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The EMC algorithm: 3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

Cornell University

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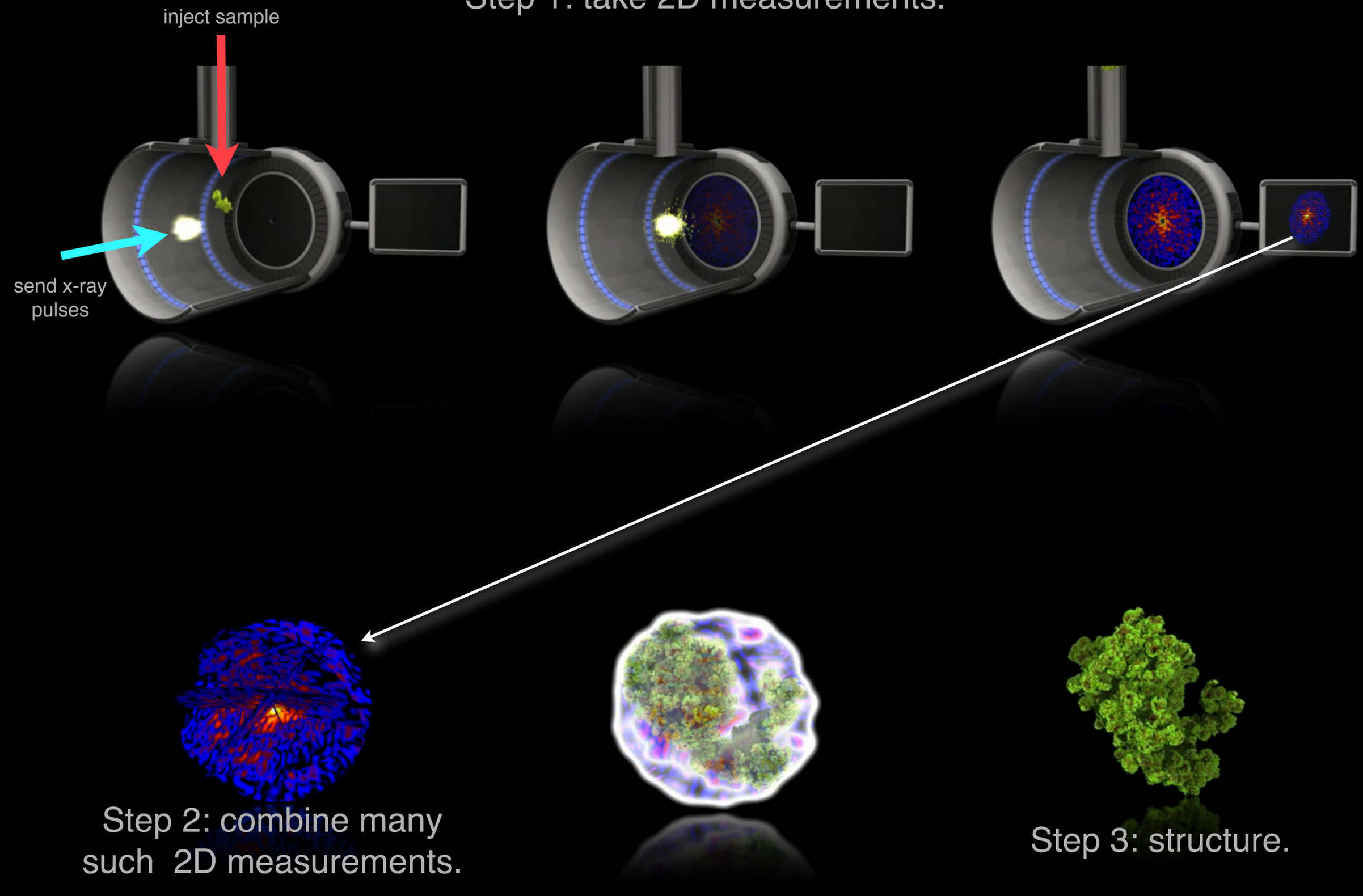
Step 1: take 2D measurements.



Step 2: combine many such 2D measurements.

Step 3: structure.

Movie stills from LCLS's website.

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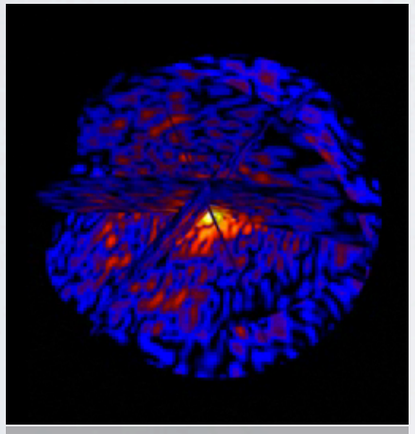
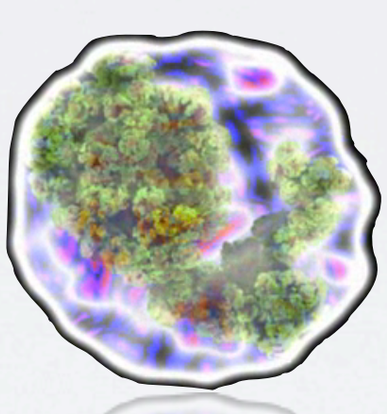
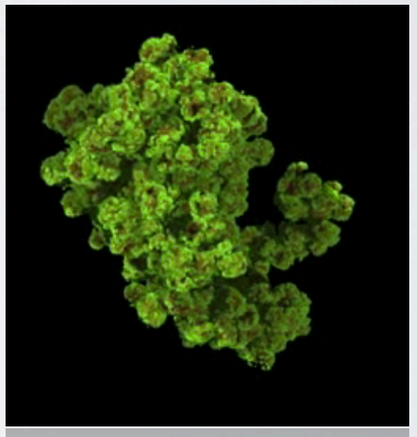
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.







Magic happens!

Movie stills from LCLS's website.

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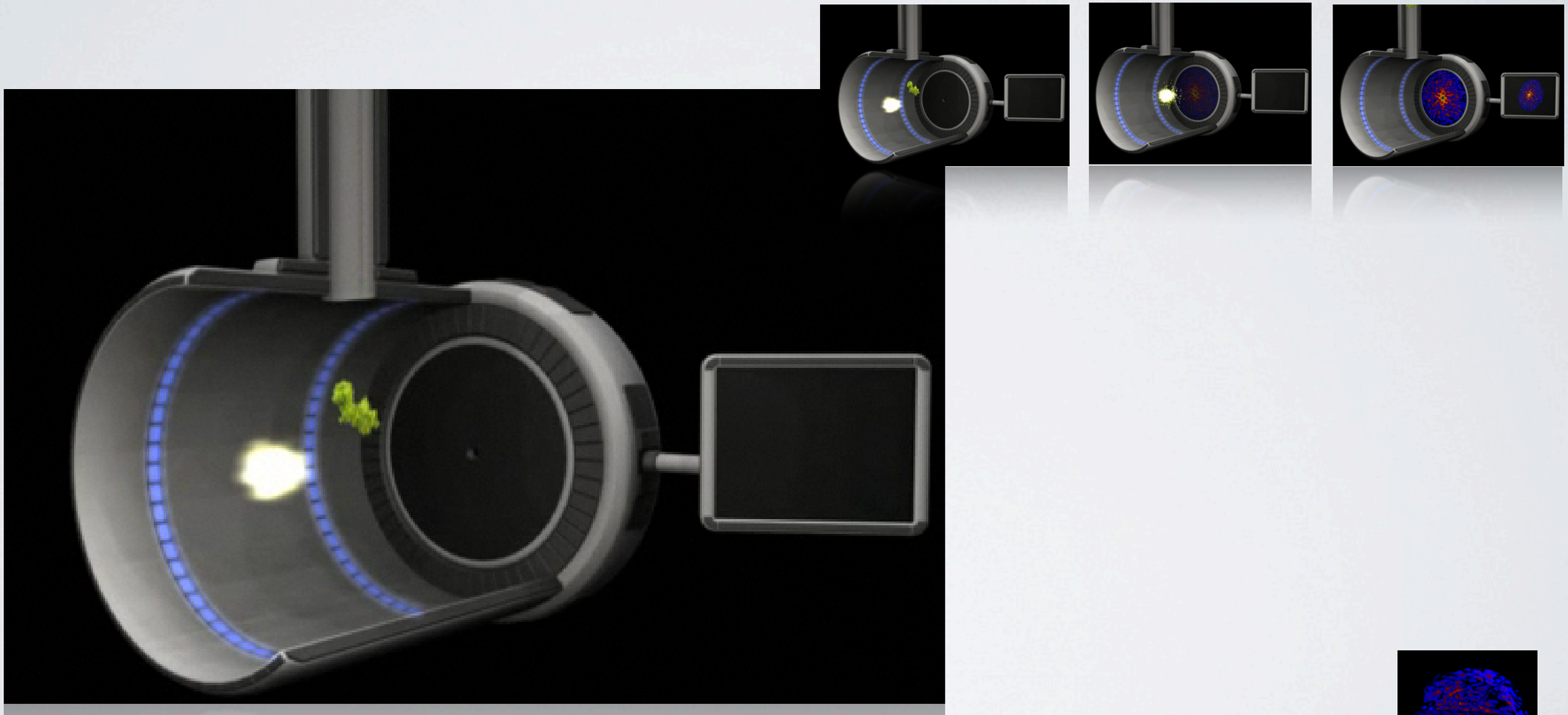
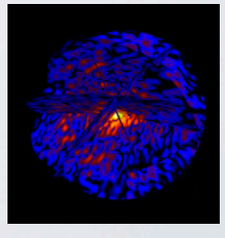
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.





Movie stills from LCLS's website.

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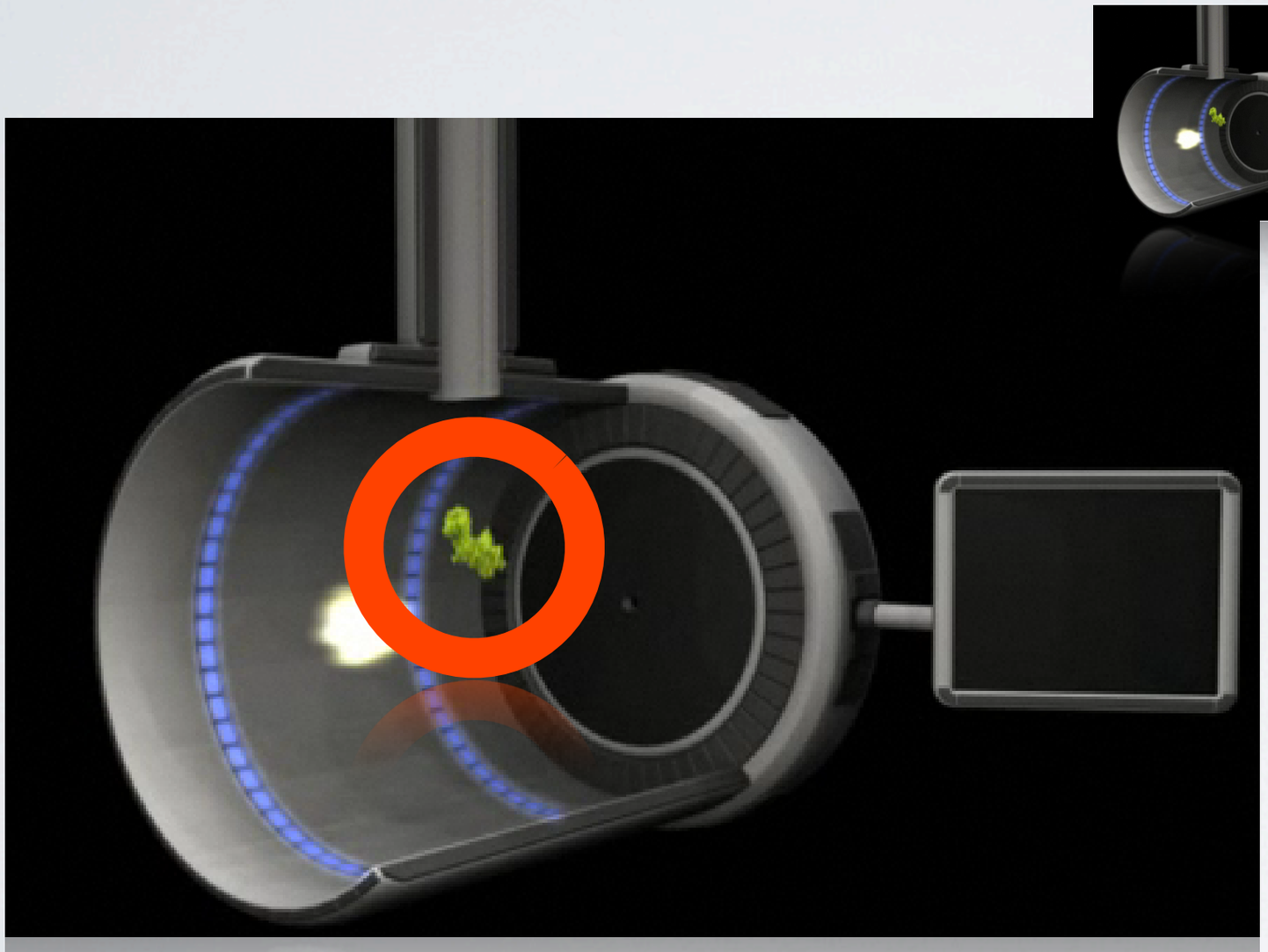
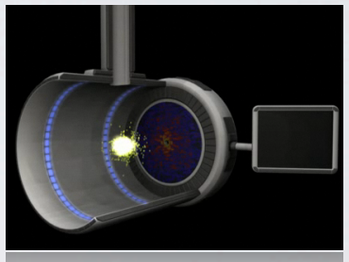
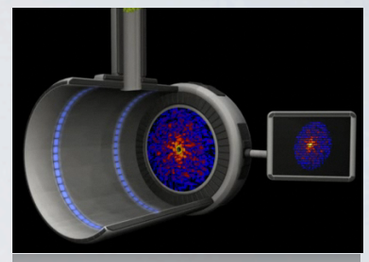
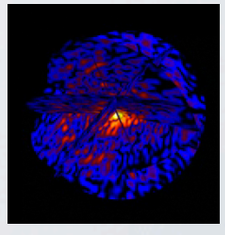
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.









Movie stills from LCLS's website.

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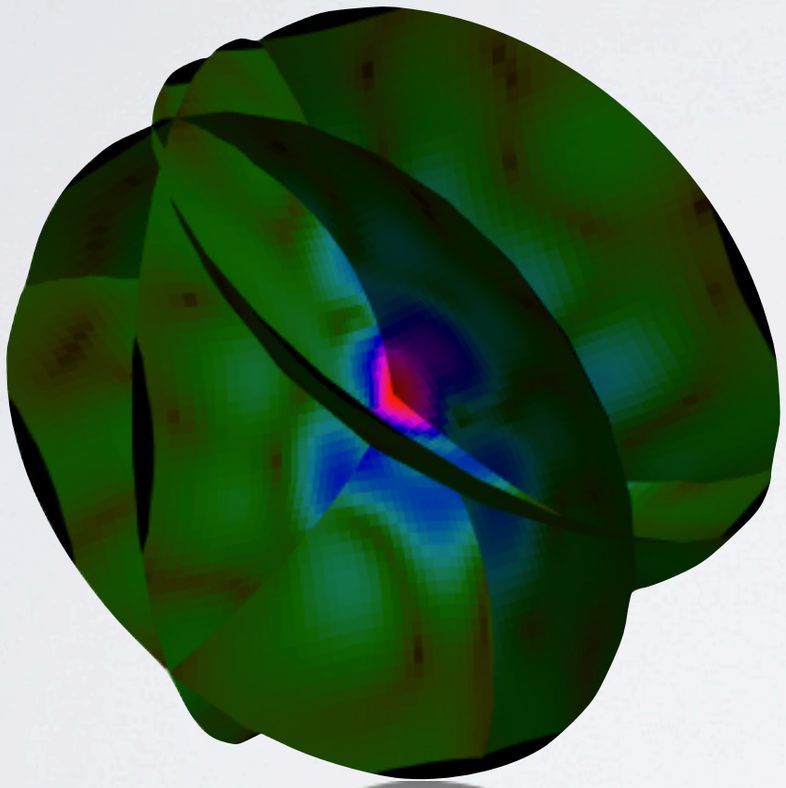
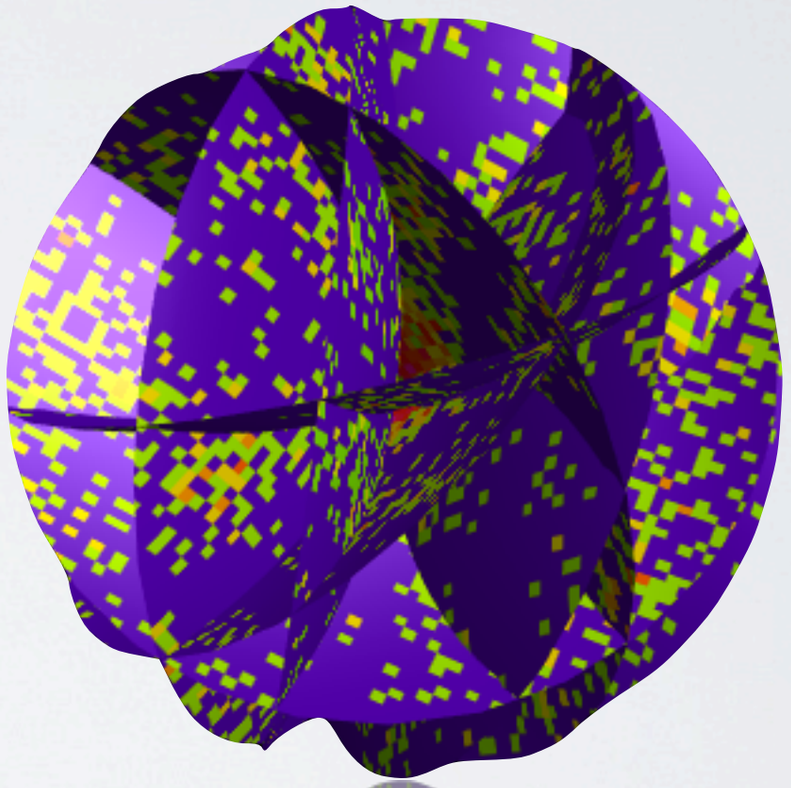
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

Noiseless diffraction.



Expected photon-limited diffraction.



Noise and unknown data orientations
make merging more challenging.

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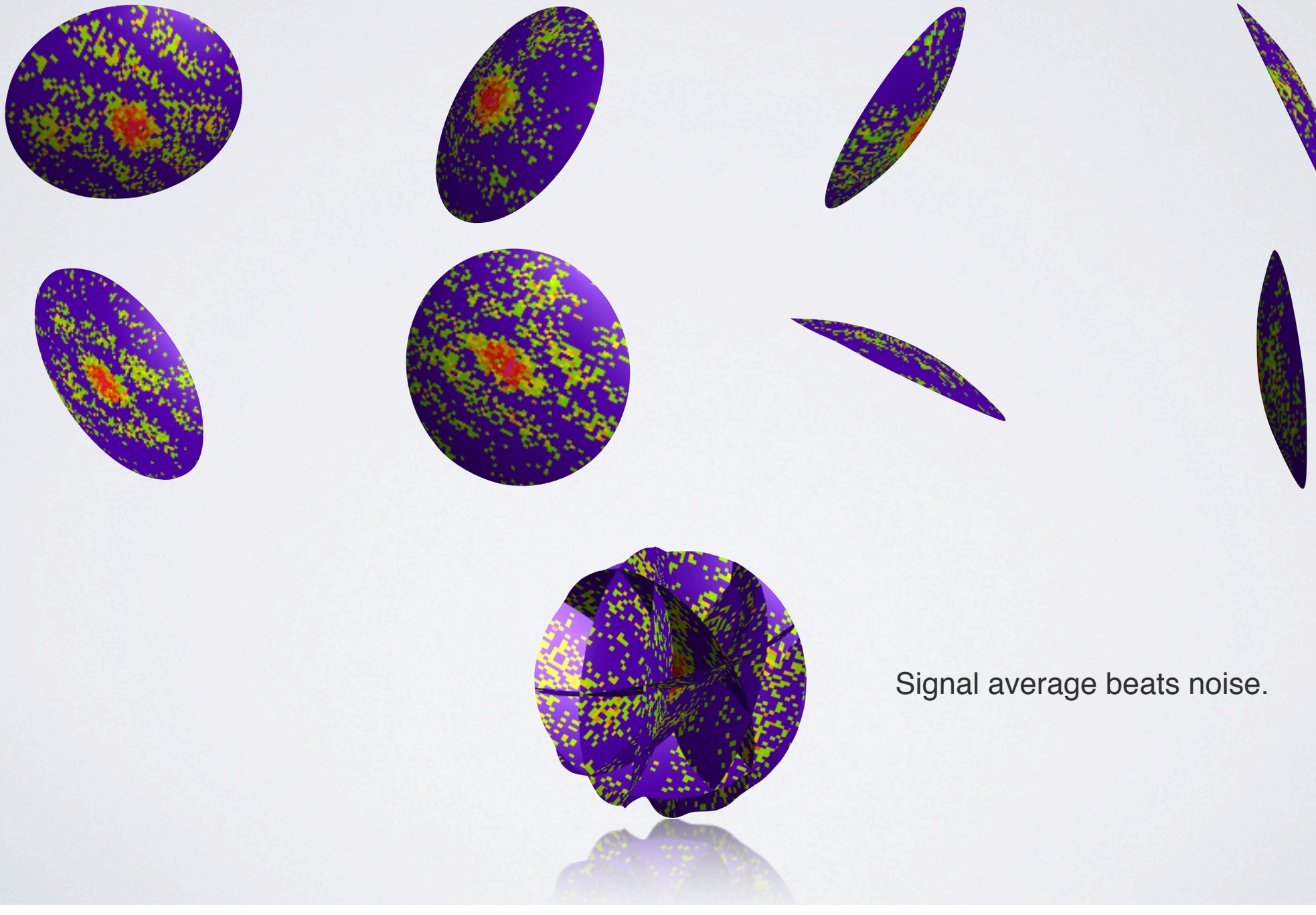
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.



Signal average beats noise.

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The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

EMC: **E**xpand-**M**aximize-**C**ompress.

Veit Elser, Cornell University.

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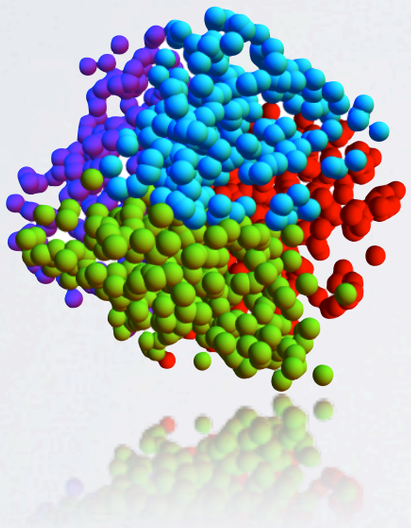
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

Heuristic;
e.g. K-means clustering.



EMC is principled.

P(orientation| data,current guess)

Poisson statistics;
no undetermined parameters

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The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

How is EMC related to:
- Maximum likelihood estimator?
- Likelihood maximization?
- Expectation maximization?

Different treatments of Likelihood function.

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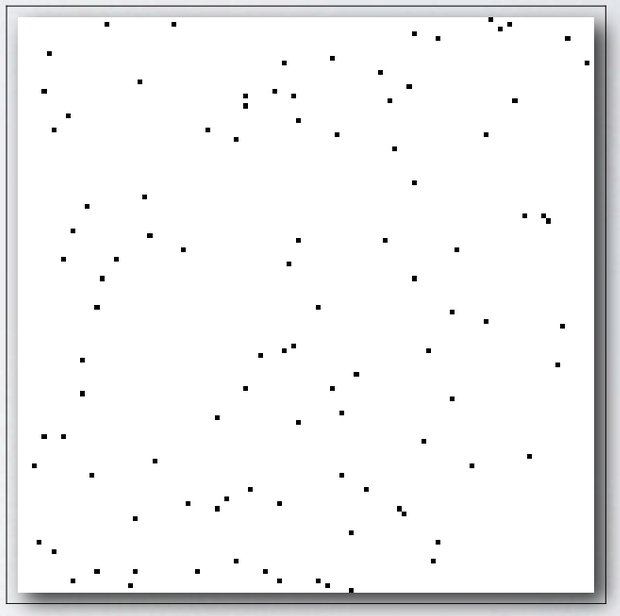
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

?

Noisy, unoriented data.



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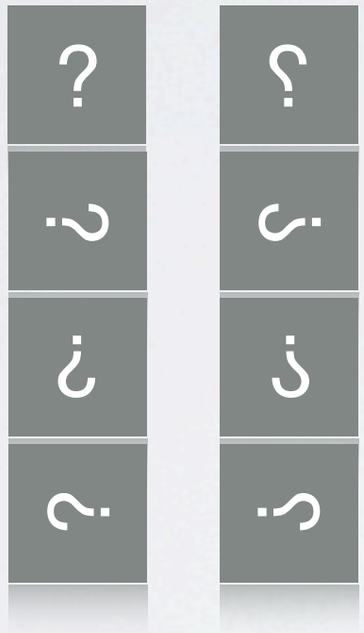
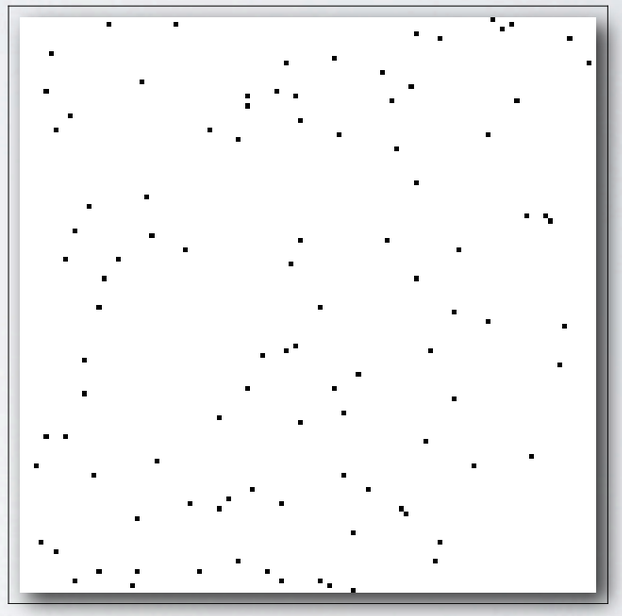
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D



Noisy, unoriented data.



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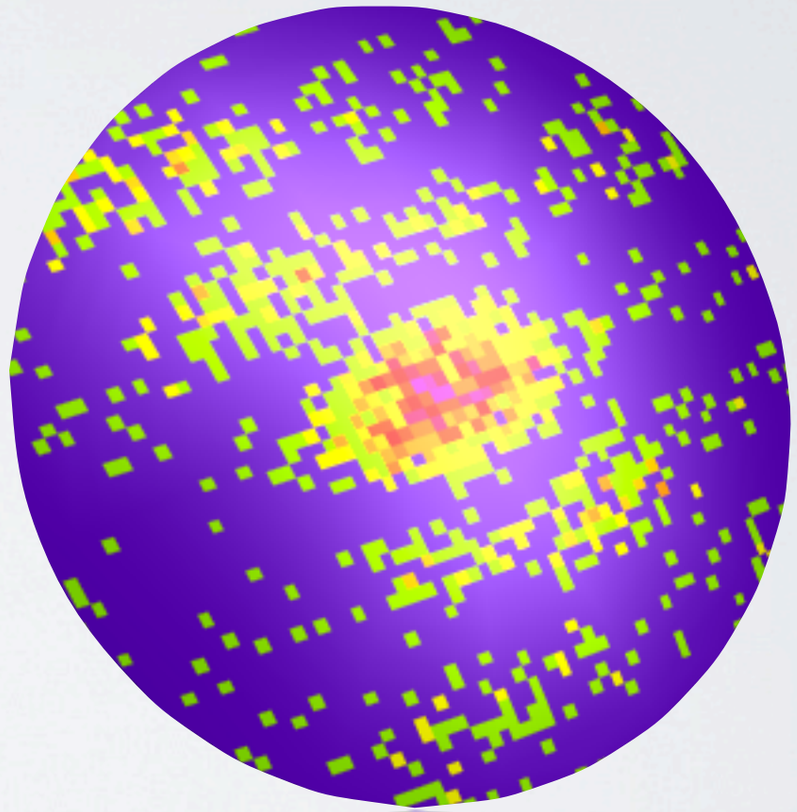
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D



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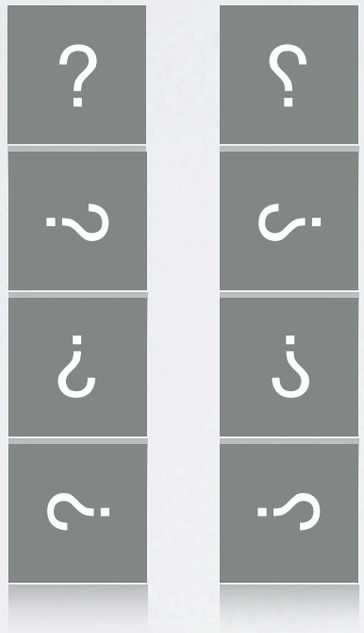
The EMC algorithm:

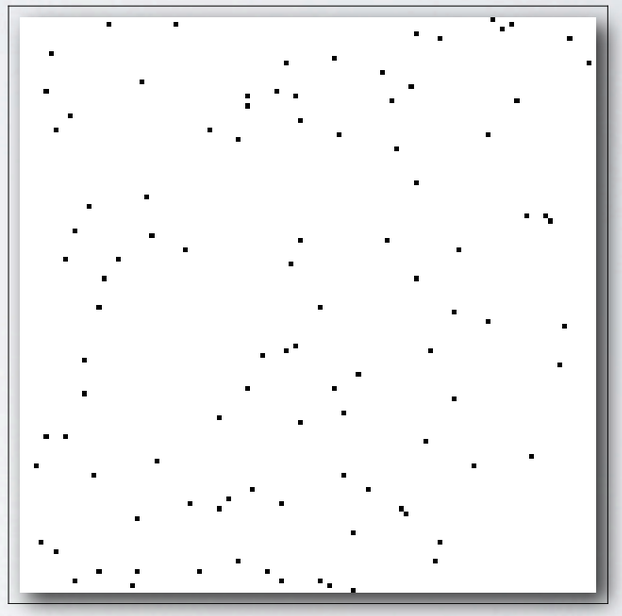
3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

How to recover data orientation if you don't know the source image?



Noisy, unoriented data.



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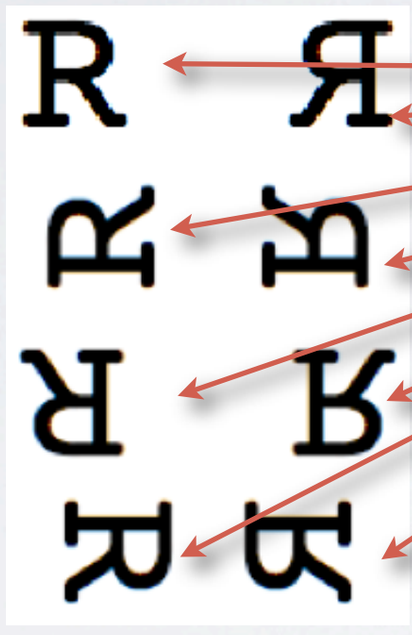
The EMC algorithm:

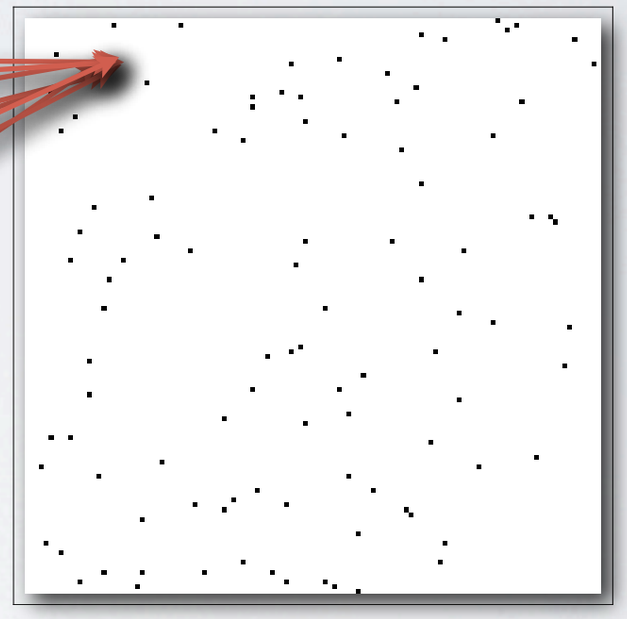
3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

What if you **knew** the source image?



Noisy, unoriented data.



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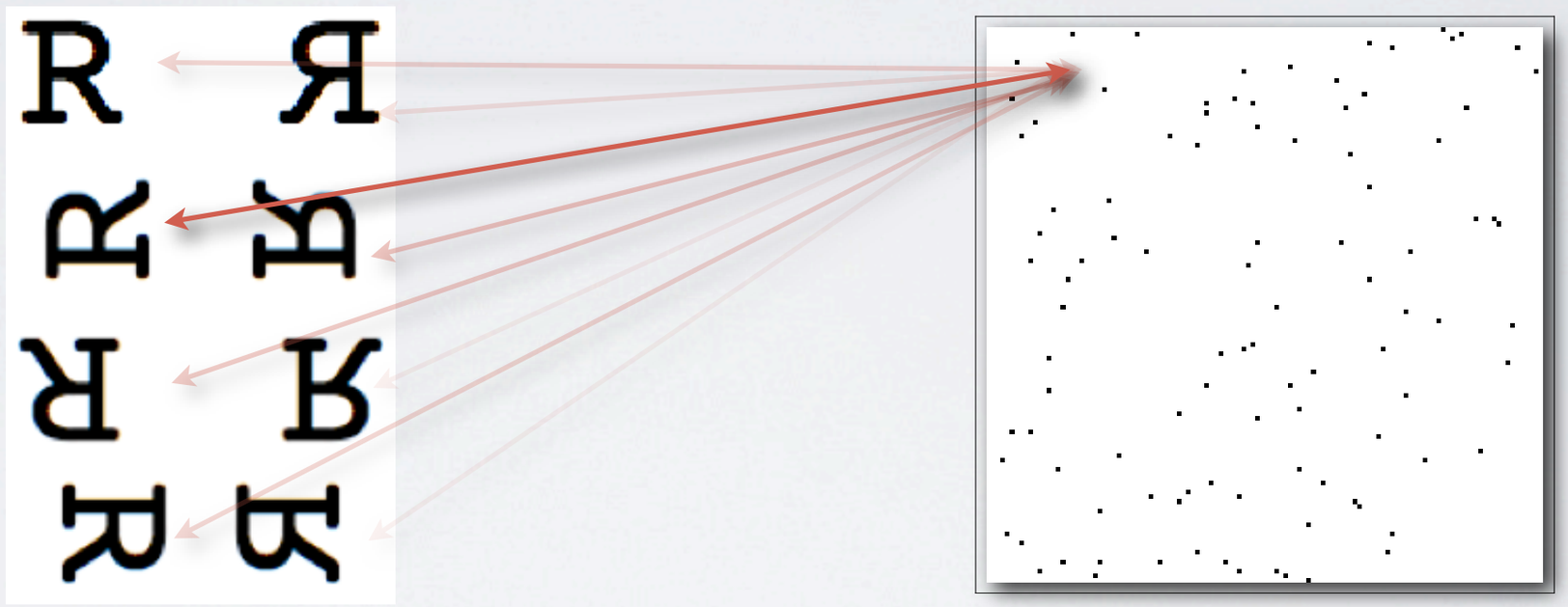
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Noisy, unoriented data.



Likelier in darker arrows.

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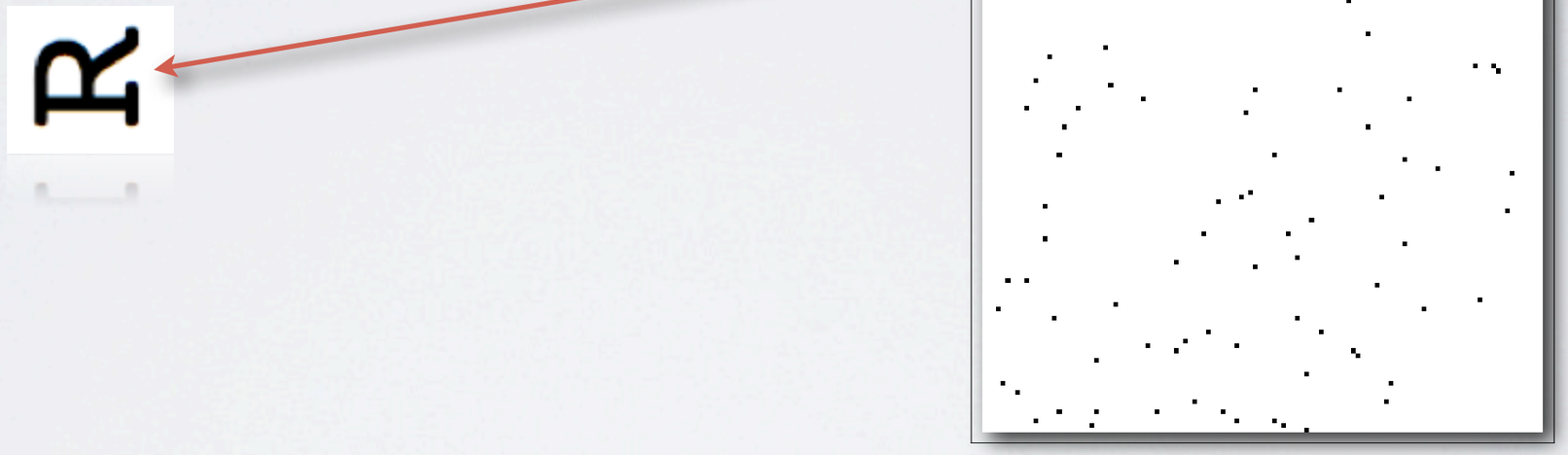
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Noisy, unoriented data.



“Hard” maximization?

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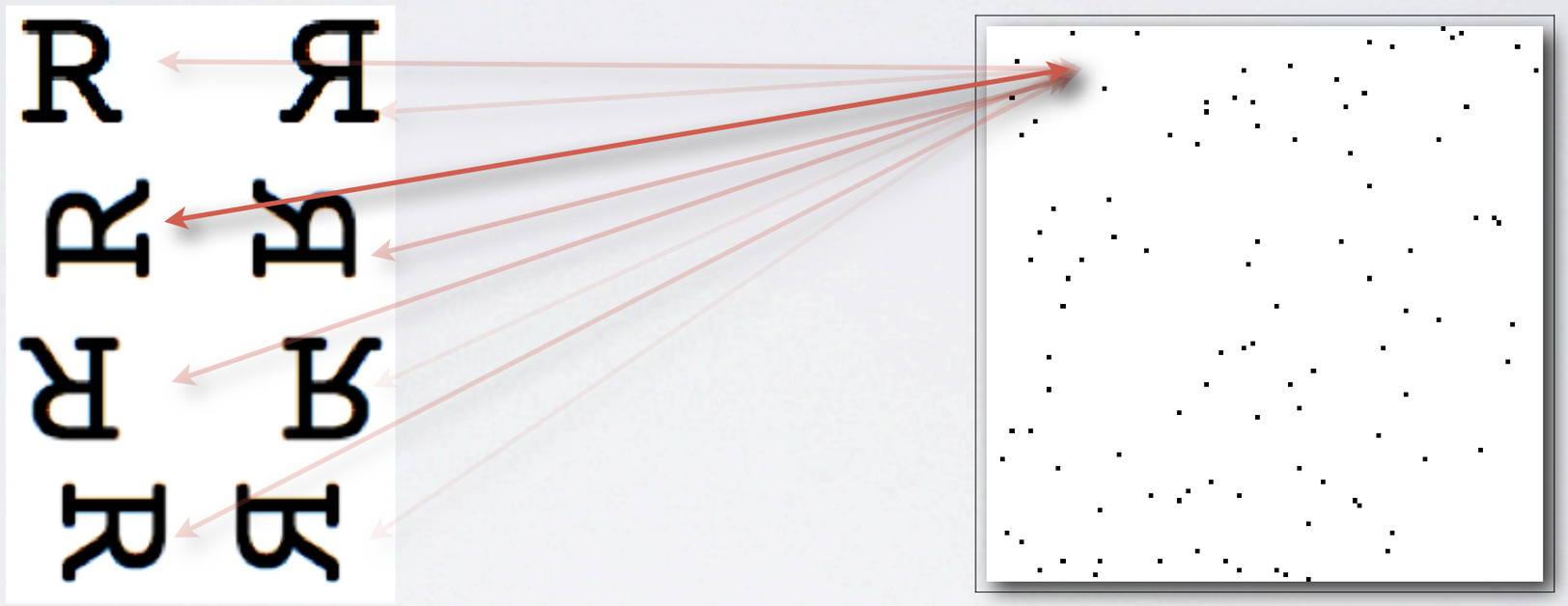
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Noisy, unoriented data.



“Soft” maximization,
because data is very noisy.

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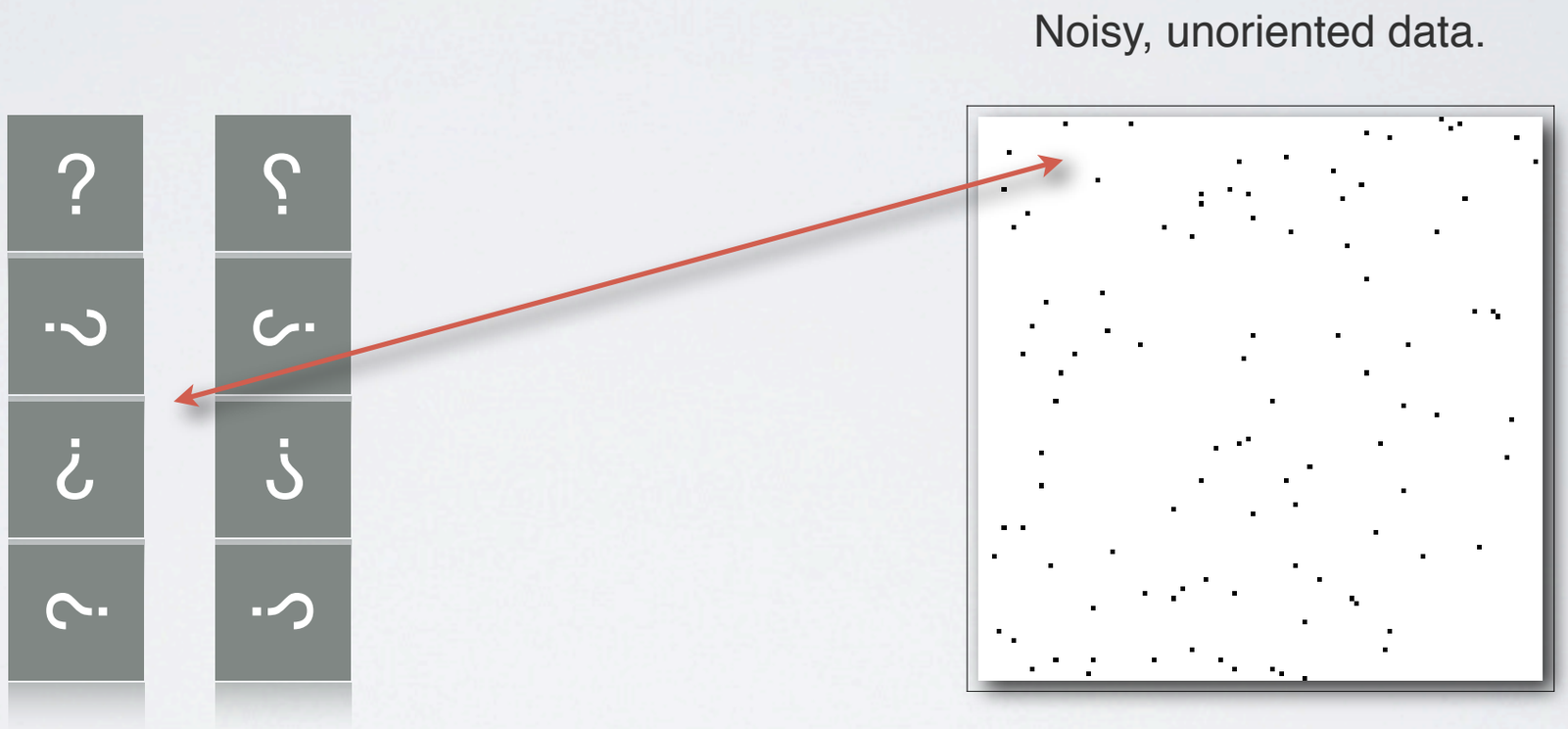
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D



How to compare?

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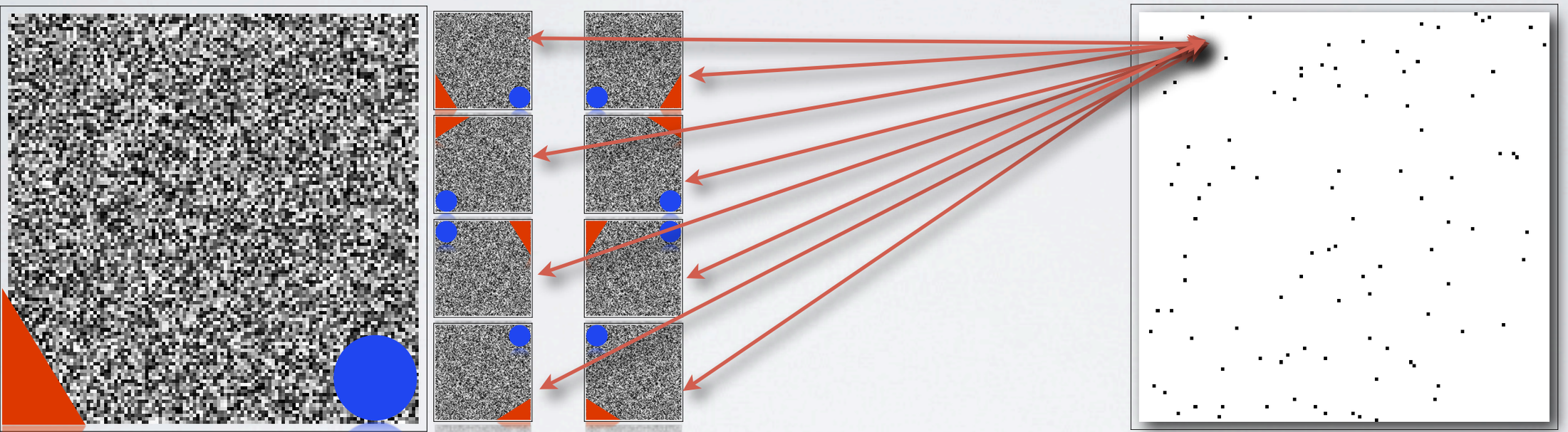
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Random guess?

Noisy, unoriented data.



Why not?

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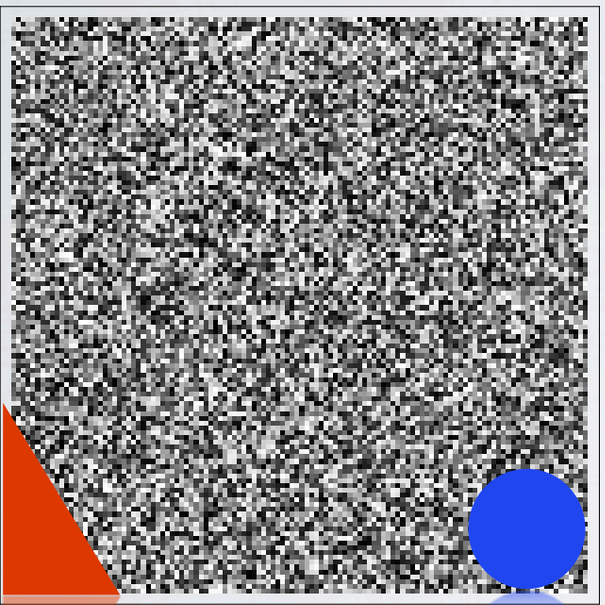
The EMC algorithm:

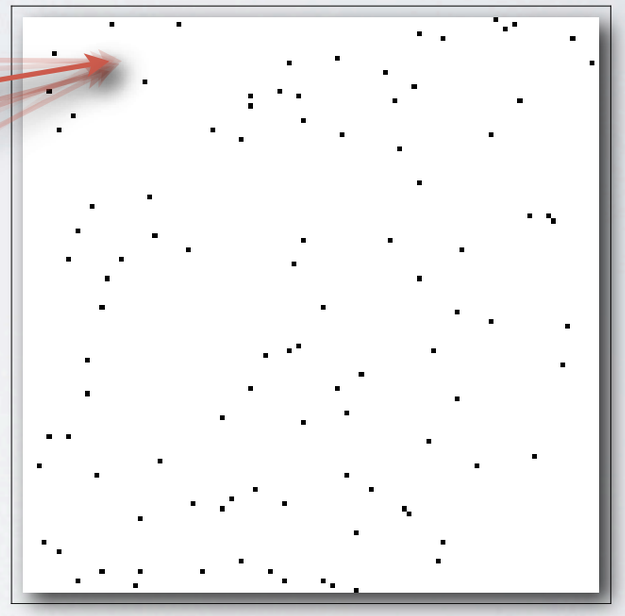
3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Random guess?



Noisy, unoriented data.



Why not?

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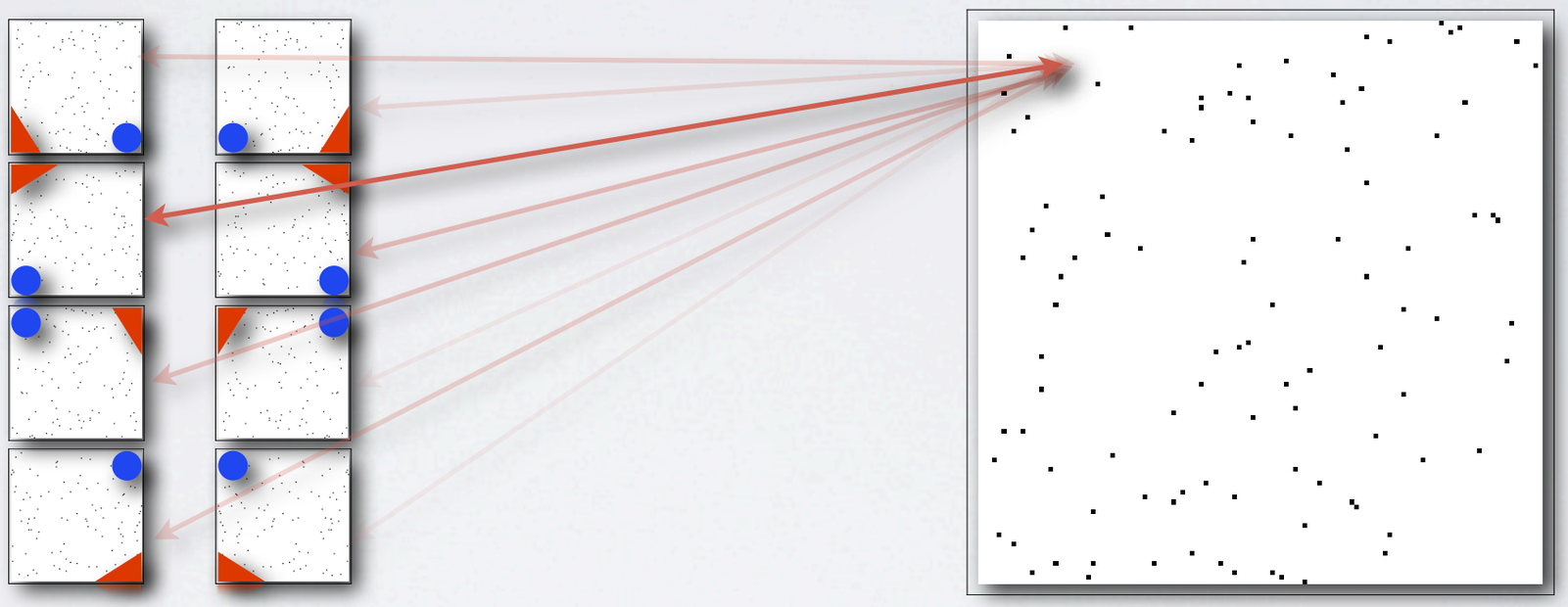
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Noisy, unoriented data.



Replace guess with data..

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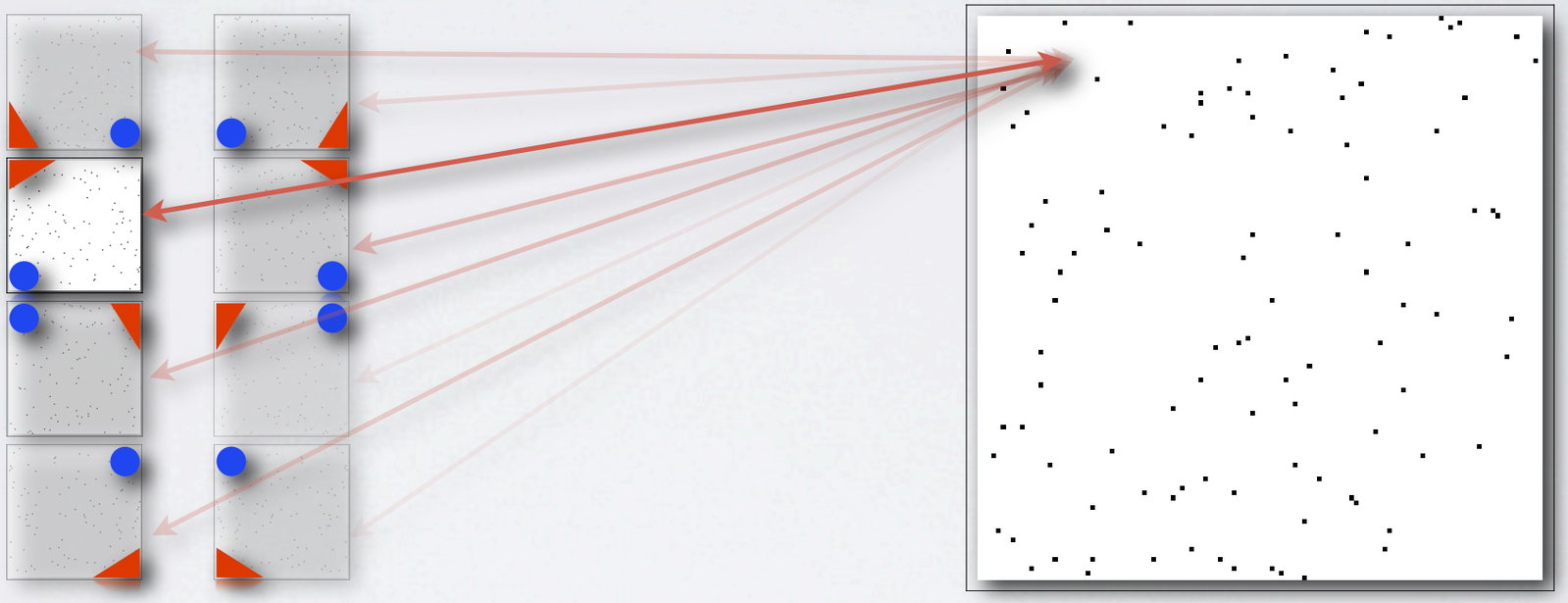
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Noisy, unoriented data.



...based on probabilities
conditional on current guess.

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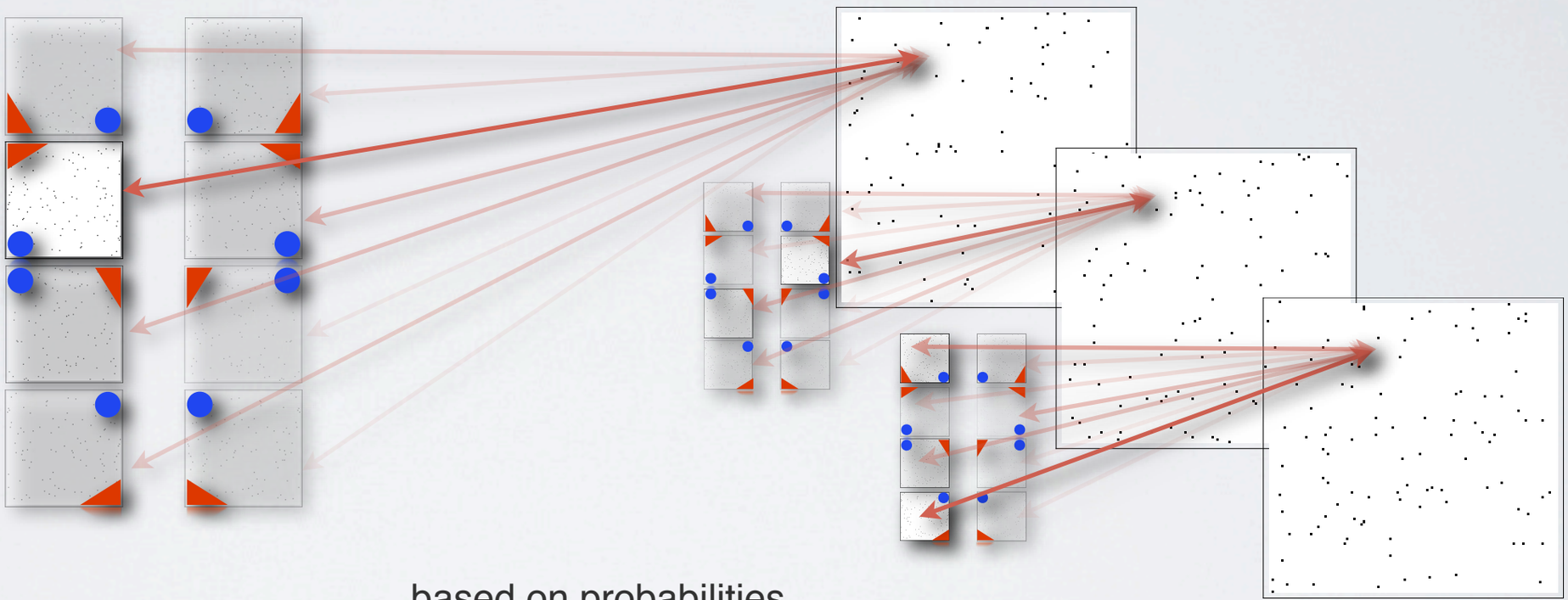
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

P(orientation| data,current guess)

Many, noisy, unoriented data.



...based on probabilities
conditional on current guess.

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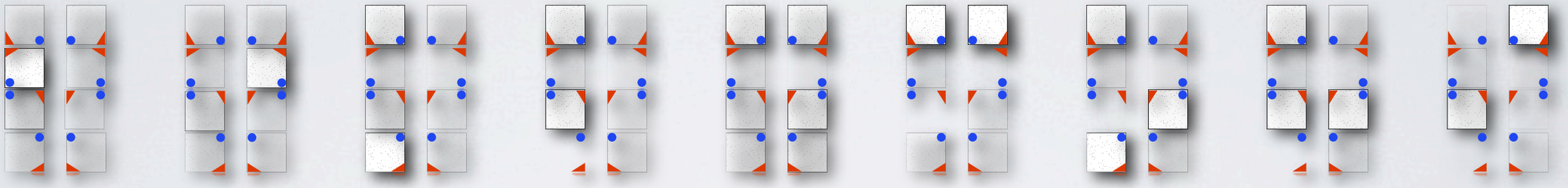
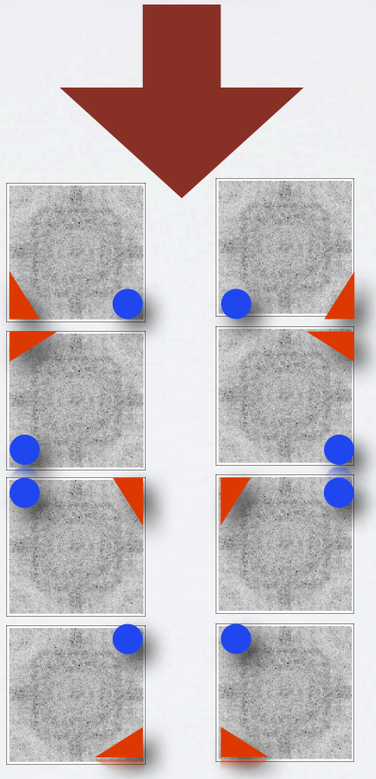
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Average results from many, noisy, unoriented data.





Iterating this, is similar to expectation maximization.

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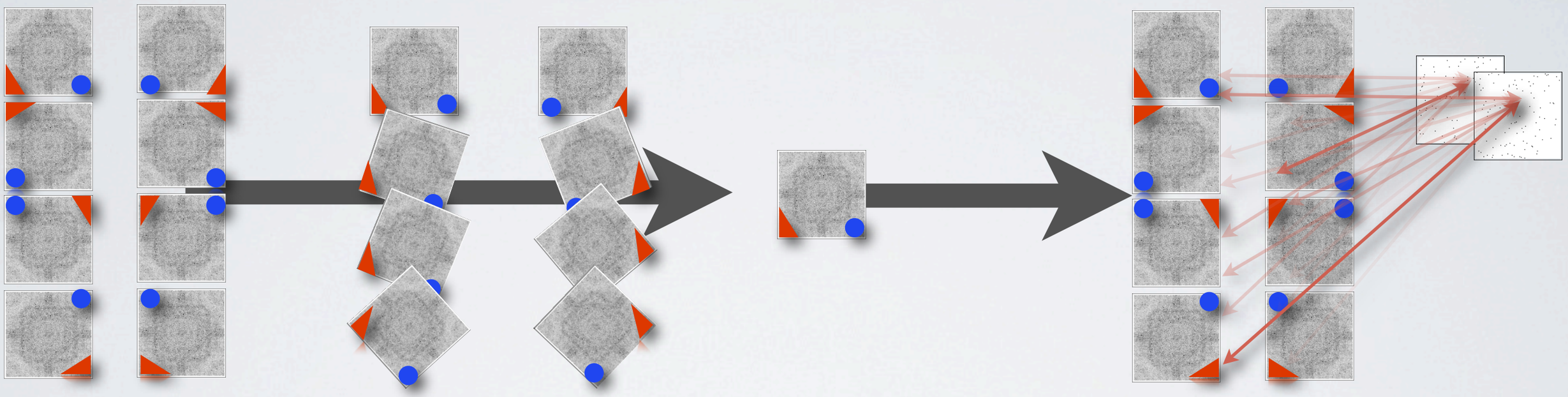
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Compress to enforce commonalities.



Expand for next round of iteration.

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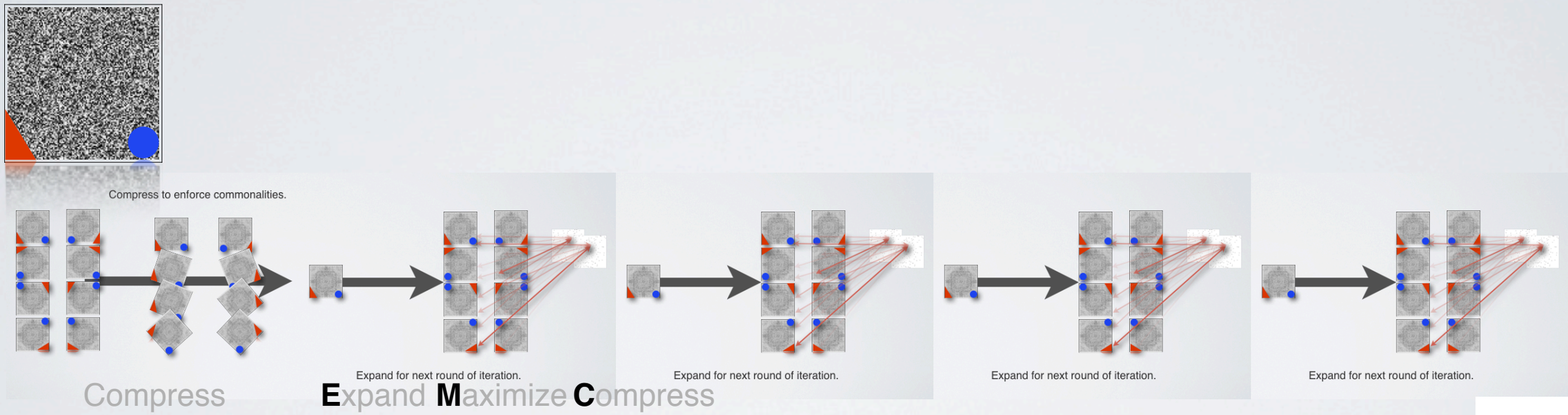
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Step1: random initial guess.



Compress **E**xpand **M**aximize **C**ompress

Step2: iterate EMC to convergence.

Step3: profit.

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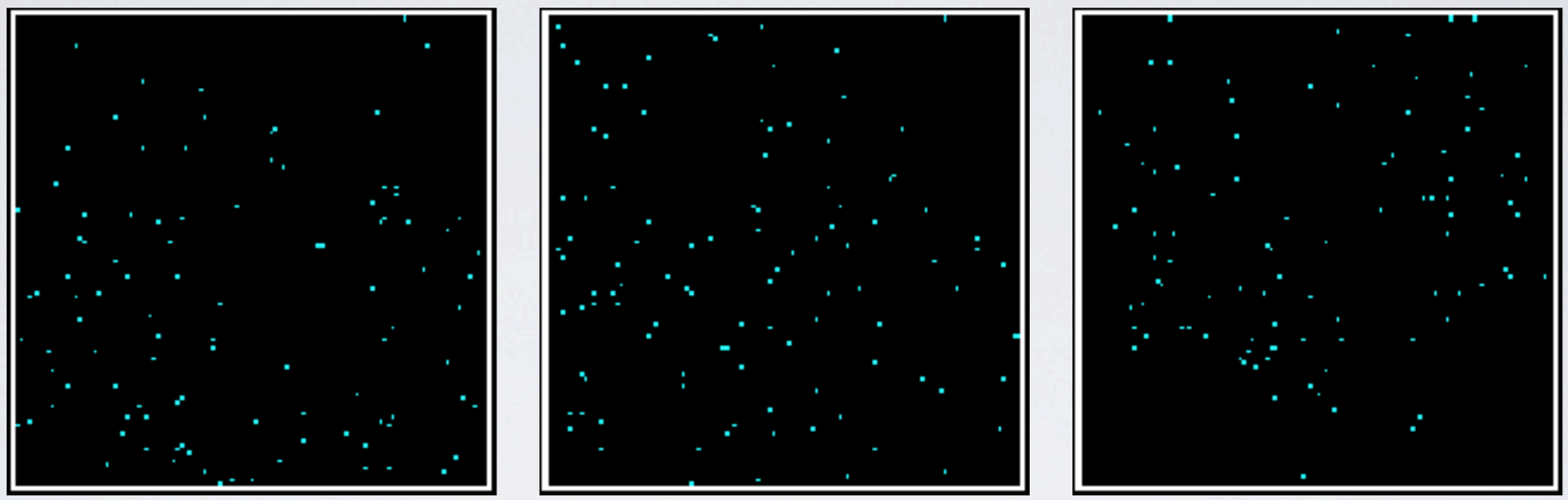
The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D



10,000 pixels

3,000 data, with average
100 photons each.

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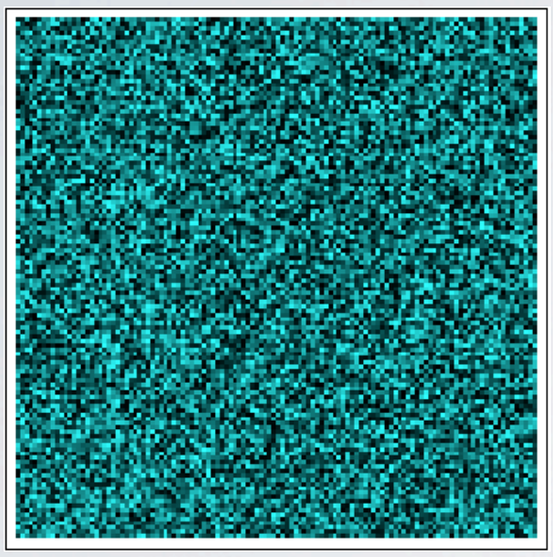
The EMC algorithm:

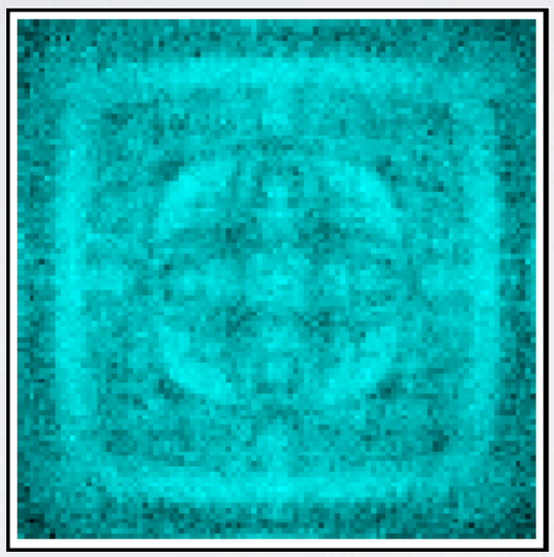
3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

How many iterations?



Random initial.



Iteration 1

2

3

4

Source image.

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The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

What if you had 100 times more data
(i.e. 3,000 to 300,000 data)?

Source image.

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The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ 2D image.

You get Veit to wear a T-shirt of your reconstruction.

Source image.

With 10^12 photons at LCLS...

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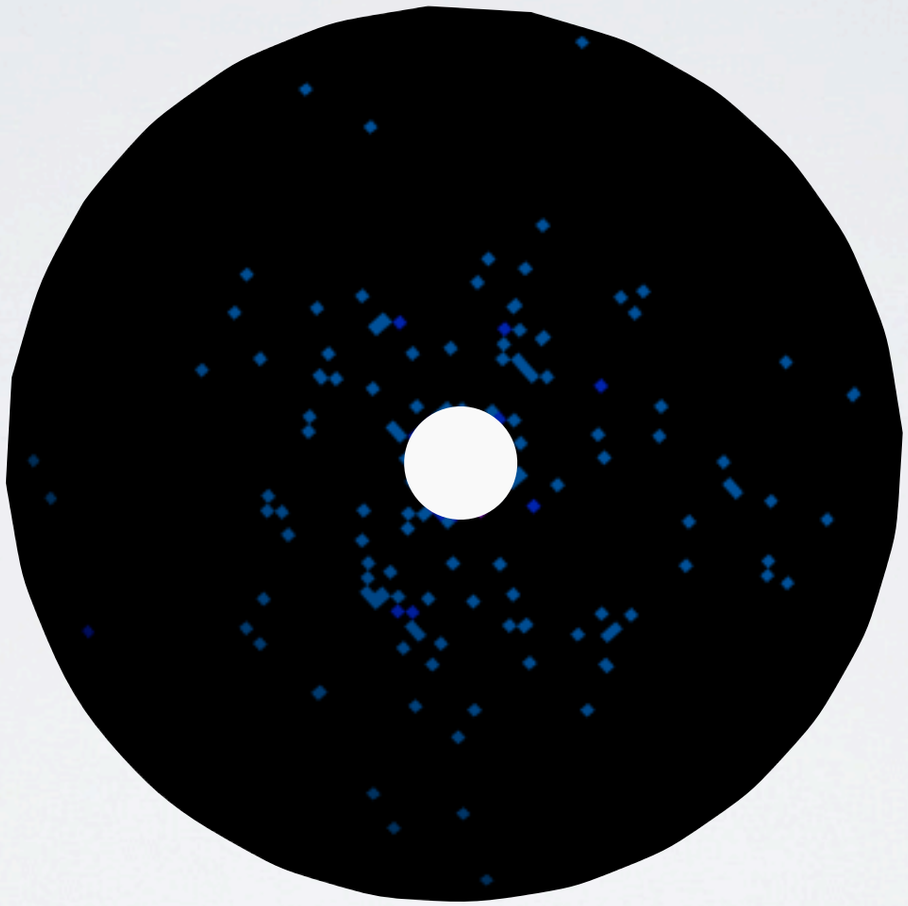
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

Average of 100 photons per diffraction data.



100,000 of such noisy, unoriented data.

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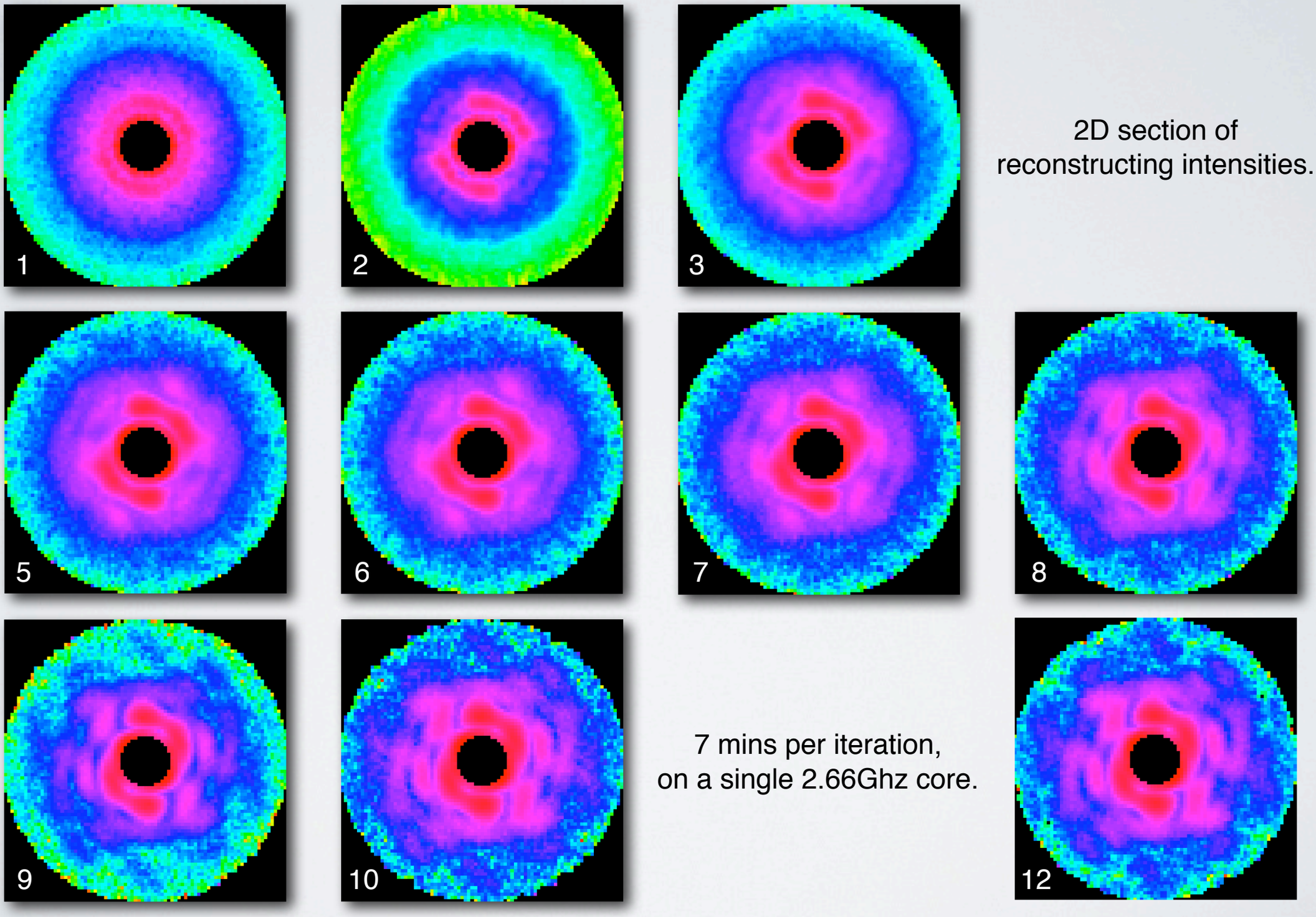
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

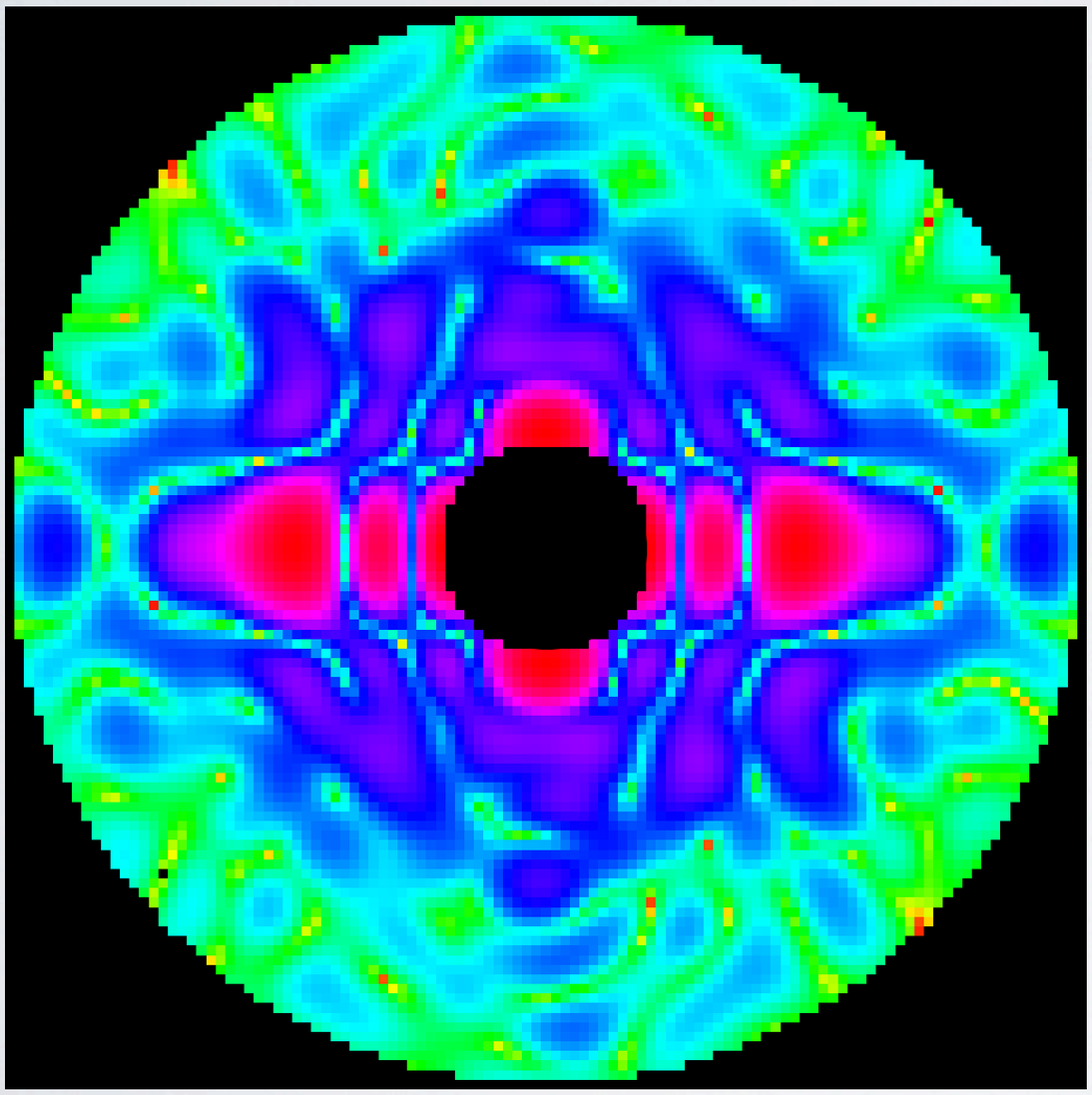


2D section of
reconstructing intensities.

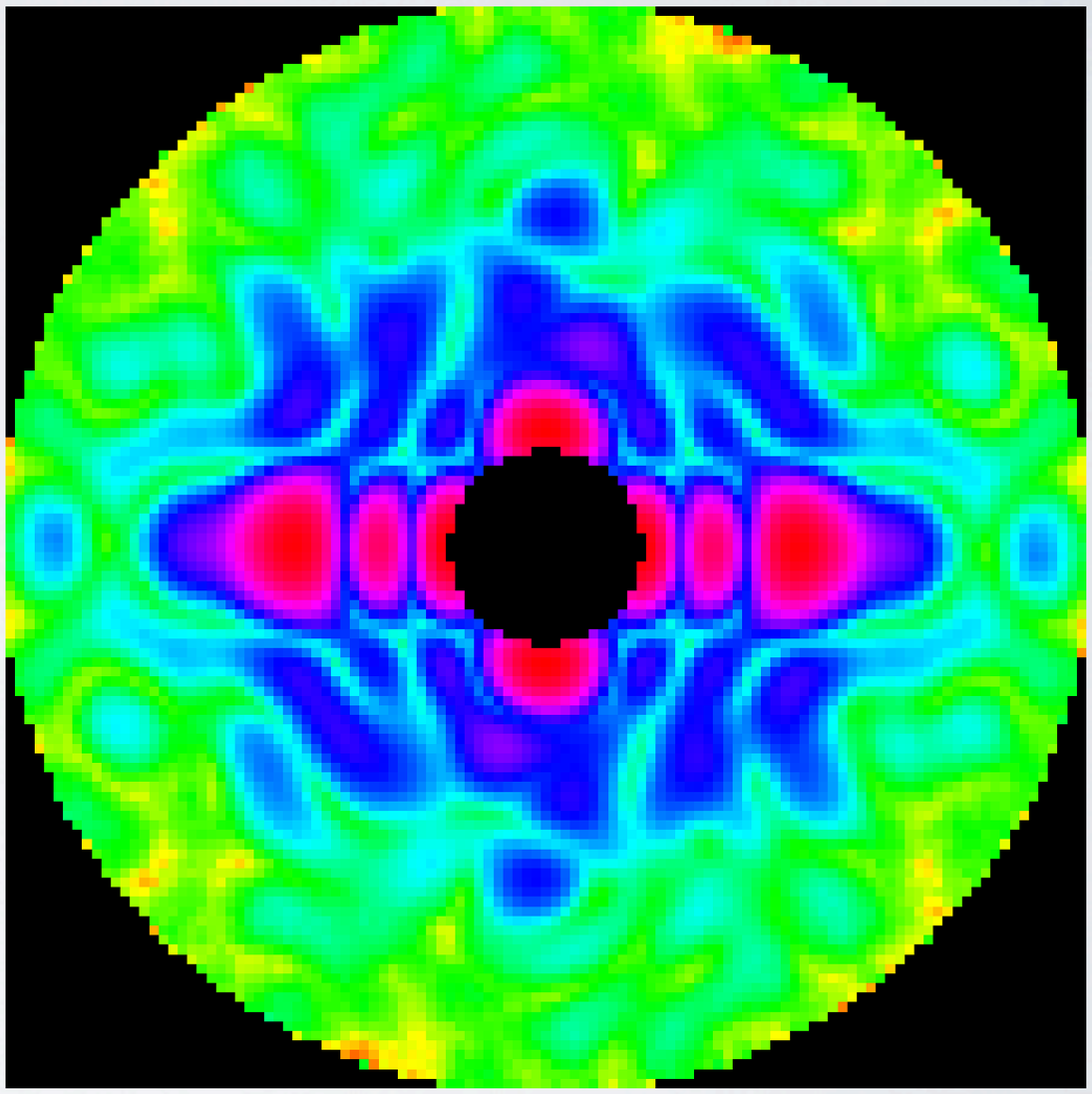
7 mins per iteration,
on a single 2.66Ghz core.

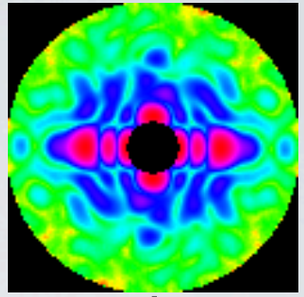
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

Solution intensities.

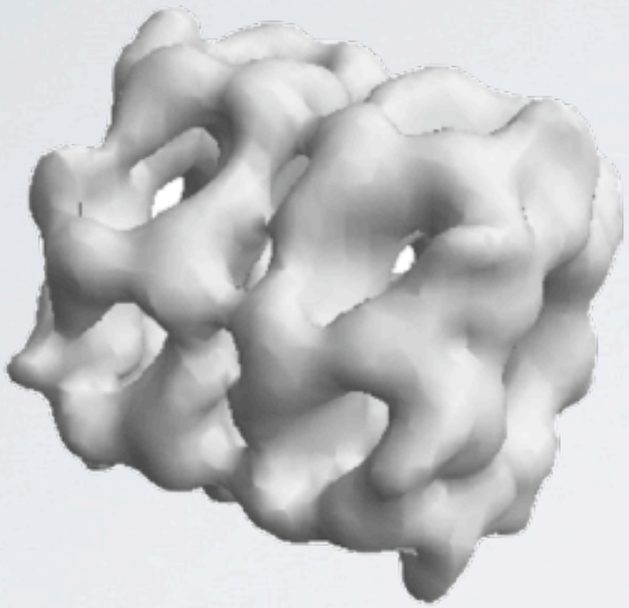


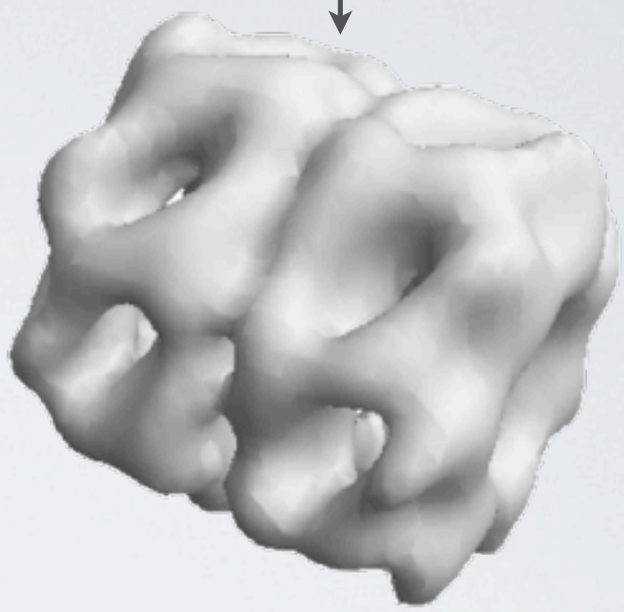
Reconstructed intensities from 10^6 data
with 100 mean photons

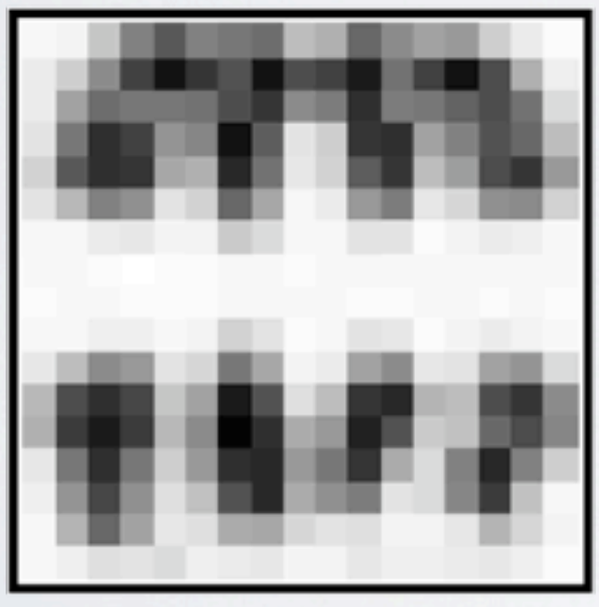




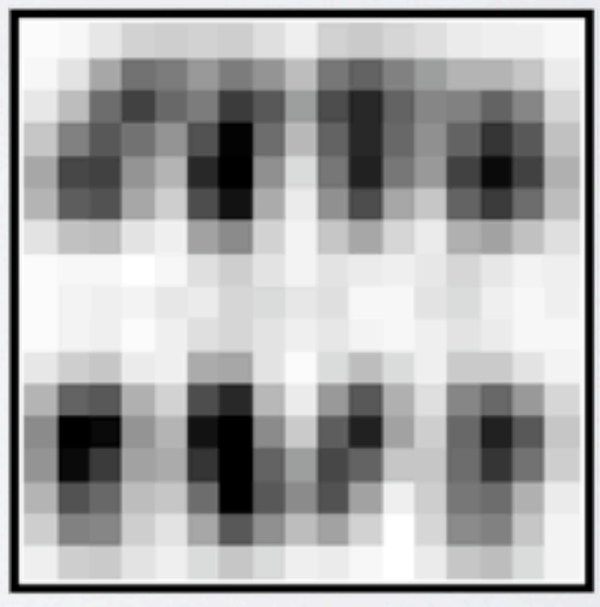
Phase retrieval







Solution, 1nm pixels



Reconstruction

Cryptotomography: an experimental demonstration.

N. D. Loh[1,2], M. J. Bogan[3], V. Elser[1], A. Barty[4], S. Boutet[3], S. Bajt[5], J. Hajdu[6], T. Ekeberg[6], F. R. N. C. Maia[6], J. Schulz[4], M. M. Seibert[6], B. Iwan[6], N. Timneanu[6], S. Marchesini[7], I. Schlichting[8,9], R. L. Shoeman[8,9], L. Lomb[8,9], M. Frank[10], M. Liang[4], and H. N. Chapman[4,11]

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[2]*Cornell High Energy Synchrotron Source (CHESS), Cornell University, Ithaca, NY 14853-2501, USA*
[3]*SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California, 94025, USA*
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[8]*Max Planck Institute for Medical Research, Jahnstr. 29, 69120 Heidelberg, Germany*
[9]*Max Planck Advanced Study Group, Center for Free-Electron Laser Science, DESY, Notkestrasse 85, Hamburg 22607, Germany*
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[11]*University of Hamburg, Luruper Chaussee 149, Hamburg 22761, Germany*

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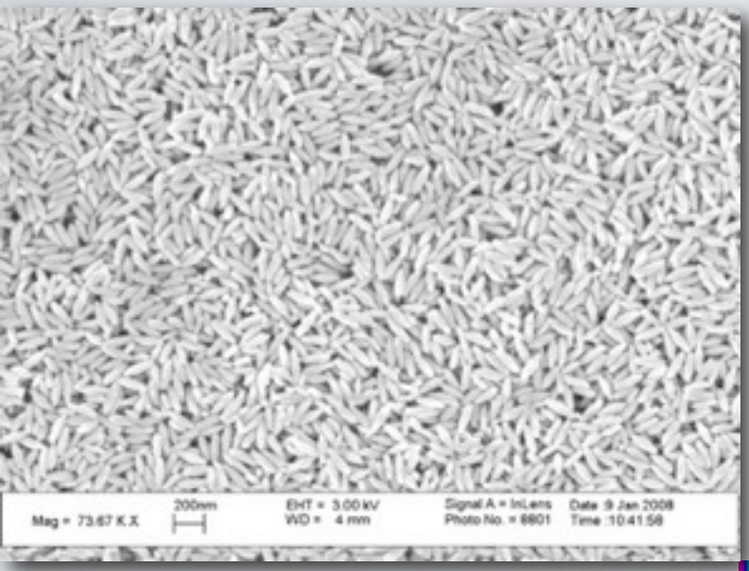
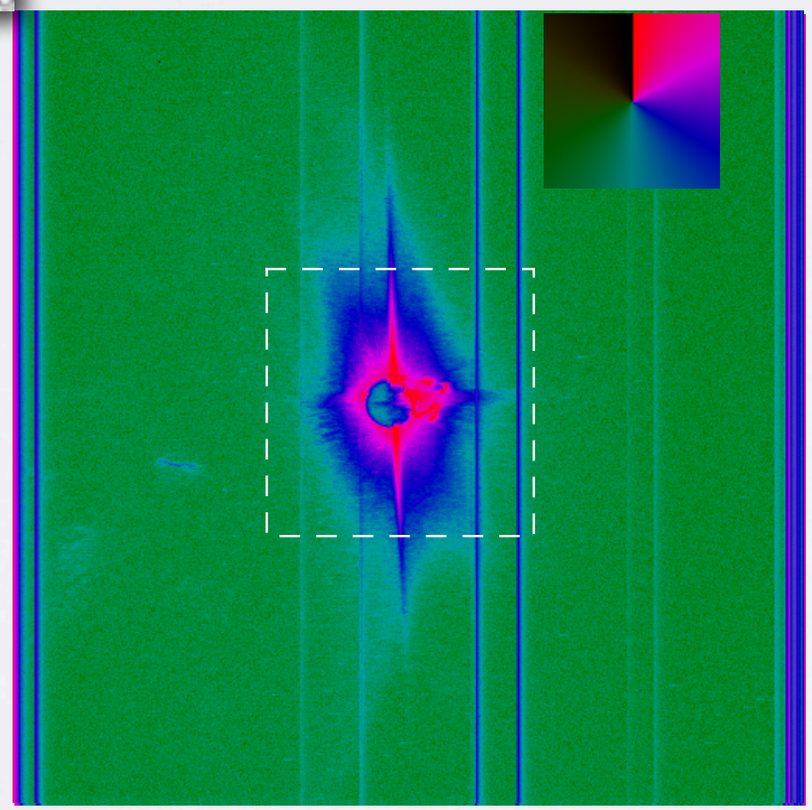
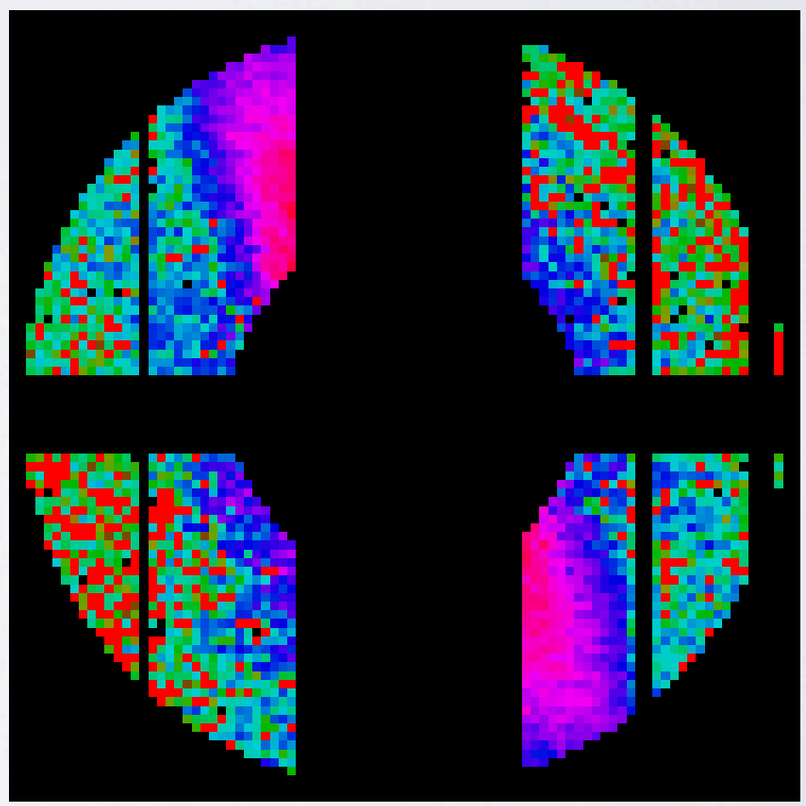
Cryptotomography: an experimental demonstration.



diffraction data



background-subtracted, low-res.



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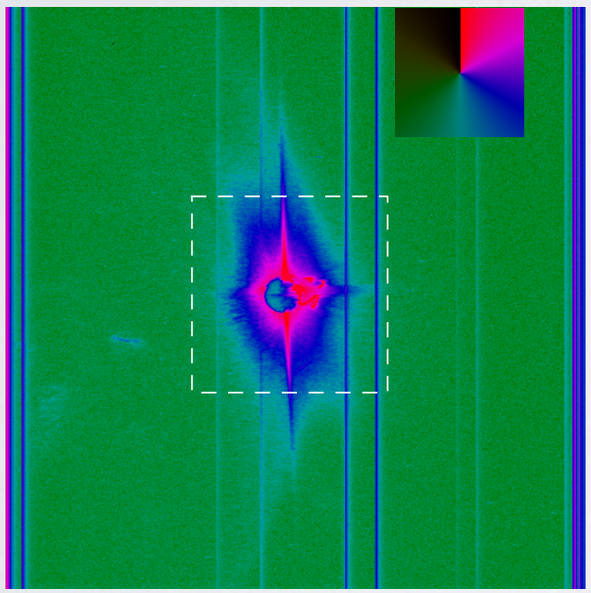
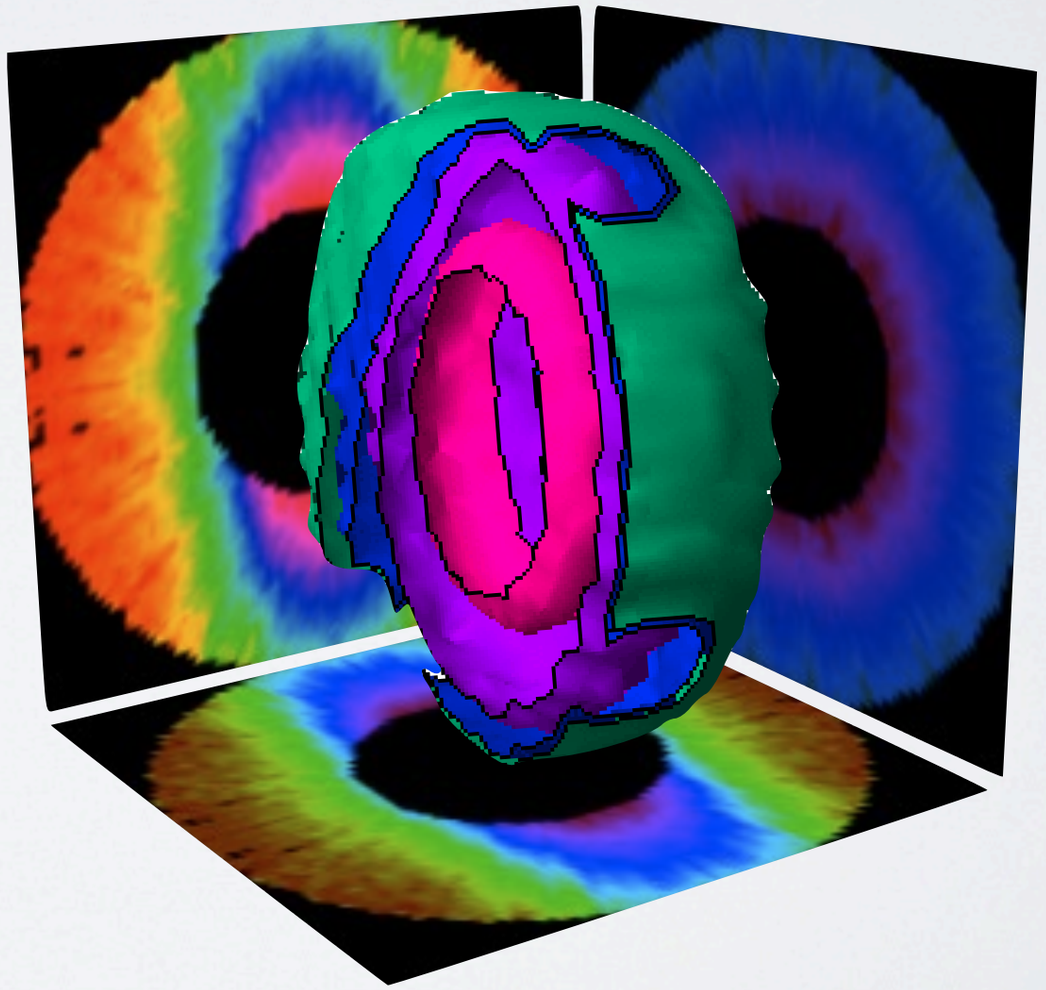
Cryptotomography: an experimental demonstration.



52 data.

Low-res. 3D reconstructed intensities.



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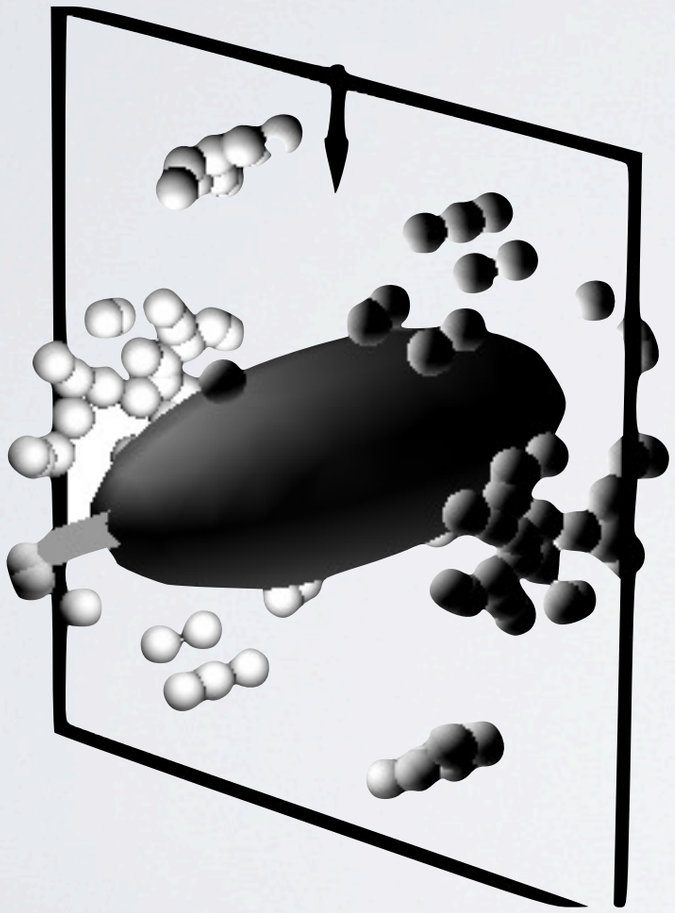
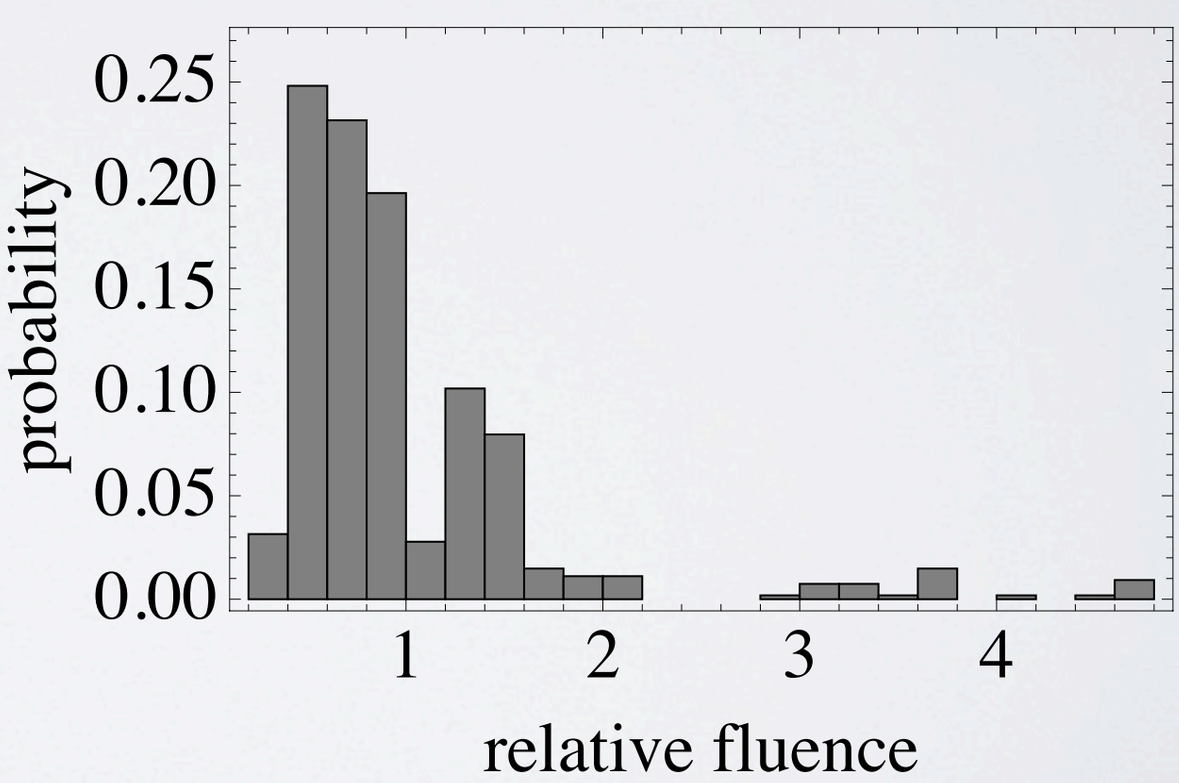
Cryptotomography: an experimental demonstration.

reconstruct orientation bias.





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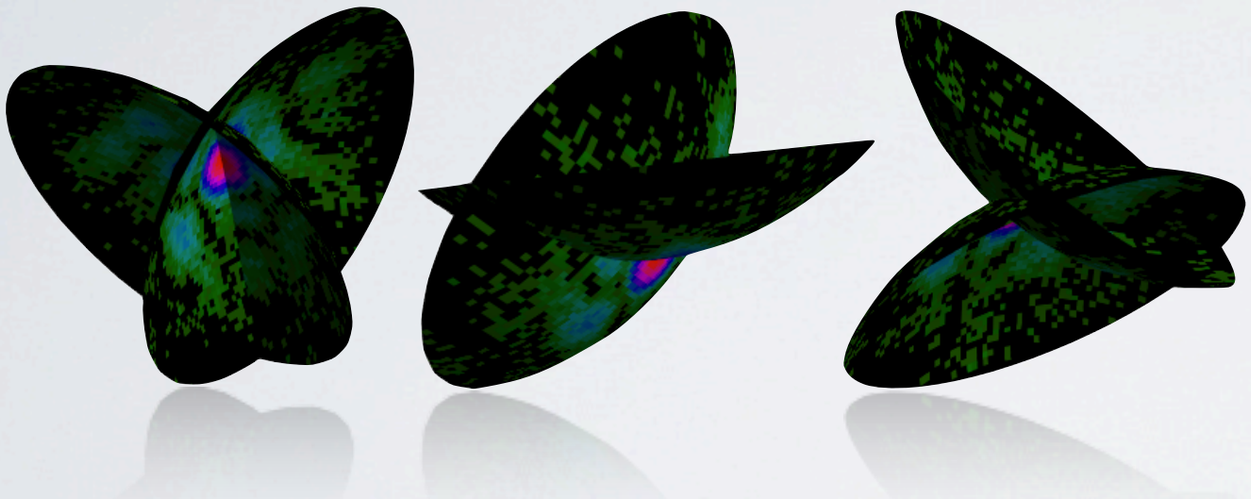
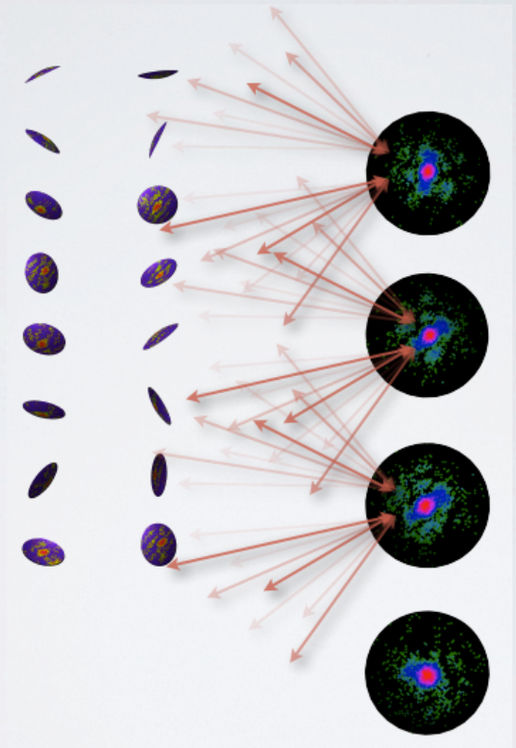
Cryptotomography: an experimental demonstration.

Data-data comparisons.



N_{data}^2

EMC.



$\text{const} \times N_{data}$

Computation time scaling.

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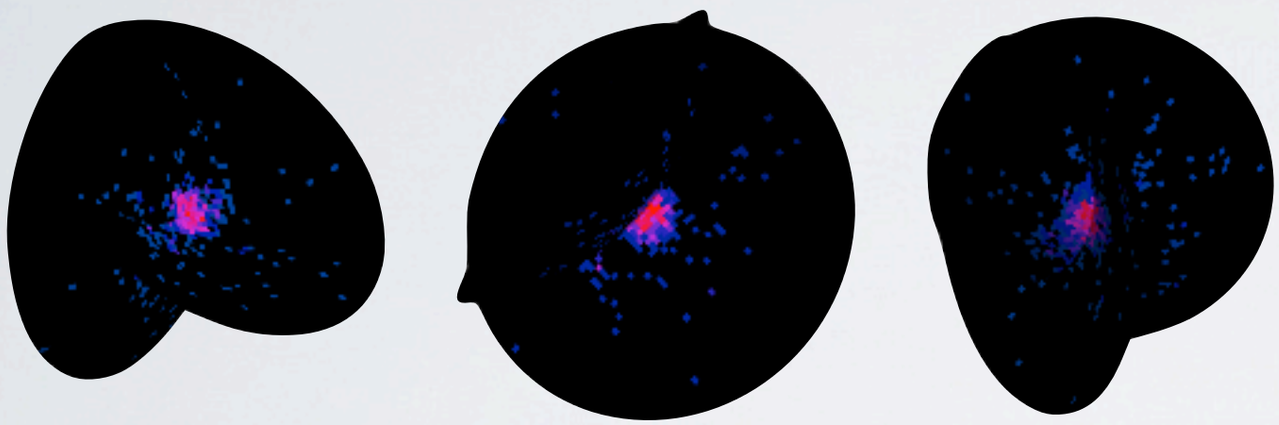
Cryptotomography: an experimental demonstration.

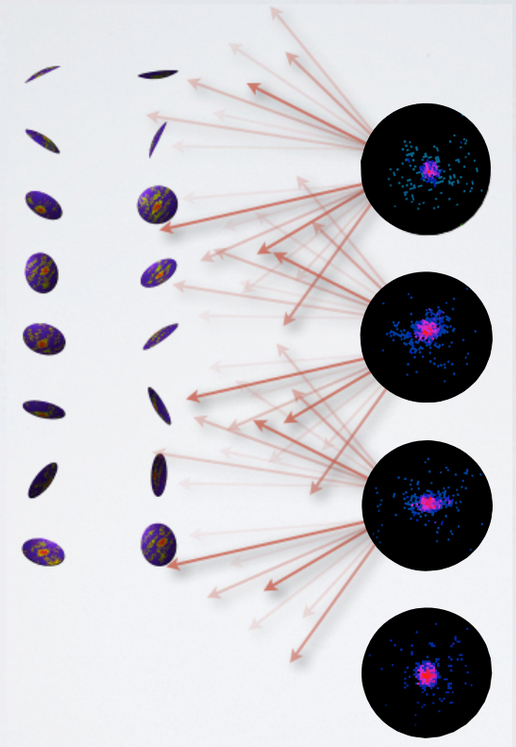
Data-data comparisons.



Still able to reconstruct?

N_{data}^2?

EMC.



$\text{const} \times N_{data}$

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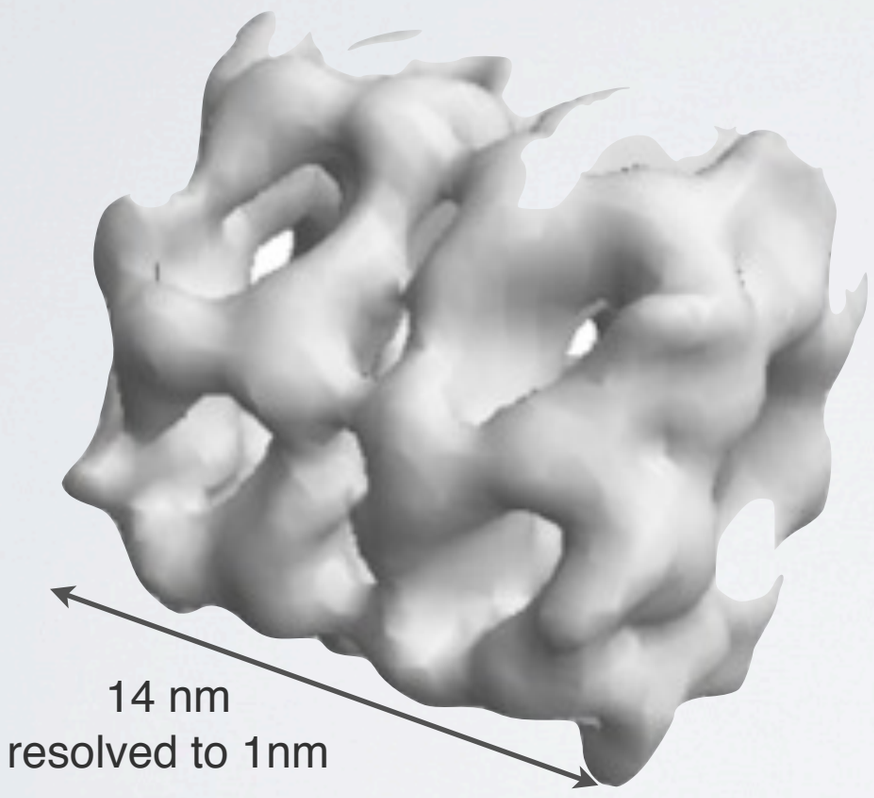
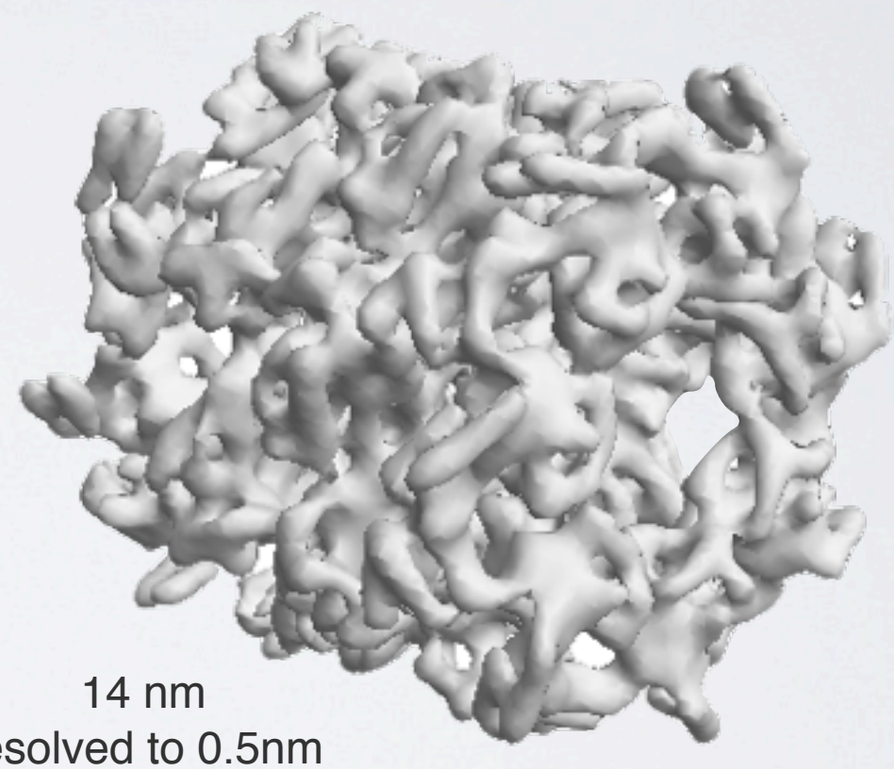
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

With 1 processor.



Distributed across 64 processors.



reconstructed GroEL

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The EMC algorithm:

3D reconstruction from noisy, unoriented, 2D ~~single-particle diffraction data~~ image.

2D

Why the hassle of expanding and compressing?

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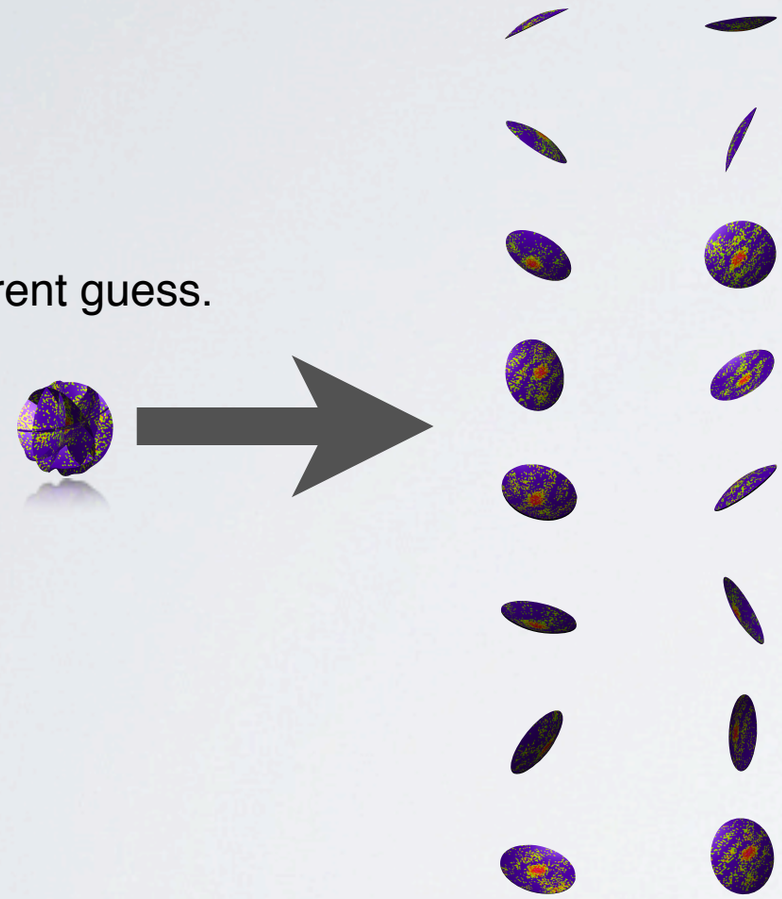
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

Expansion of current guess.

Current guess.



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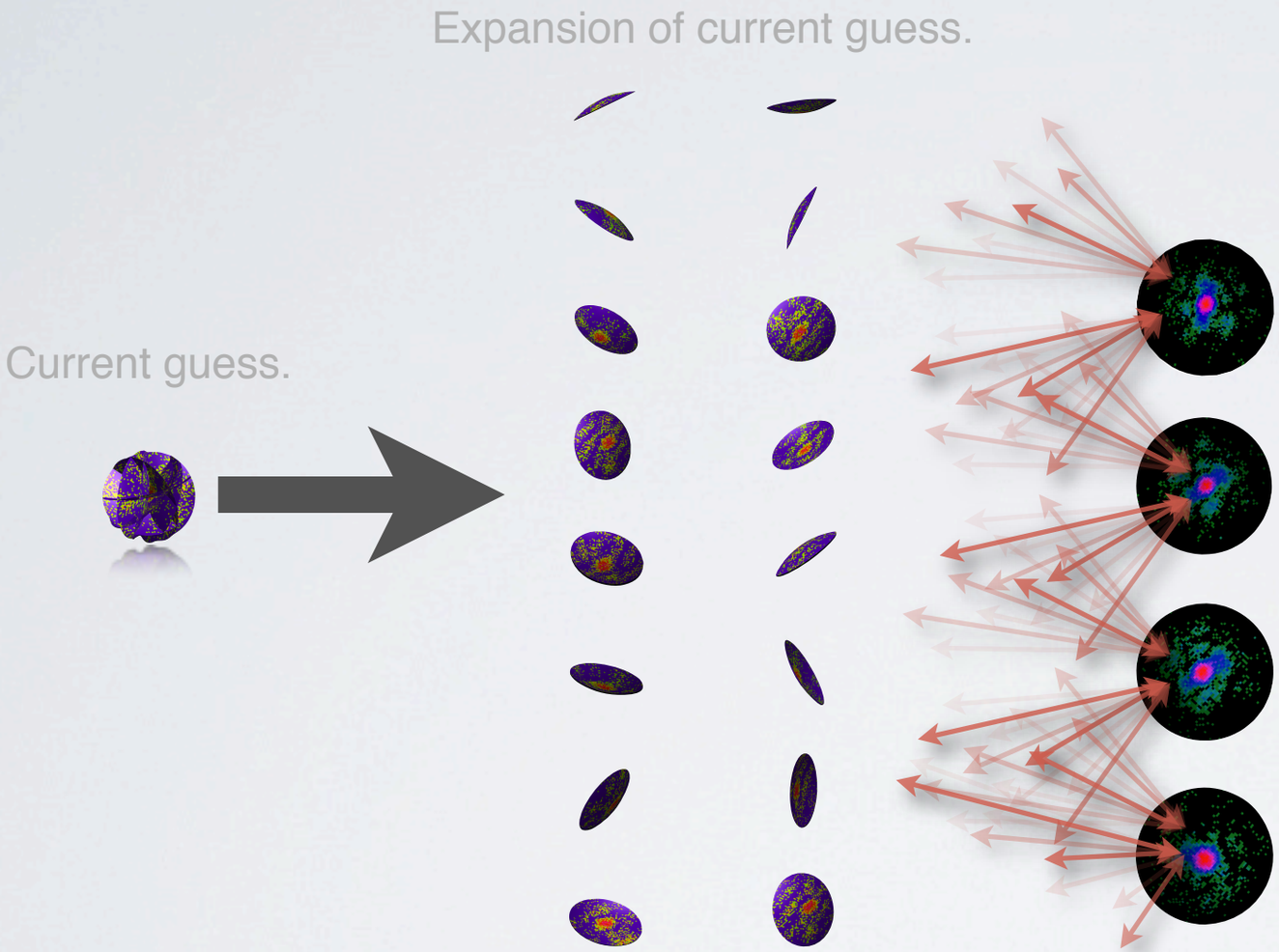
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.



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The EMC algorithm:
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Expansion of current guess.

Current guess.

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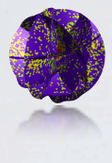
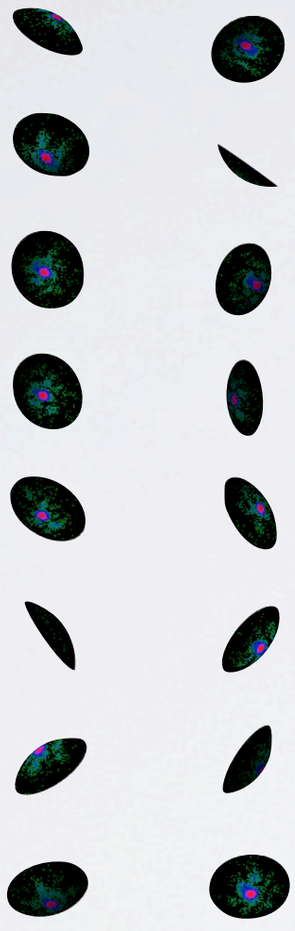
The EMC algorithm:
3D reconstruction from noisy, unoriented, 2D single-particle diffraction data.

Current guess.



Expansion of current guess.



Compress;
enforce
commonalities.