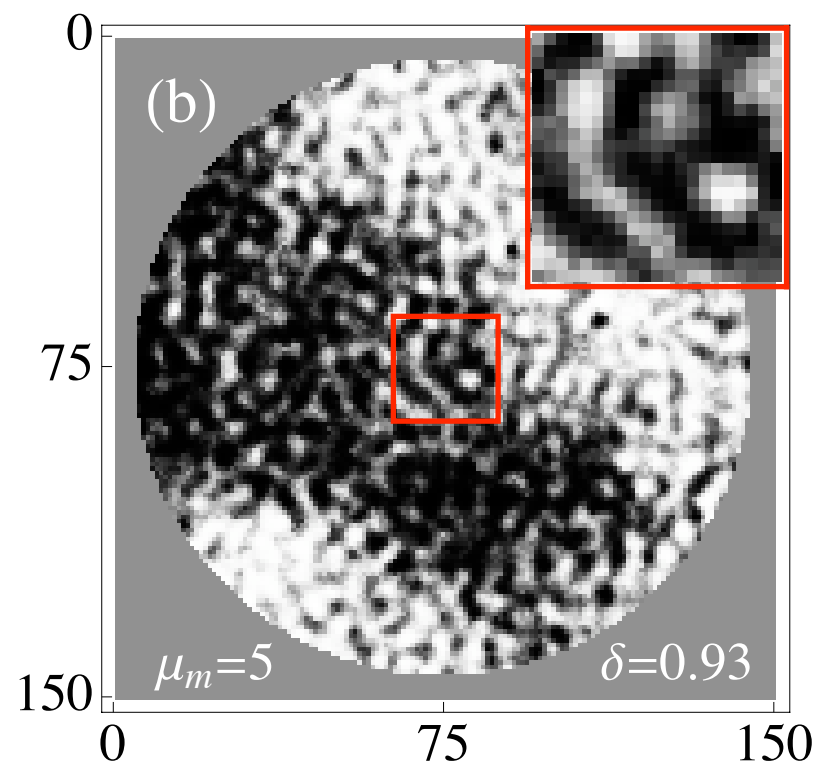
simulated data







# Fourier transform holography\* simulations



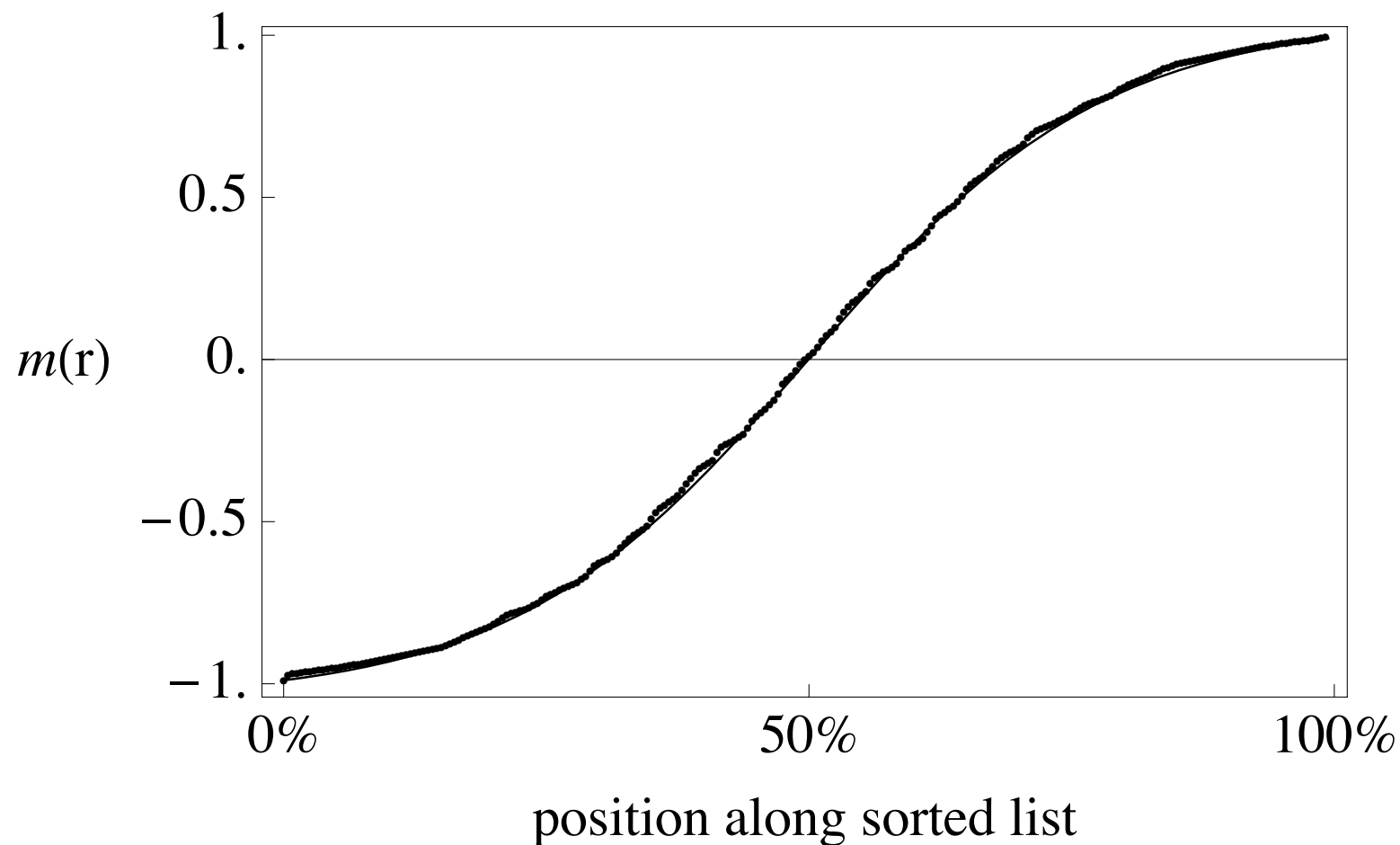
\* Eisebitt et al., Nature 432, 885-888 (2004)

## decoding tricks:

- histogram constraint on contrast
- speckle-filter intensity
- error-stabilized algorithm

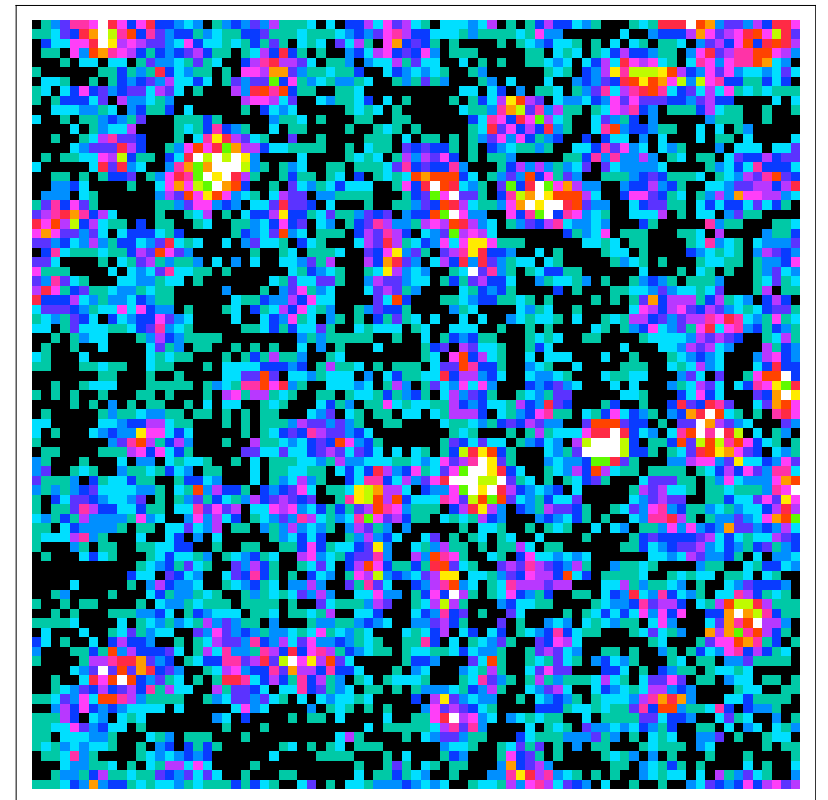
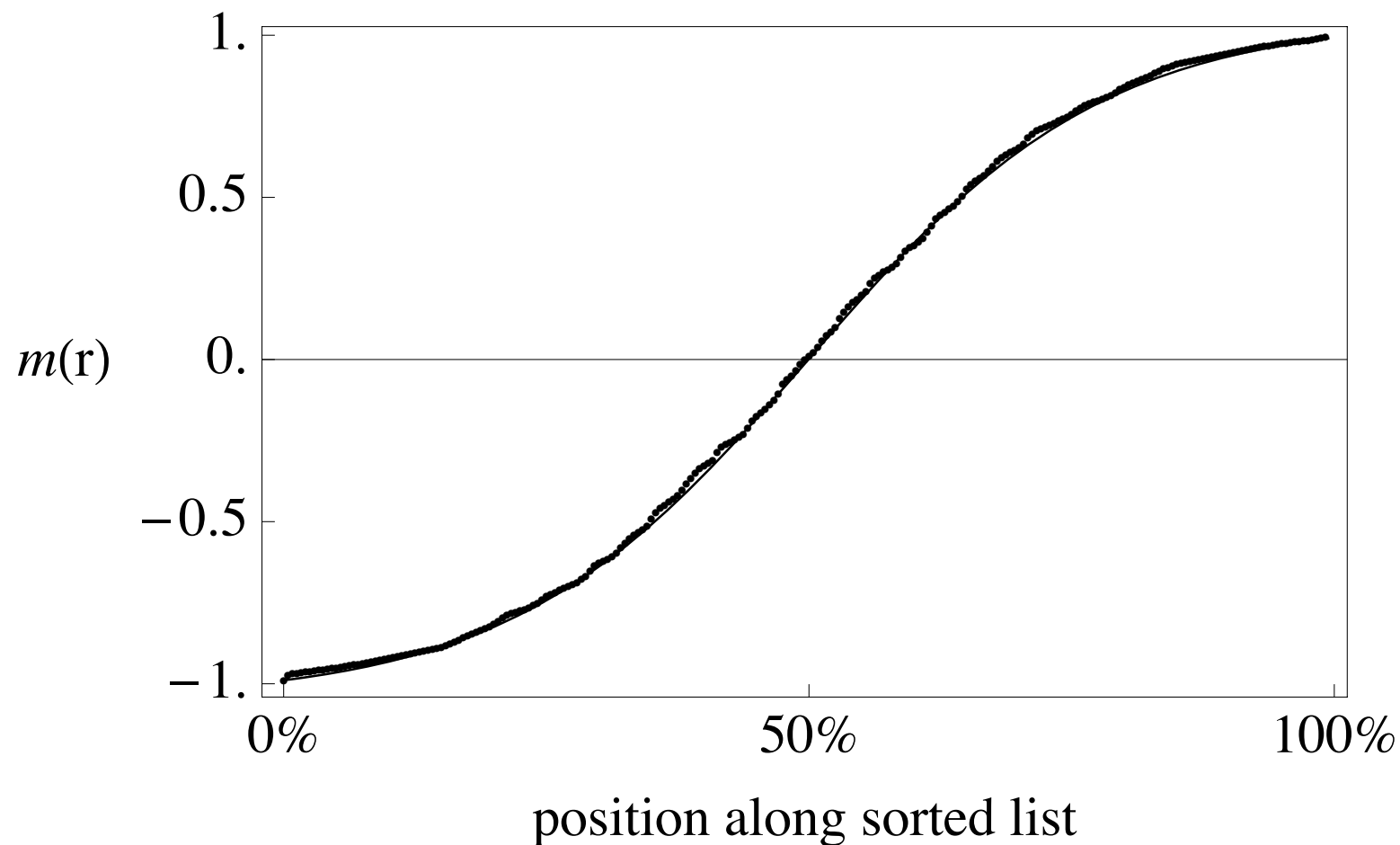
## decoding tricks:

- histogram constraint on contrast
- speckle-filter intensity
- error-stabilized algorithm



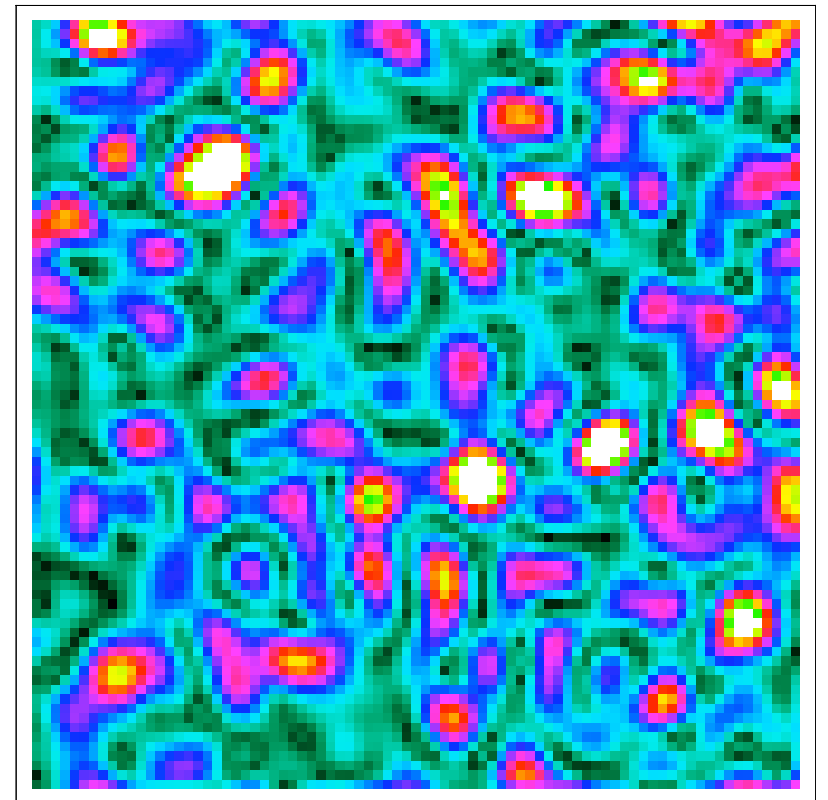
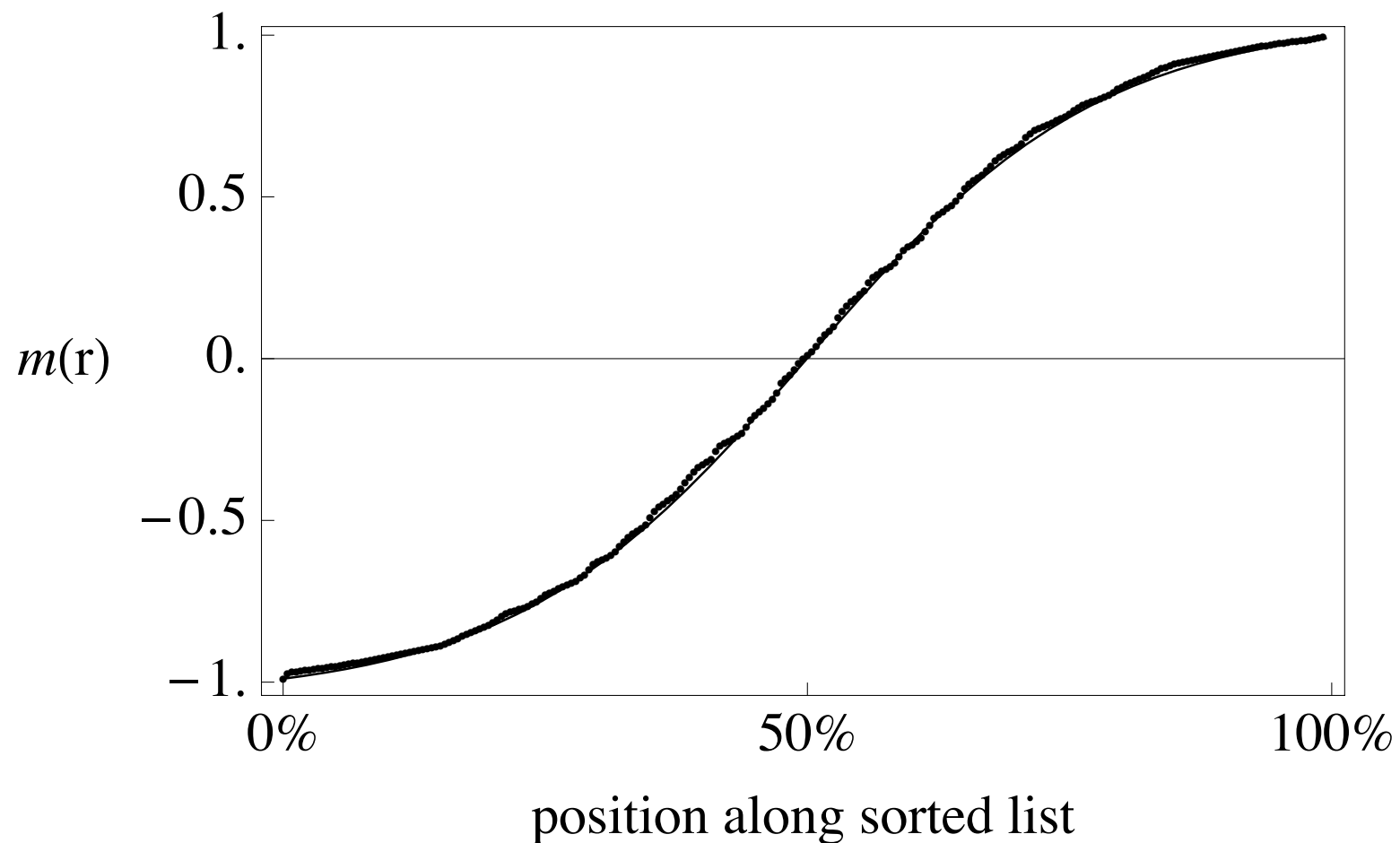
# decoding tricks:

- histogram constraint on contrast
- speckle-filter intensity
- error-stabilized algorithm

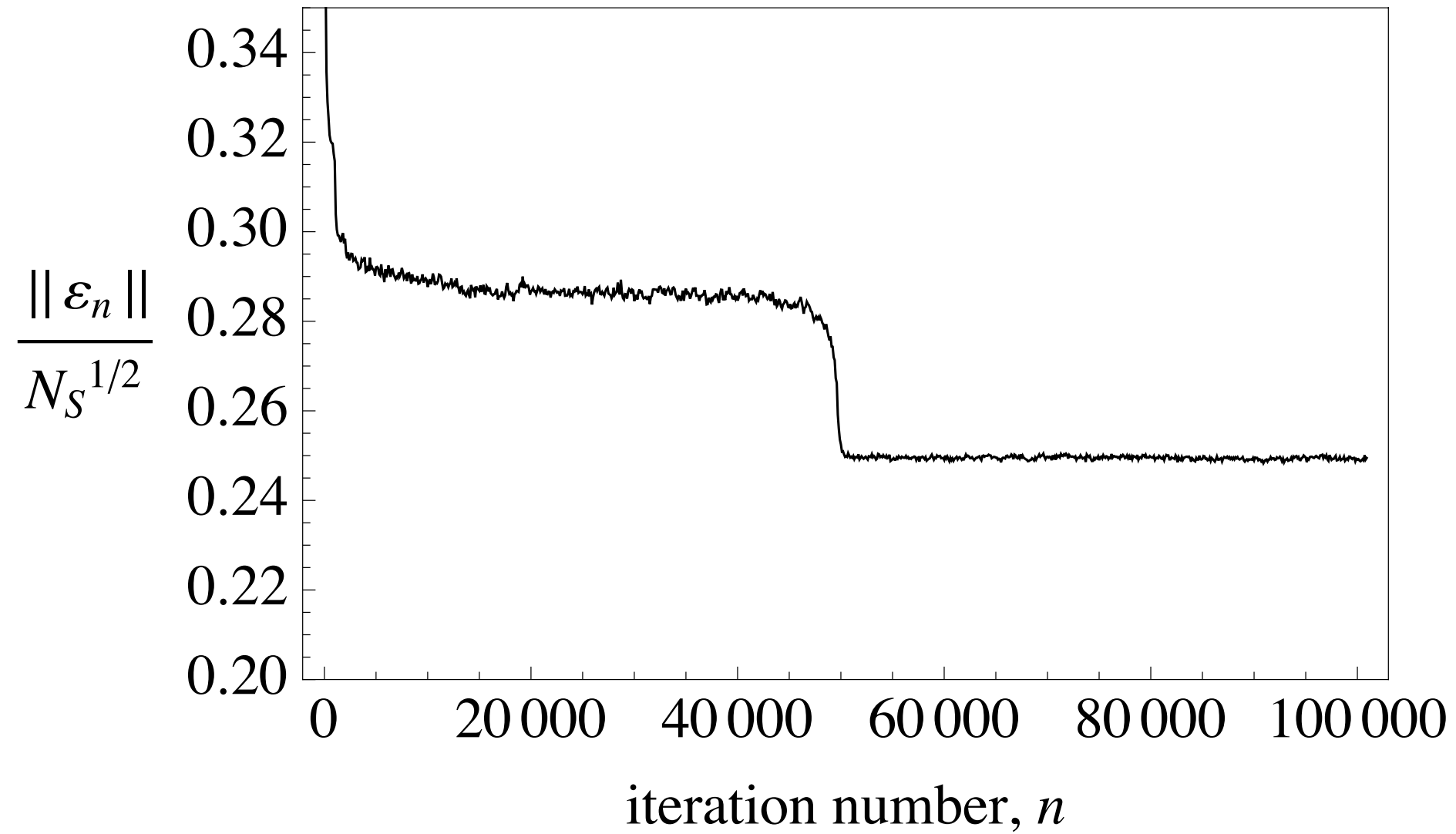


# decoding tricks:

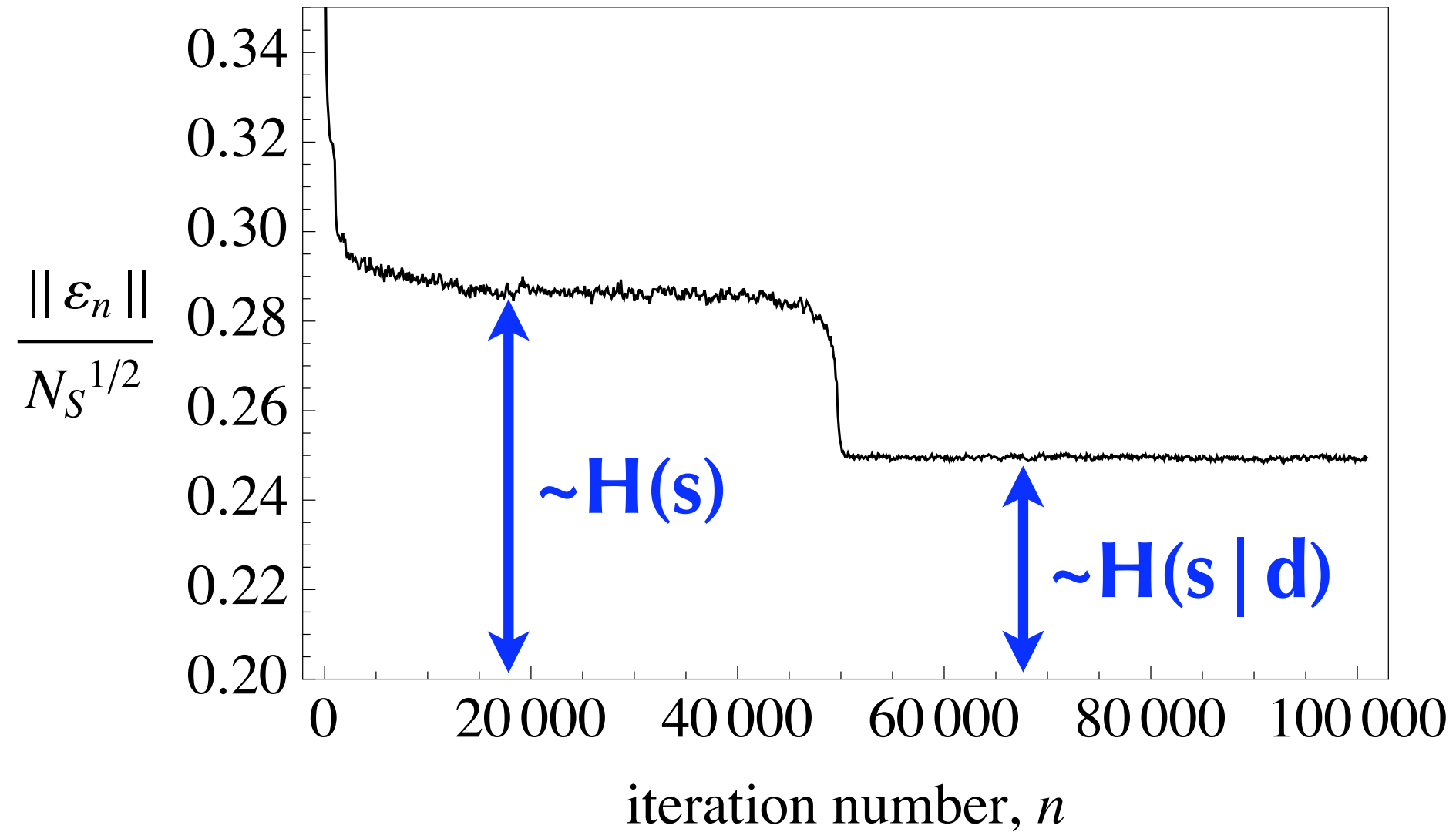
- histogram constraint on contrast
- speckle-filter intensity
- error-stabilized algorithm



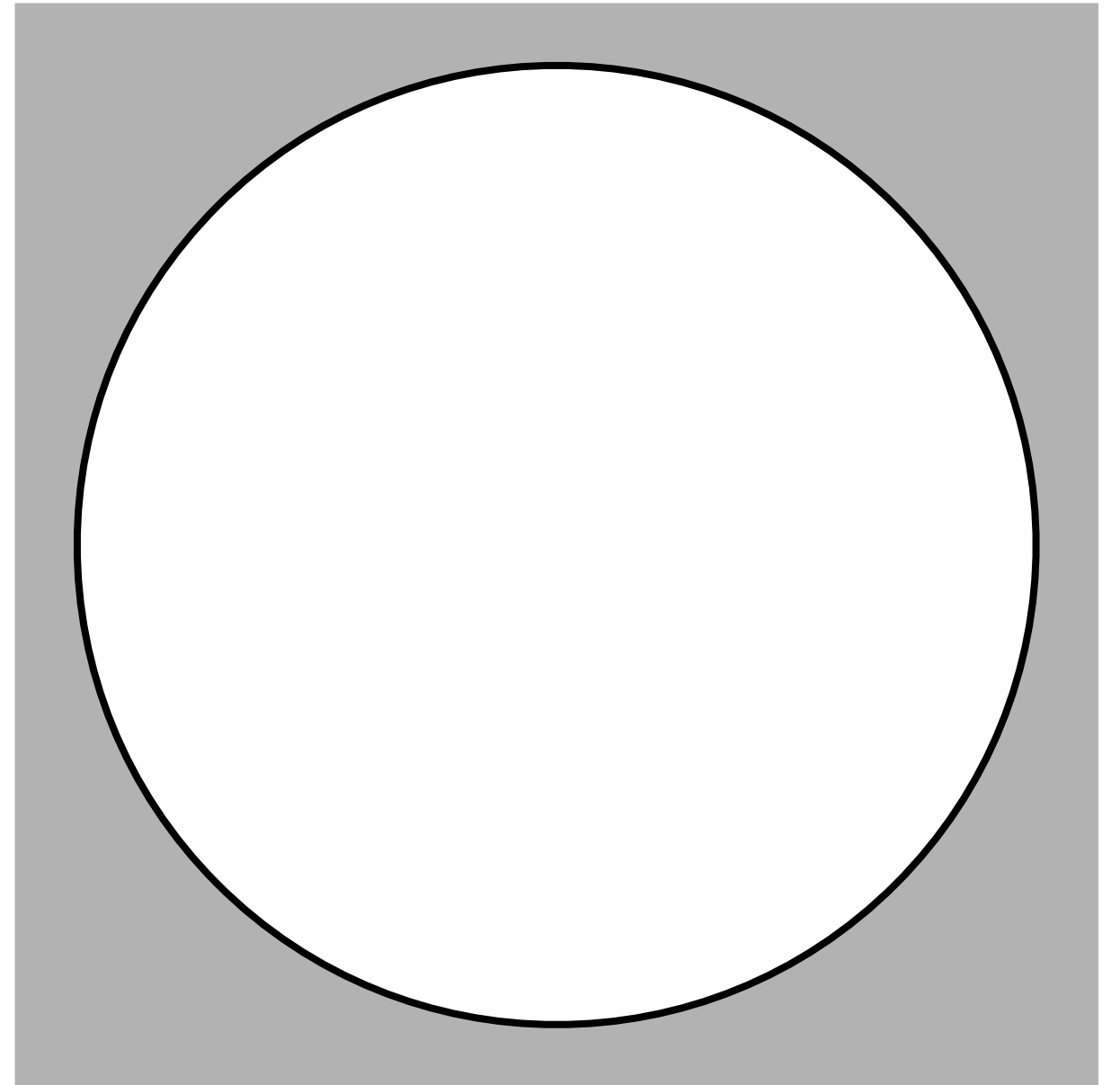
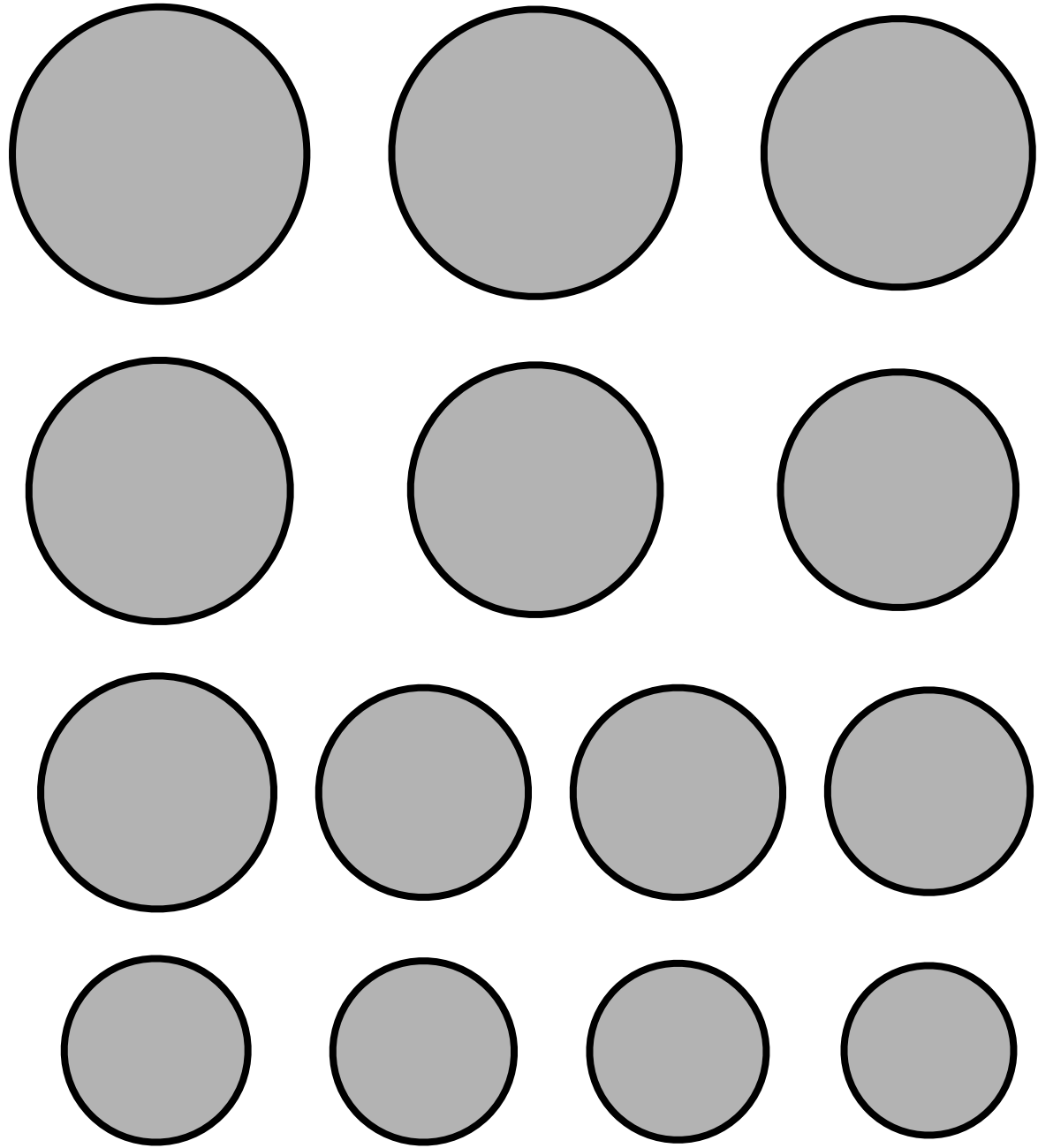
# reconstruction (decoding) algorithm



# reconstruction (decoding) algorithm







# information measures for single particle imaging



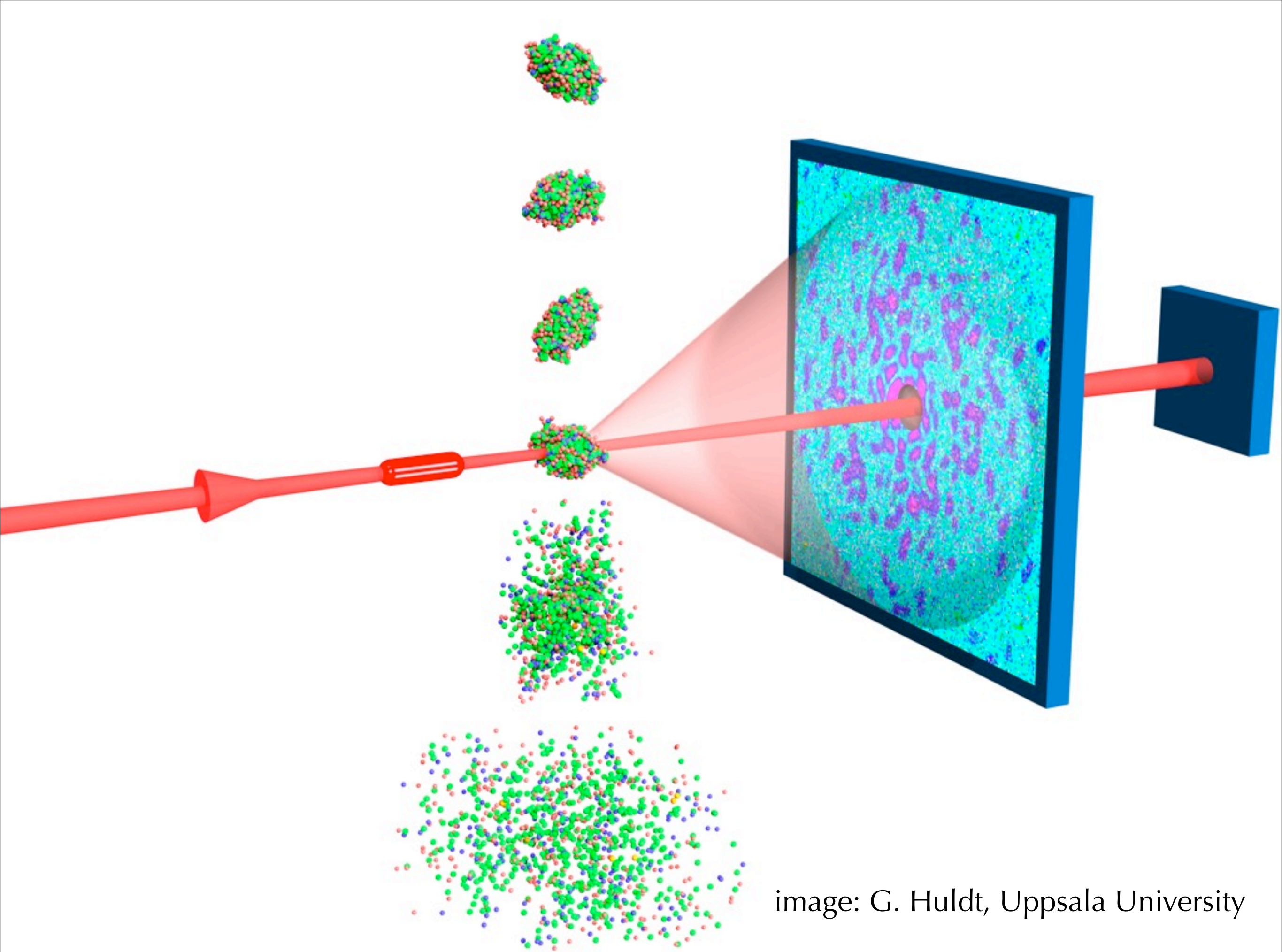
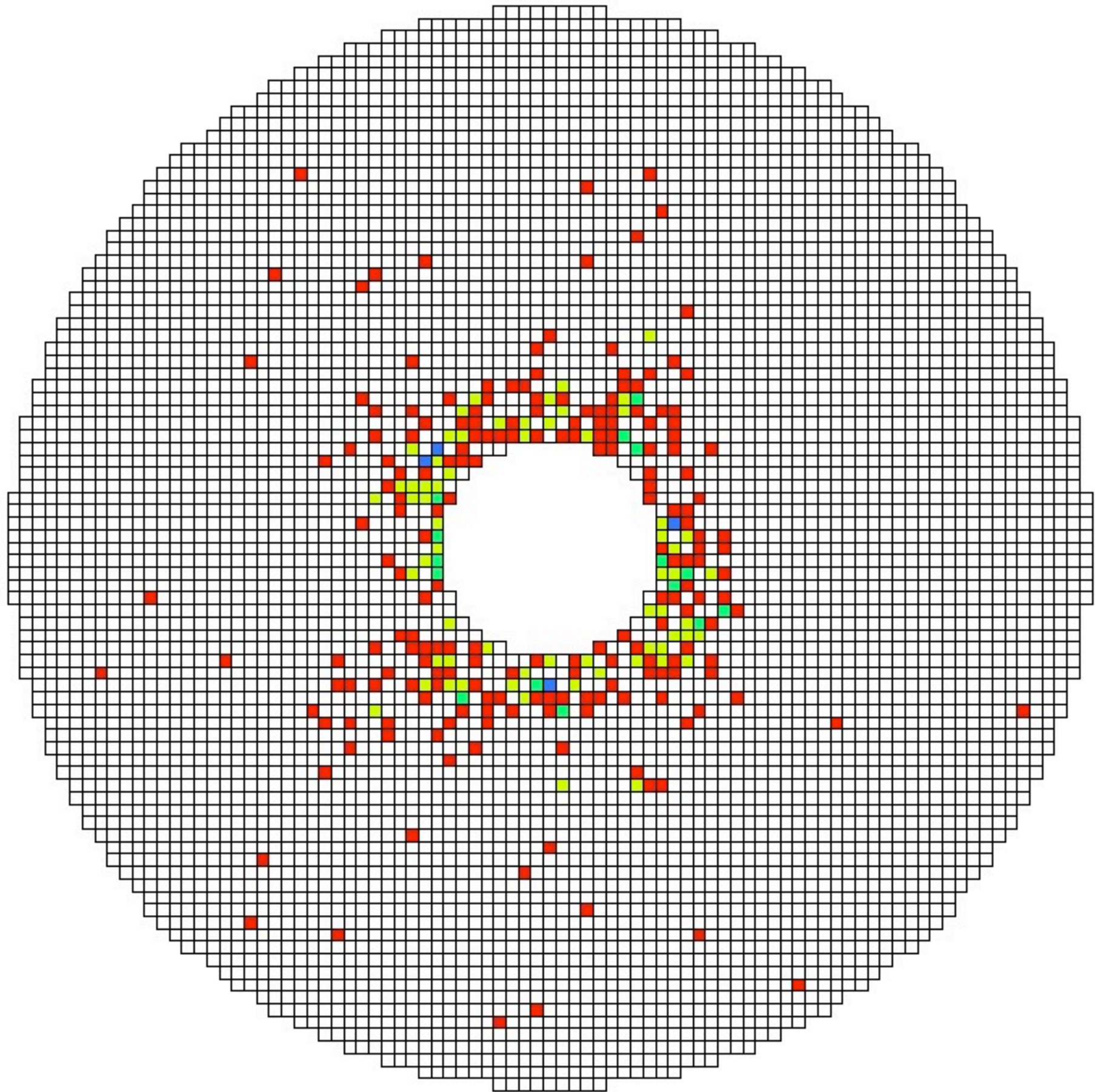
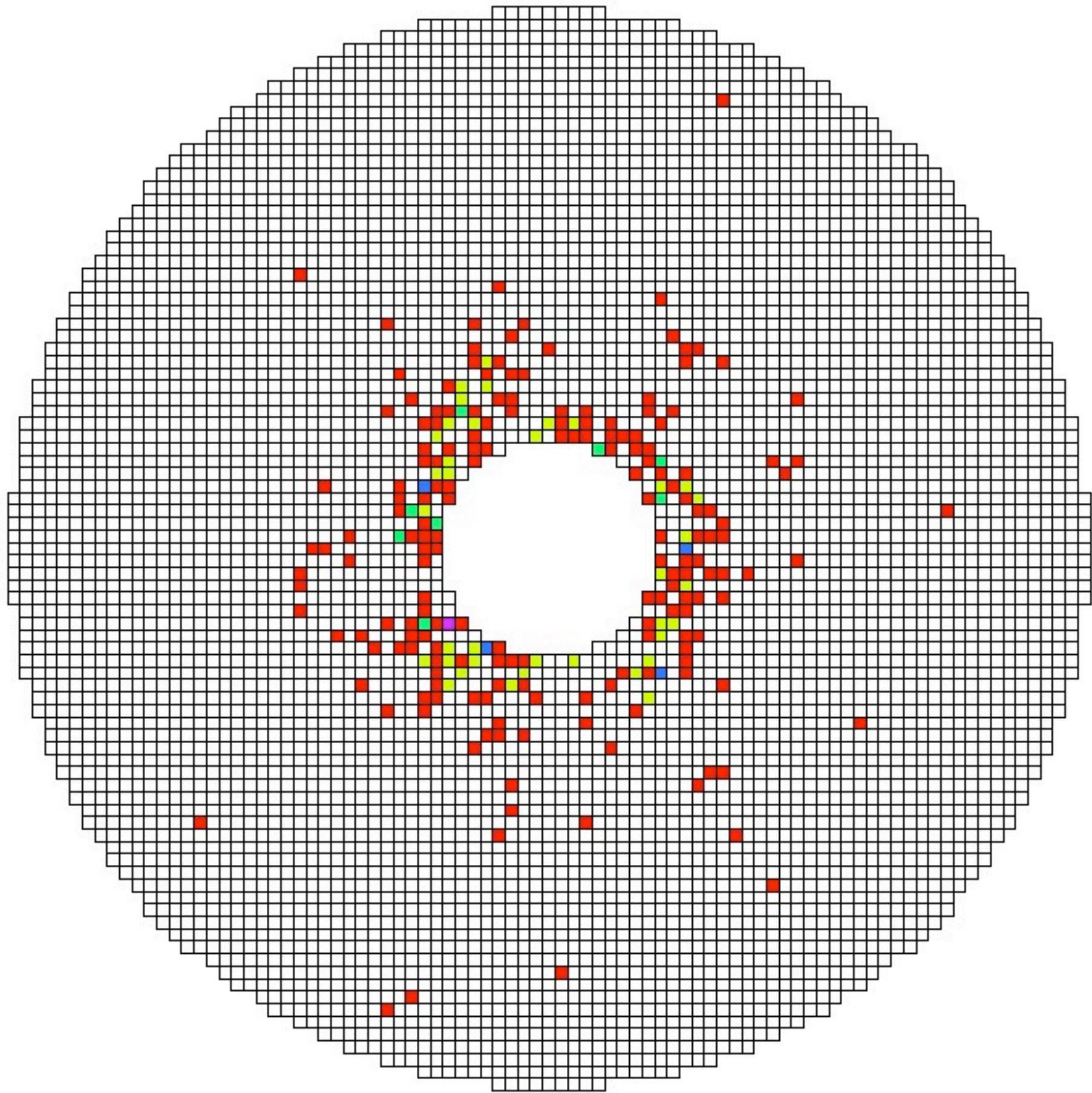


image: G. Huldt, Uppsala University







diffraction data:  $D = \{K_1, K_2, \dots, K_N\}$  (N hits)

diffraction data:  $D = \{K_1, K_2, \dots, K_N\}$  (N hits)

particle orientations:  $R = \{\Omega_1, \Omega_2, \dots, \Omega_N\}$  (unknown)

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3D intensity:  $W$  (to be determined)



diffraction data:  $D = \{K_1, K_2, \dots, K_N\}$  (N hits)

particle orientations:  $R = \{\Omega_1, \Omega_2, \dots, \Omega_N\}$  (unknown)

3D intensity:  $W$  (to be determined)

information capacity of experiment:  $I(\{W, R\}, D)$

diffraction data:  $D = \{K_1, K_2, \dots, K_N\}$  (N hits)

particle orientations:  $R = \{\Omega_1, \Omega_2, \dots, \Omega_N\}$  (unknown)

3D intensity:  $W$  (to be determined)

information capacity of experiment:  $I(\{W, R\}, D)$

but  $N \sim 10^6 - 10^7 \dots$

need more practical information measures

data from one hit:  $K$

particle orientation in one hit:  $\Omega$

3D intensity:  $W$

data from one hit:  $K$

particle orientation in one hit:  $\Omega$

3D intensity:  $W$

$I(K,W)$  = information rate in experiment  
with **unknown** orientation

data from one hit:  $K$

particle orientation in one hit:  $\Omega$

3D intensity:  $W$

$I(K,W)$  = information rate in experiment  
with **unknown** orientation

$I(K,W)|_{\Omega}$  = information rate in experiment  
with **known** orientation

# reduced information rate

$$r = \frac{I(K, W)}{I(K, W)|_{\Omega}} = \text{ratio of information rates without/with orientation}$$

V. Elser, IEEE Trans. Information Theory 55, 4715-22 (2009)

# reduced information rate

$$r = \frac{I(K, W)}{I(K, W) |_{\Omega}} = \text{ratio of information rates} \\ \text{without/with orientation}$$

$$r = \frac{I(K, W)}{I(K, W) + I(K, \Omega) |_W}$$

V. Elser, IEEE Trans. Information Theory 55, 4715-22 (2009)

# reduced information rate

$$r = \frac{I(K, W)}{I(K, W) |_{\Omega}} = \text{ratio of information rates without/with orientation}$$

$$r = \frac{I(K, W)}{I(K, W) + I(K, \Omega) |_W}$$

**$r = 1/2$  :**

information in one hit

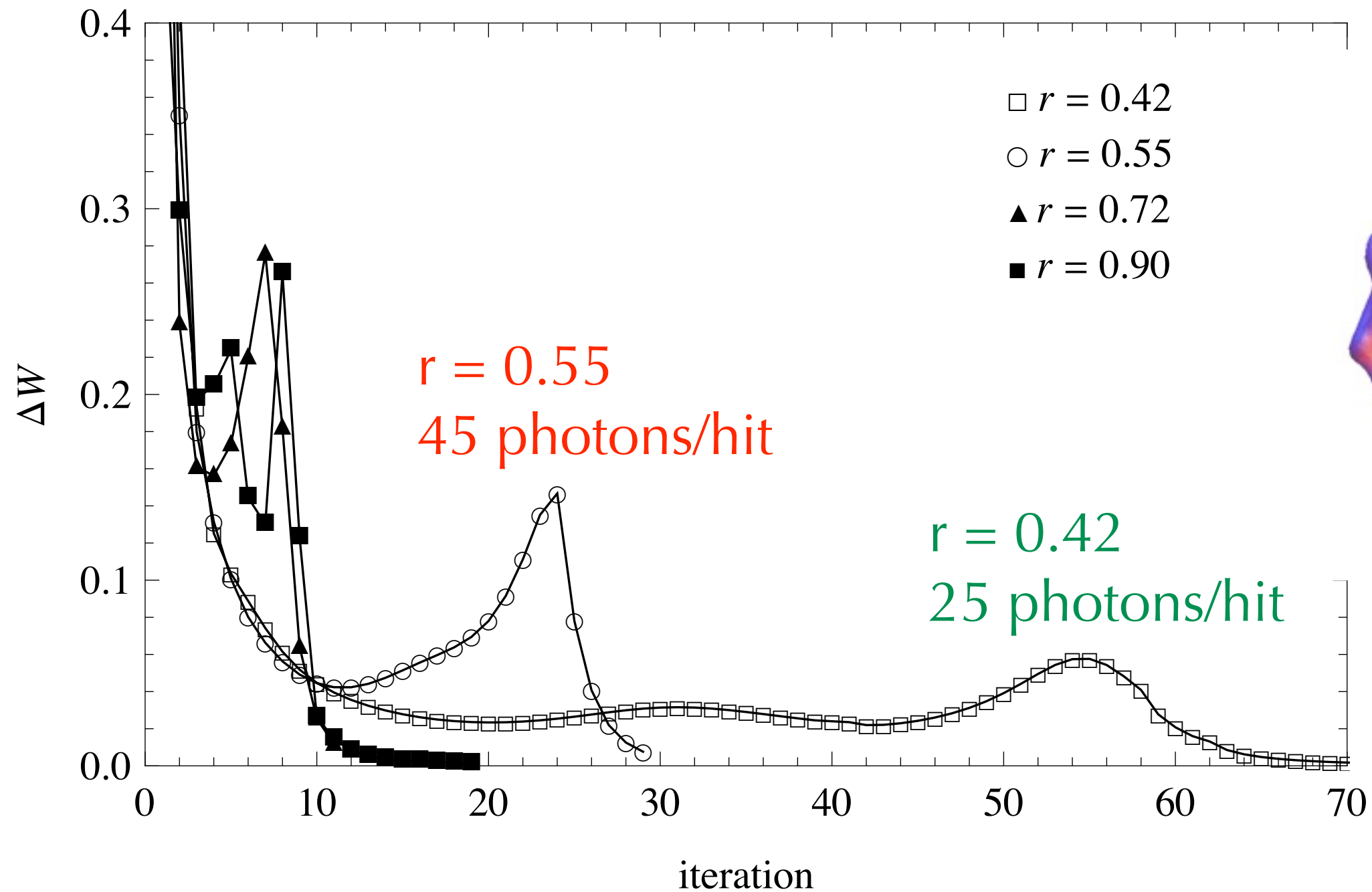
=

information obtained about **orientation**

V. Elser, IEEE Trans. Information Theory 55, 4715-22 (2009)

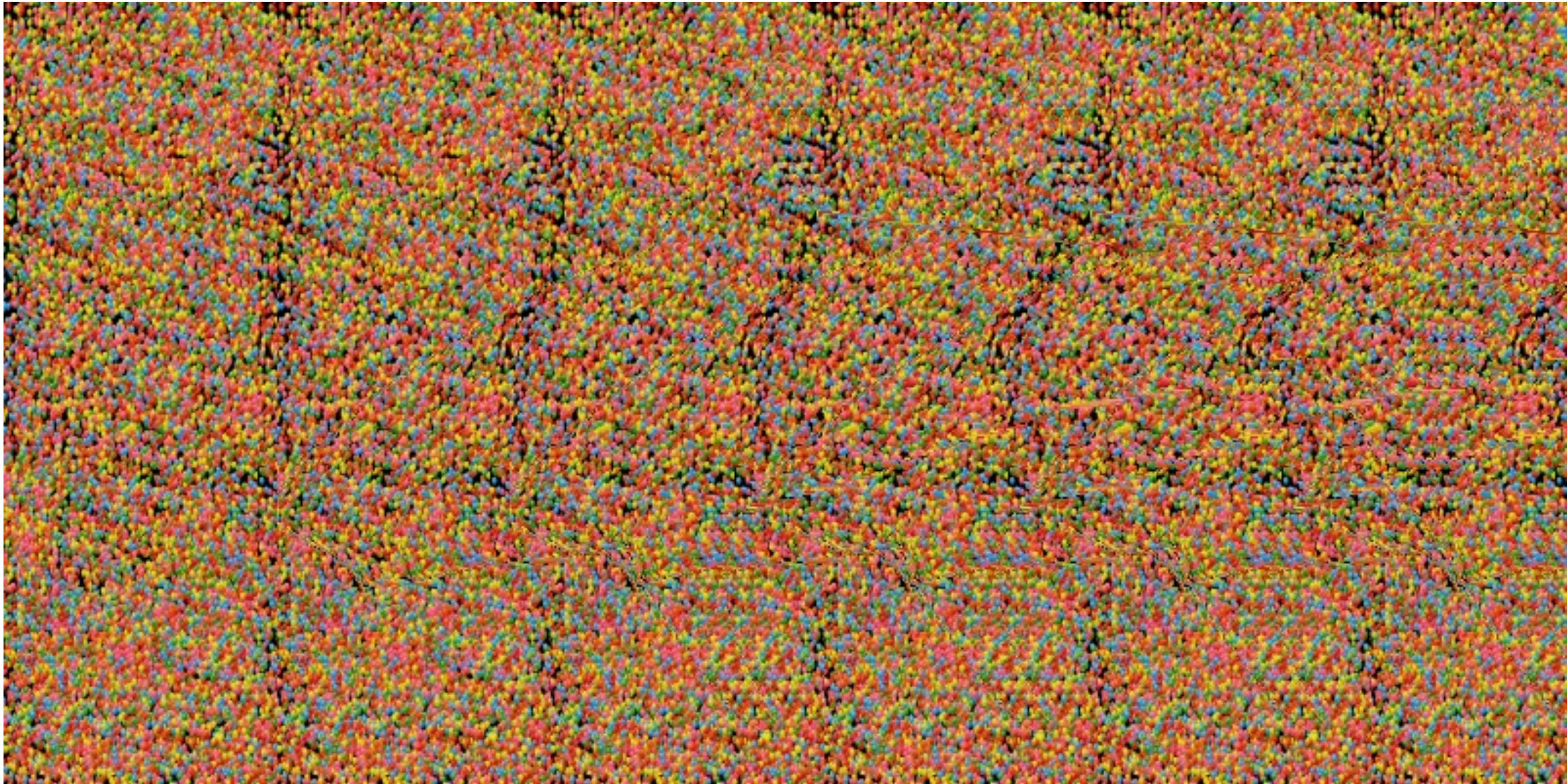


# EMC algorithm convergence



Loh & Elser, Phys. Rev. E 80, 026705 (2009)





Thank you for your attention