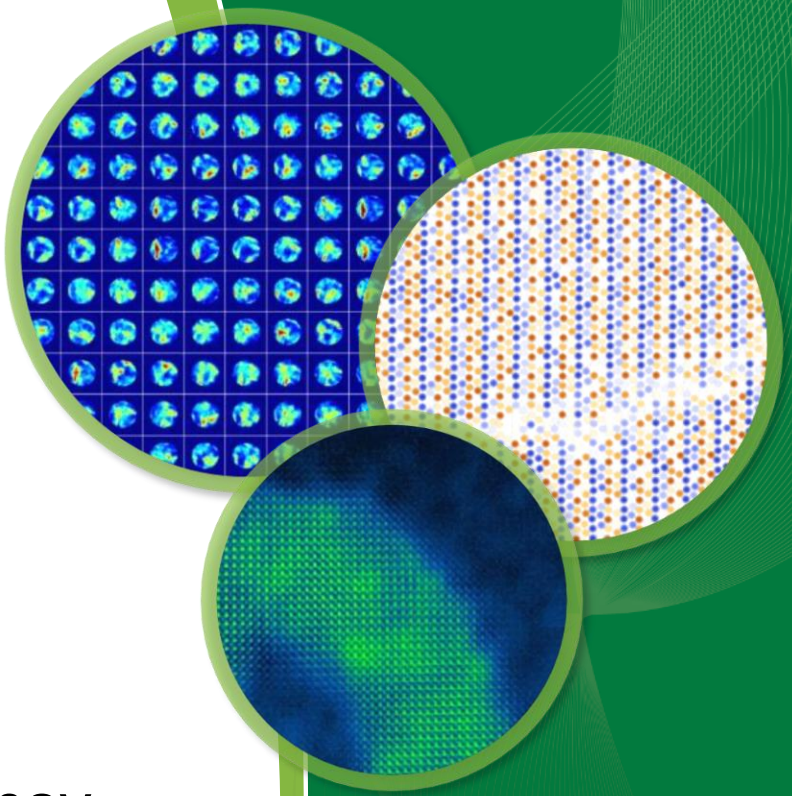
Processing of Atomic Resolution Images and Multispectral Data



Stephen Jesse, Alex Belianninov, Suhas Somnath, Chris Smith, Rama Vasudevan, Noumanne Laanait

ORNL is managed by UT-Battelle
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Outline

- Setting up images for multivariate analysis
- Multivariate analysis on imaging data
  - De-noising
  - PCA
  - K-means
  - Atom finding (pattern matching)
  - Analysis on found atoms
- 4D-STEM with multivariate analysis

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Image Processing using SVD

How can you express 2D images in a way that you can use Multivariate Techniques?

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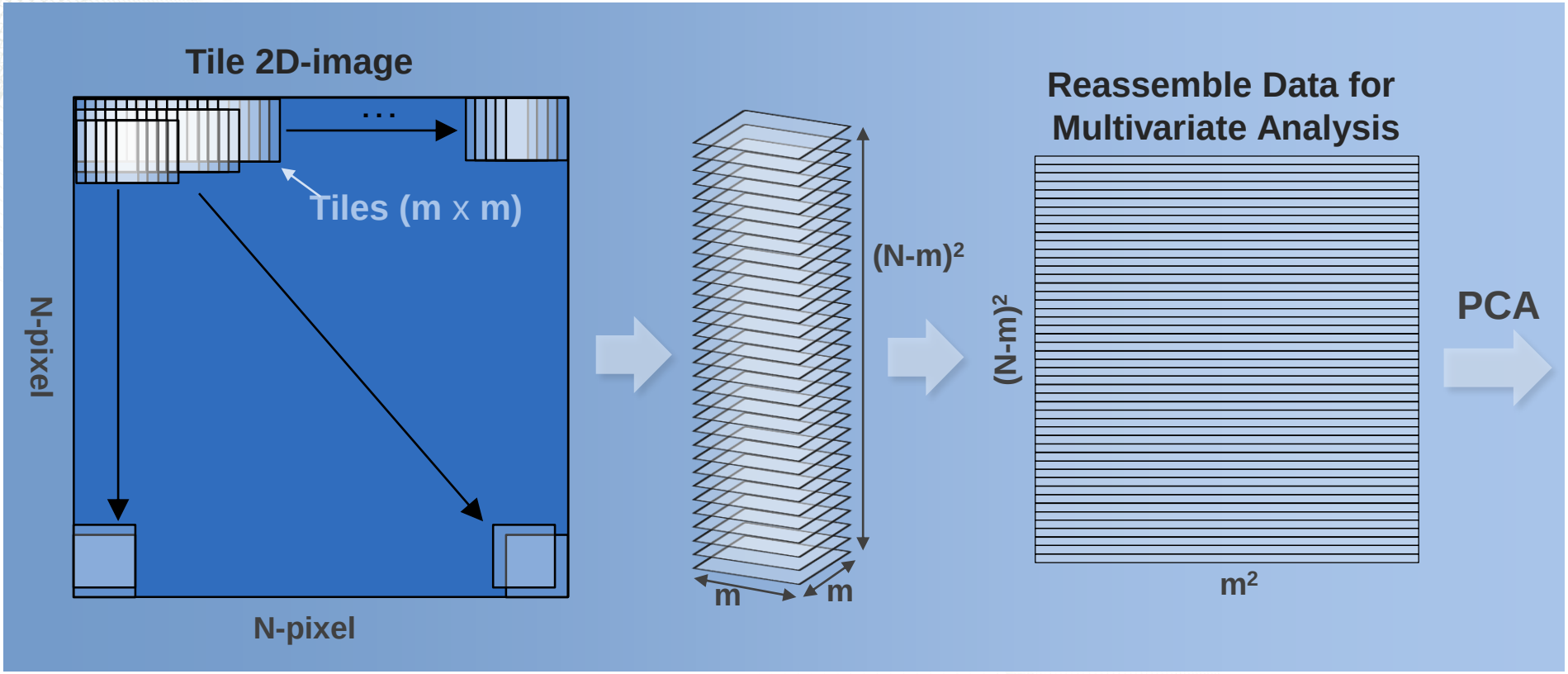
Image Cleaning: Sliding Window PCA



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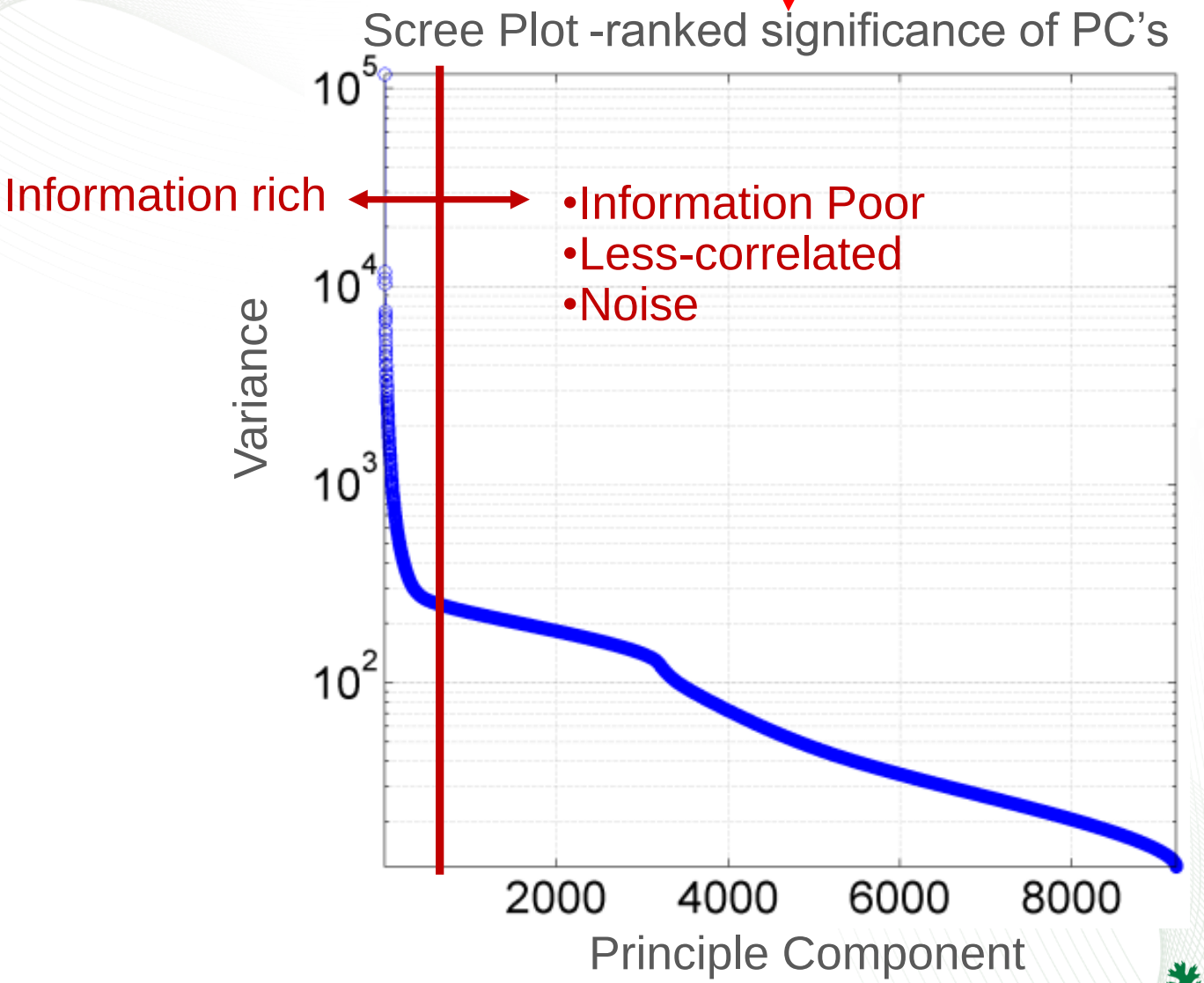
Principal Component Analysis (PCA)

$$D \rightarrow USV^*$$



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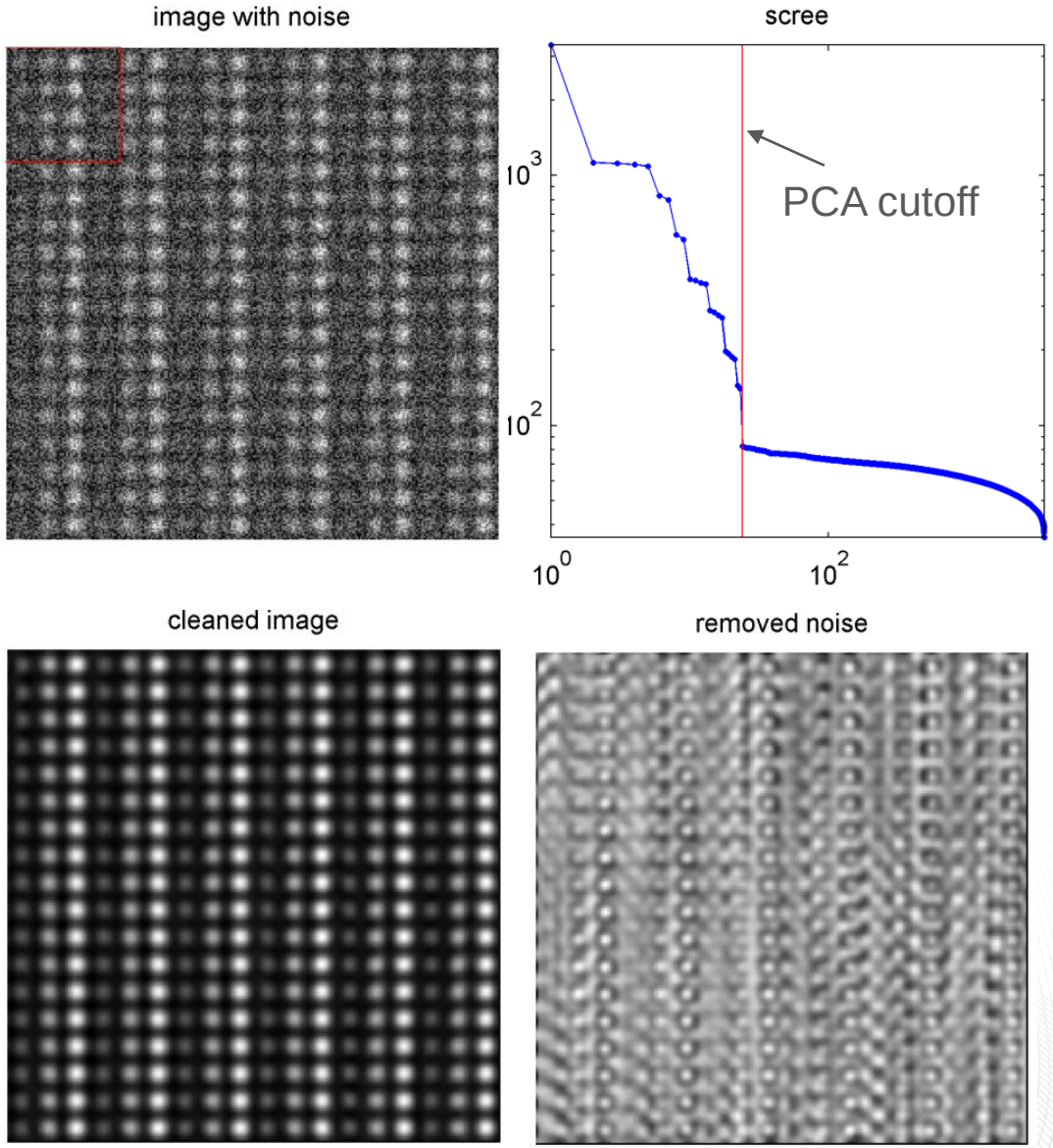
Sliding Window PCA: De-noising

Model Image



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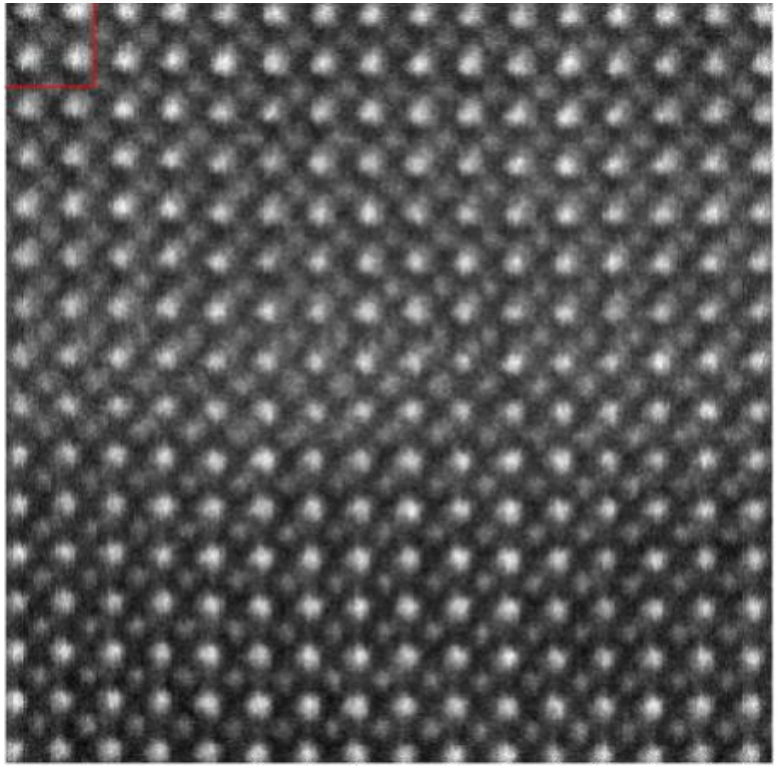
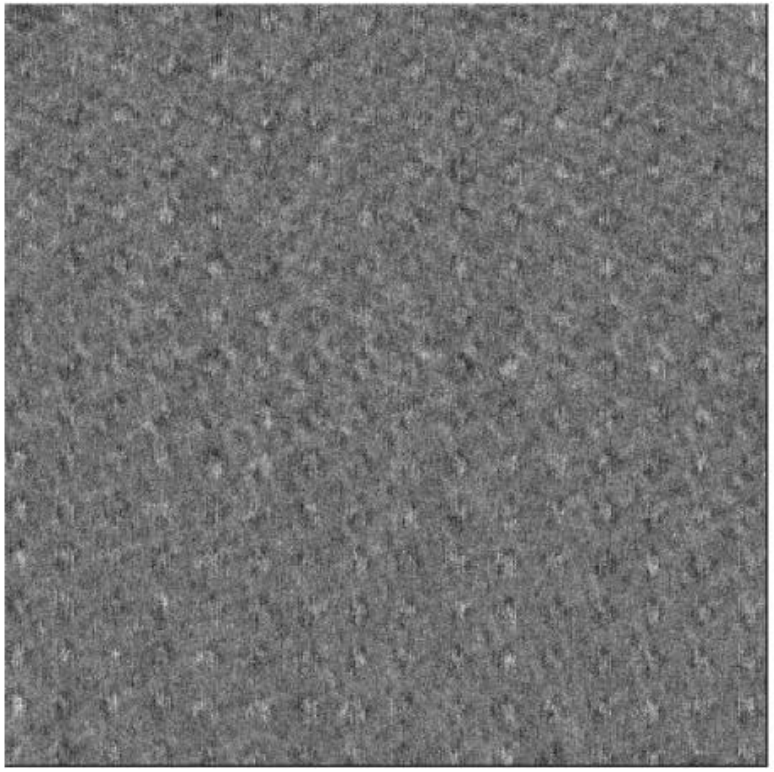
Sliding Window PCA: De-noising

Experimental Image

Original Image



Removed Noise



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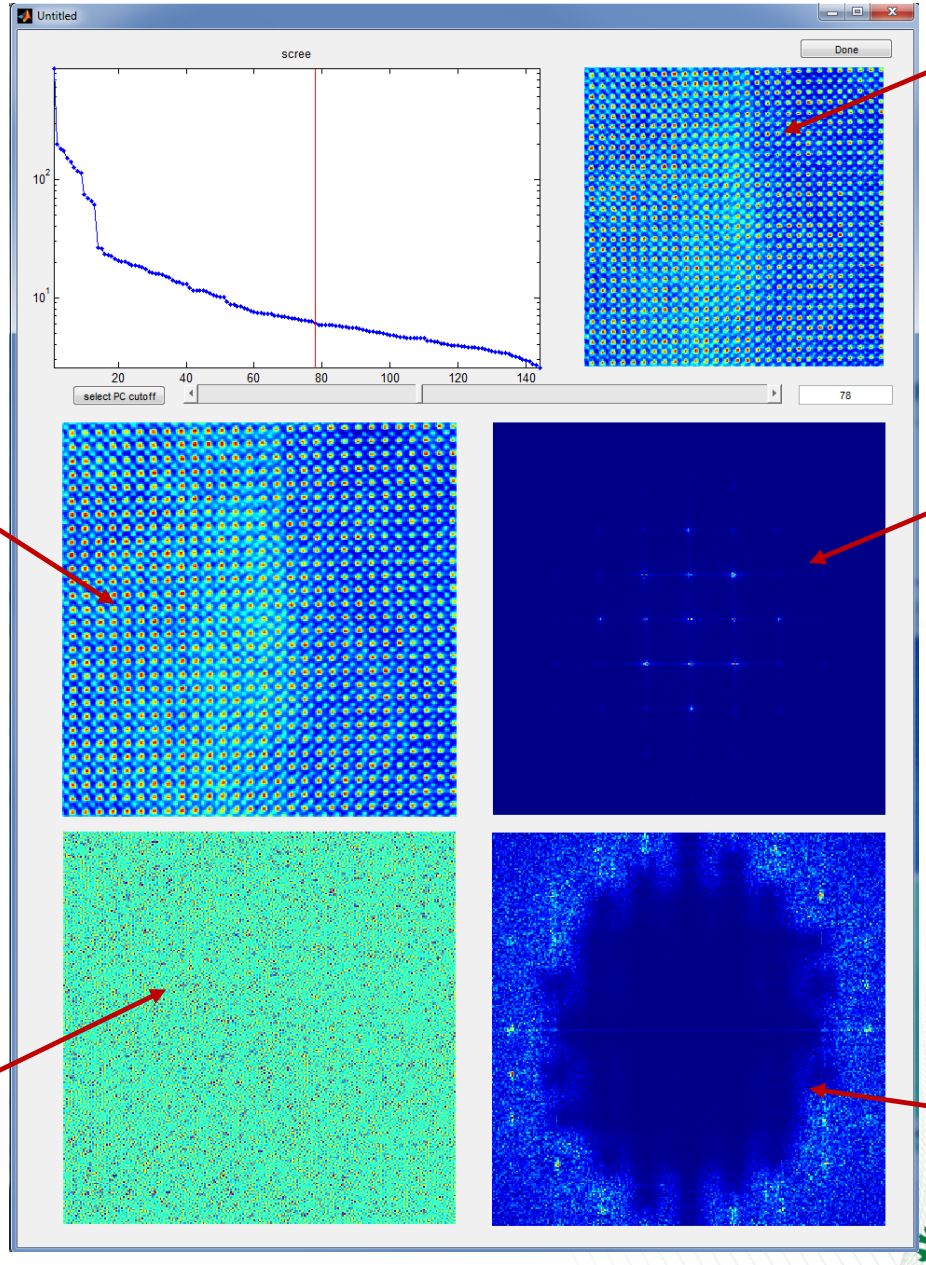
Effects of Number of Retained PC's



Original image

Cleaned Image

FFT of Cleaned Image

Removed Noise

FFT of noise

Higher PC's tend to contain higher frequency Fourier peaks

Automatically removes noise between peaks

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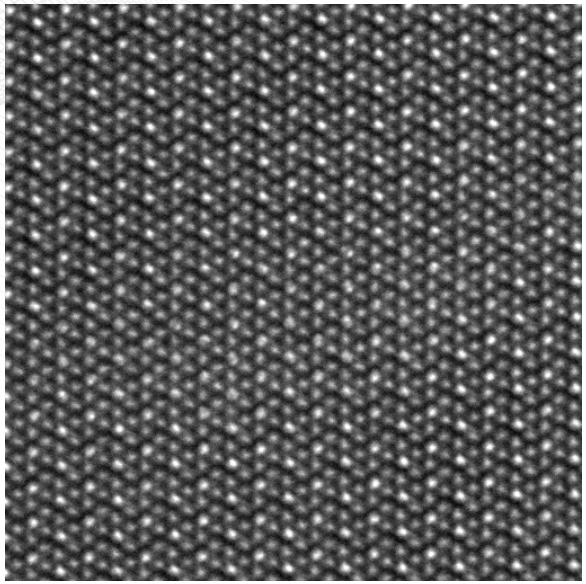
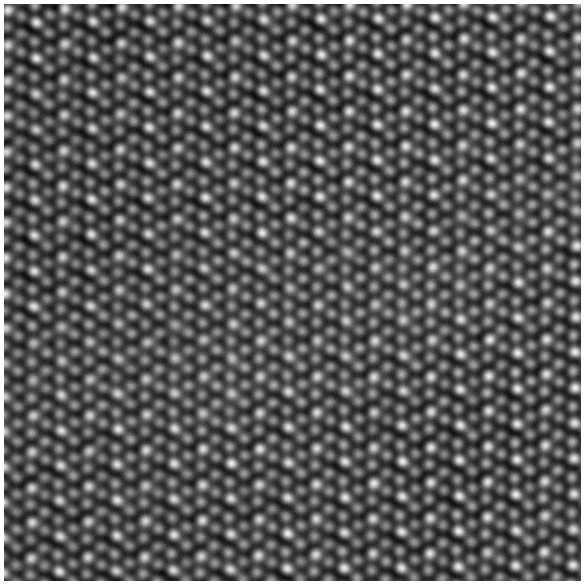
Sliding Window PCA-based Pattern Finding

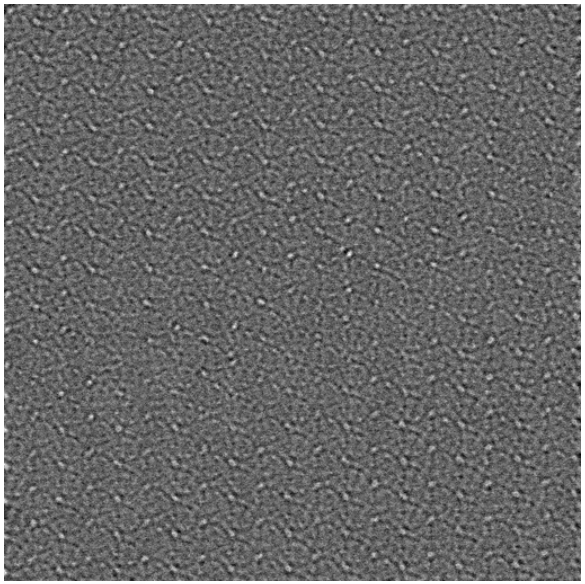
original

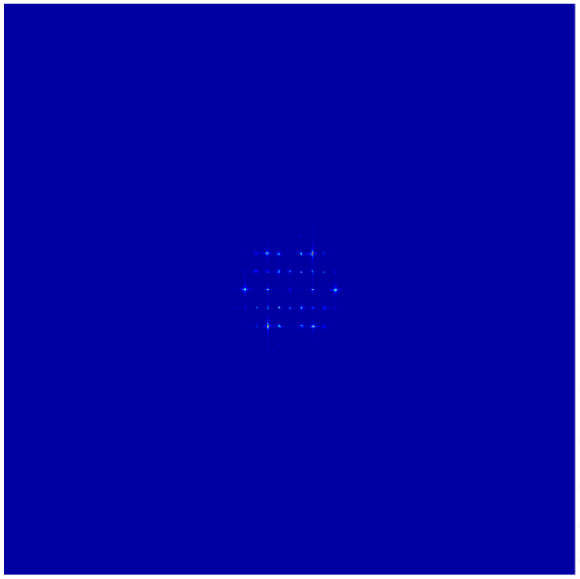


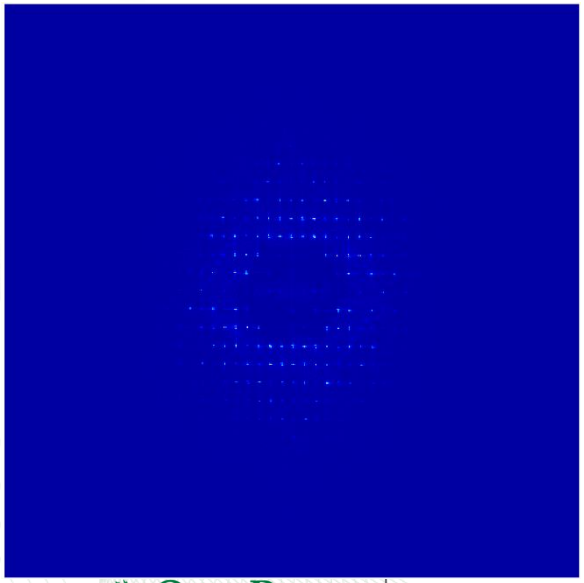
cleaned



removed noise







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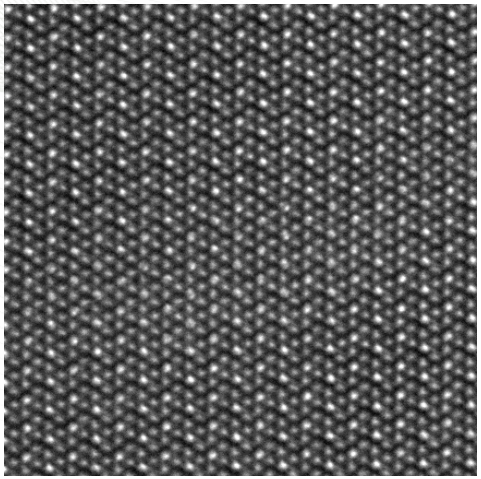
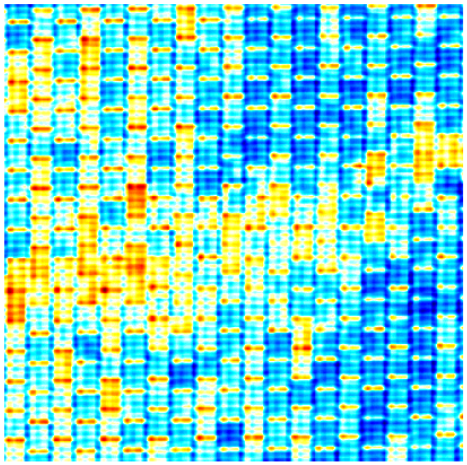
Sliding Window PCA-based Pattern Finding

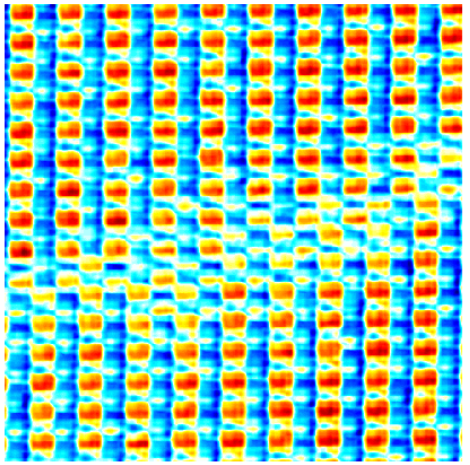
Original Image



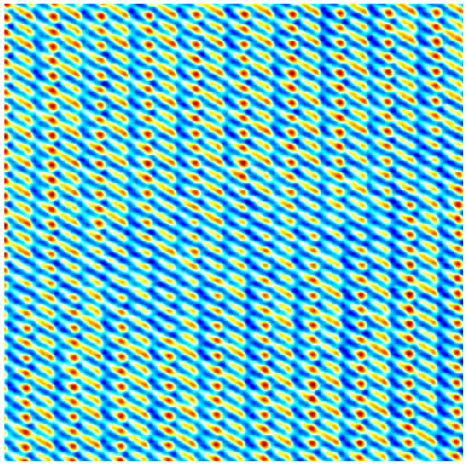
PC map 1



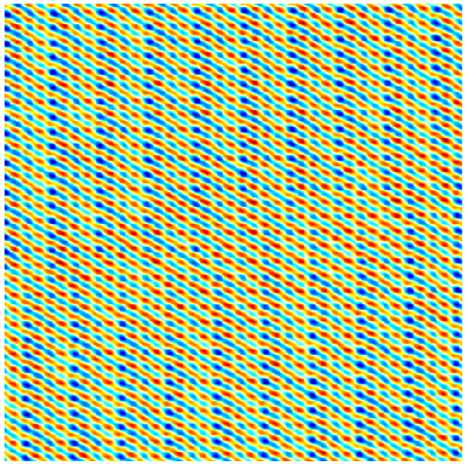
PC map 2



PC map 3



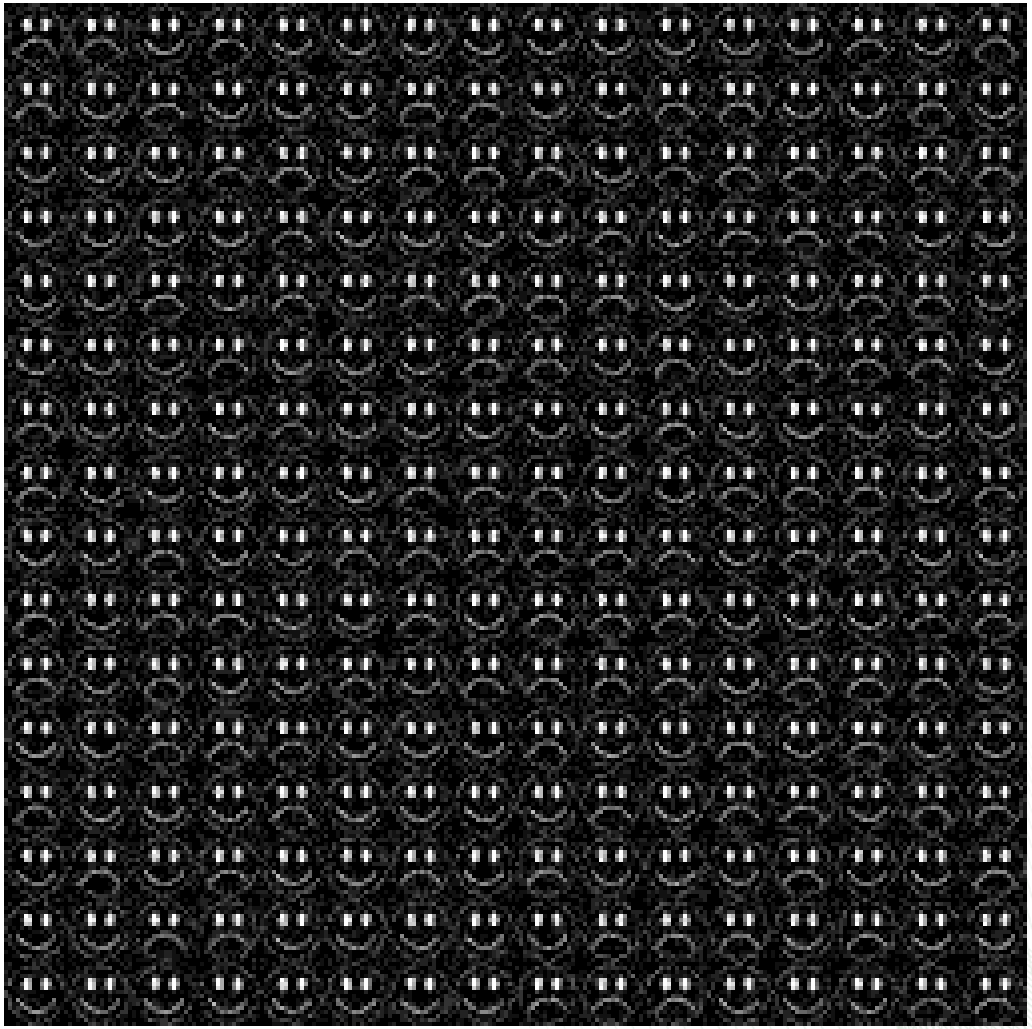
PC map 4



Sliding Window PCA can reveal patterns in images on its own without the need to identify features

Sliding Window PCA-based Pattern Finding ☺☹

Start with a random grid
of smiley and frowny faces



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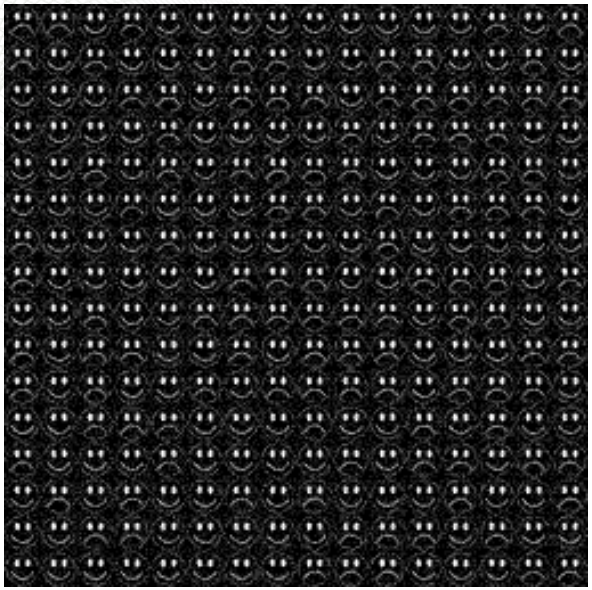
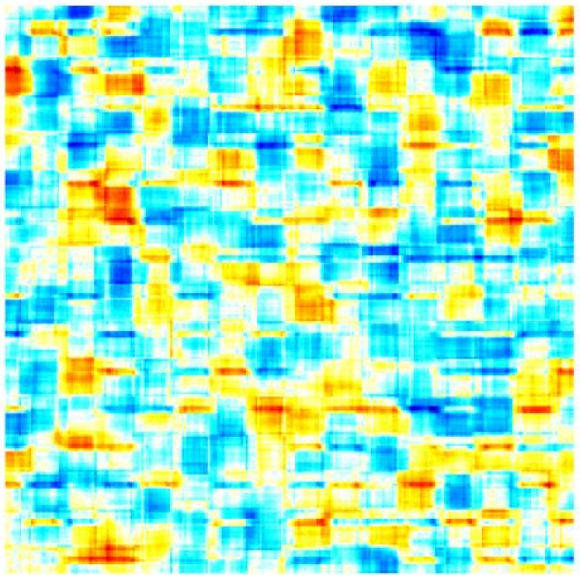
Sliding Window PCA-based Pattern Finding ☺☹



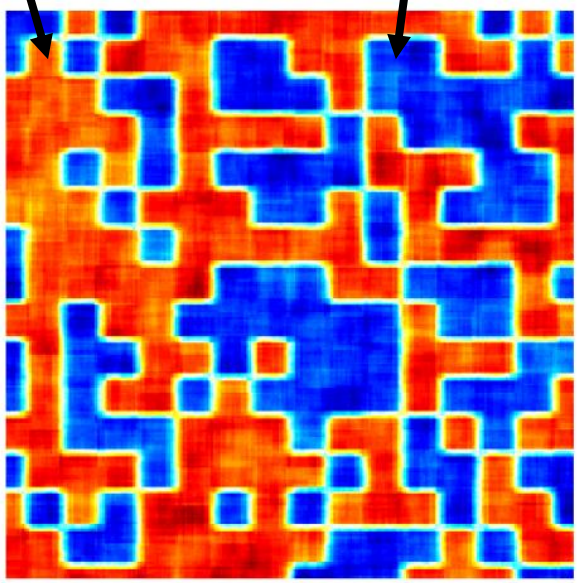
Happy face (red)

Sad face (blue)

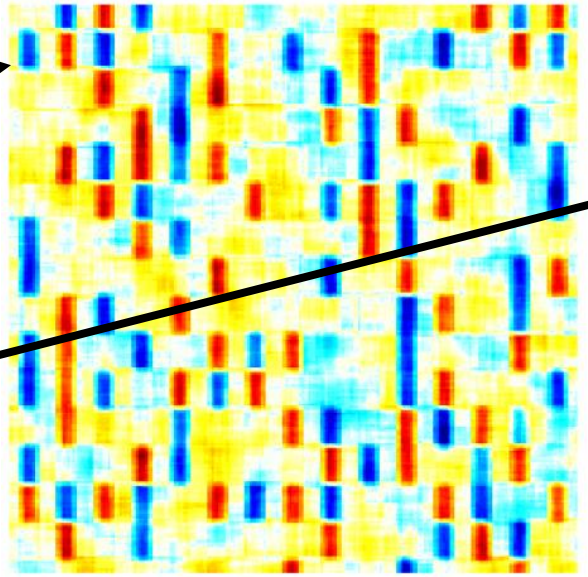
PC map 1



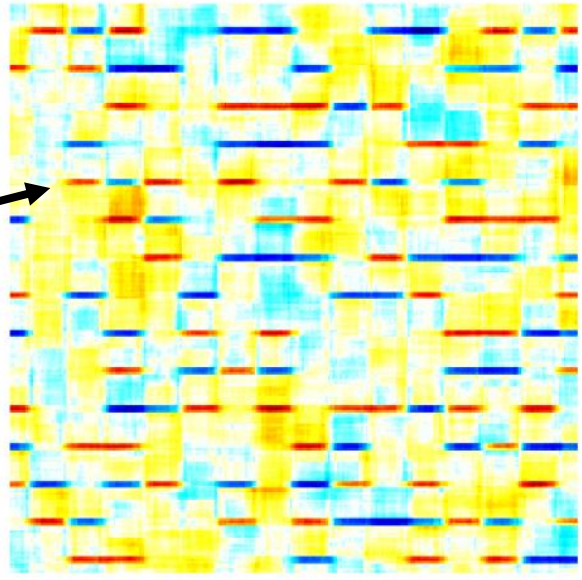
PC map 2



PC map 3



PC map 4



Horizontal Transitions
(changes in emotion)

Vertical Transitions

Clustering and Pattern Matching for Atom Finding

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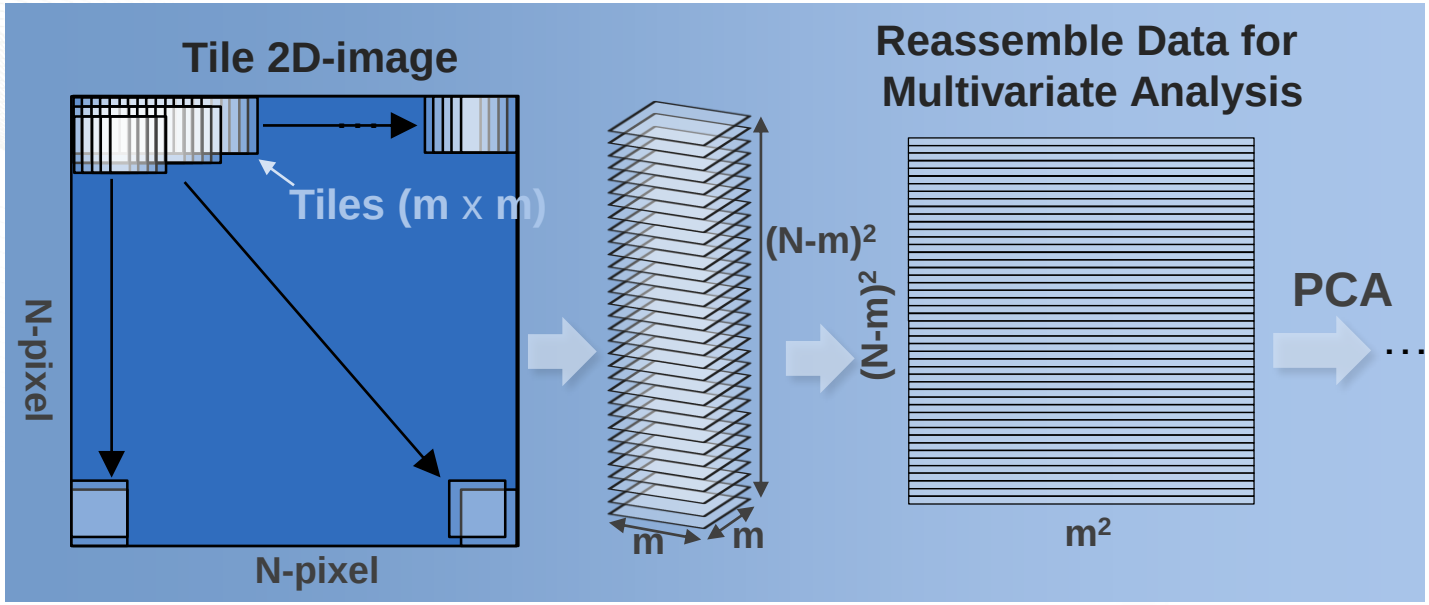
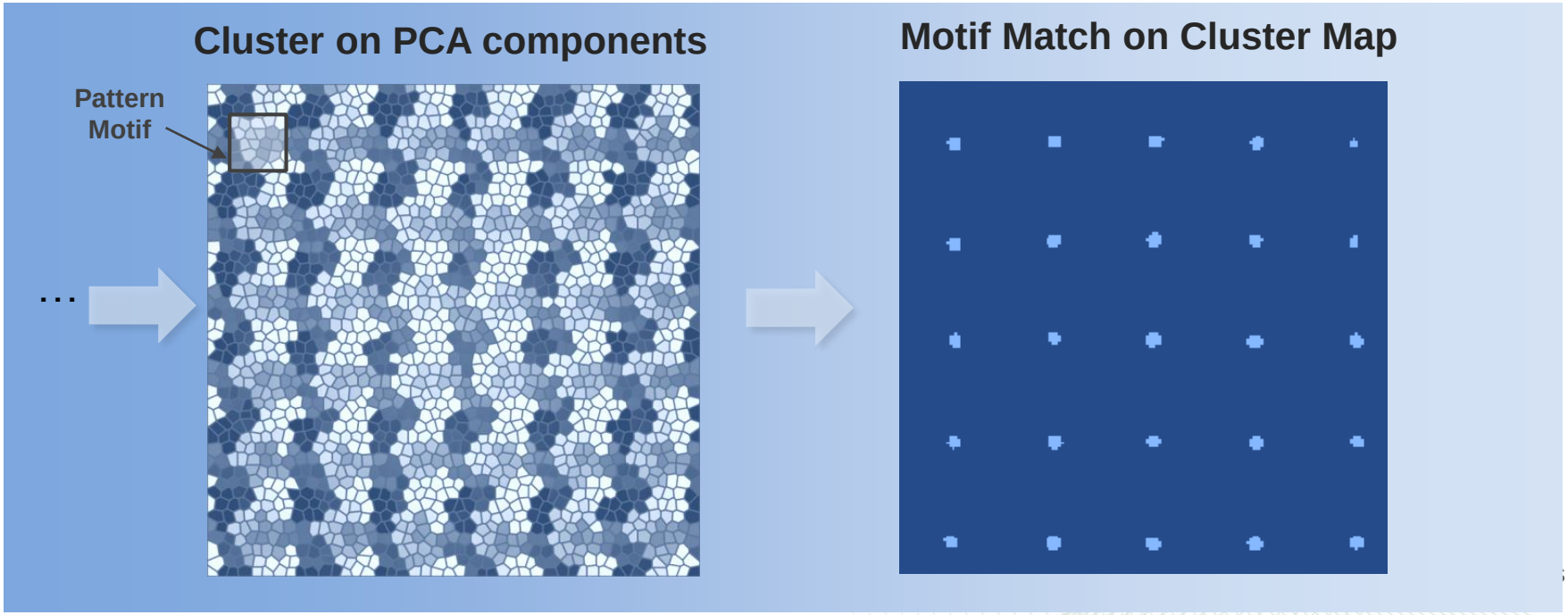
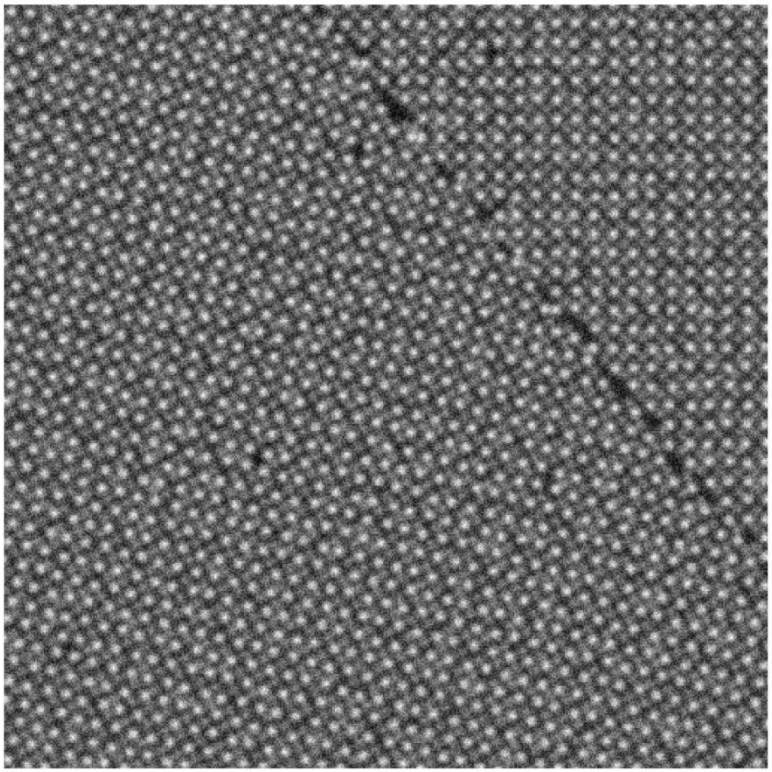
Sliding Window PCA + Clustering

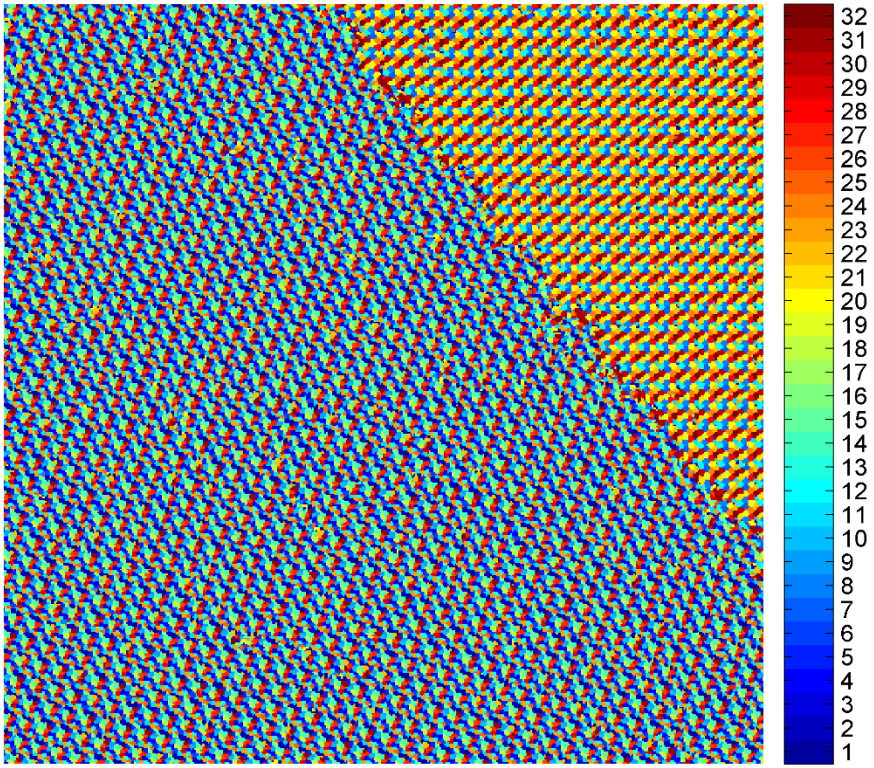




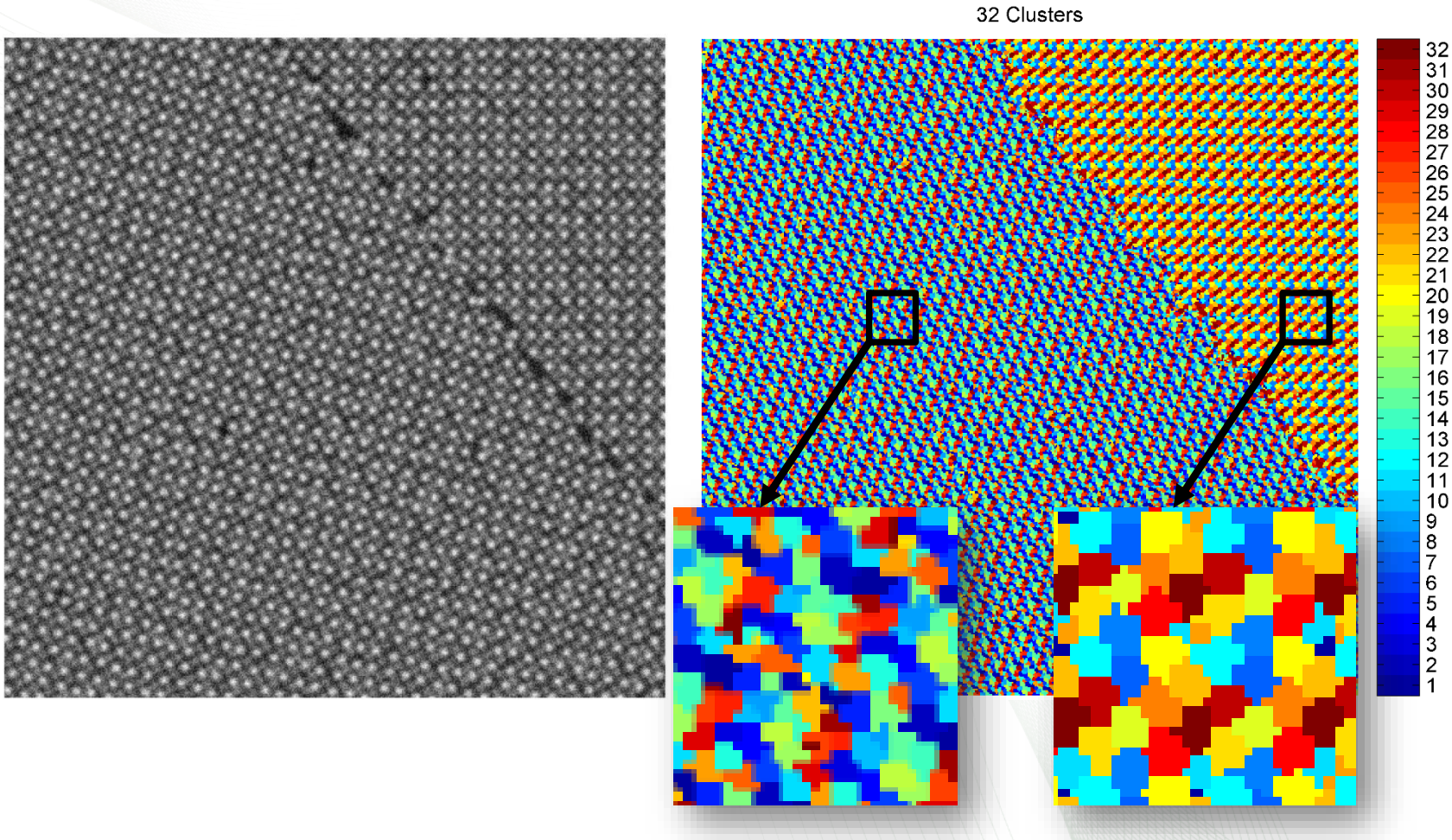
Cluster analysis

Perform clustering on PCA weighting vector from every pixel





Cluster analysis



We can use local motifs to locate similar atomic arrangements across an image

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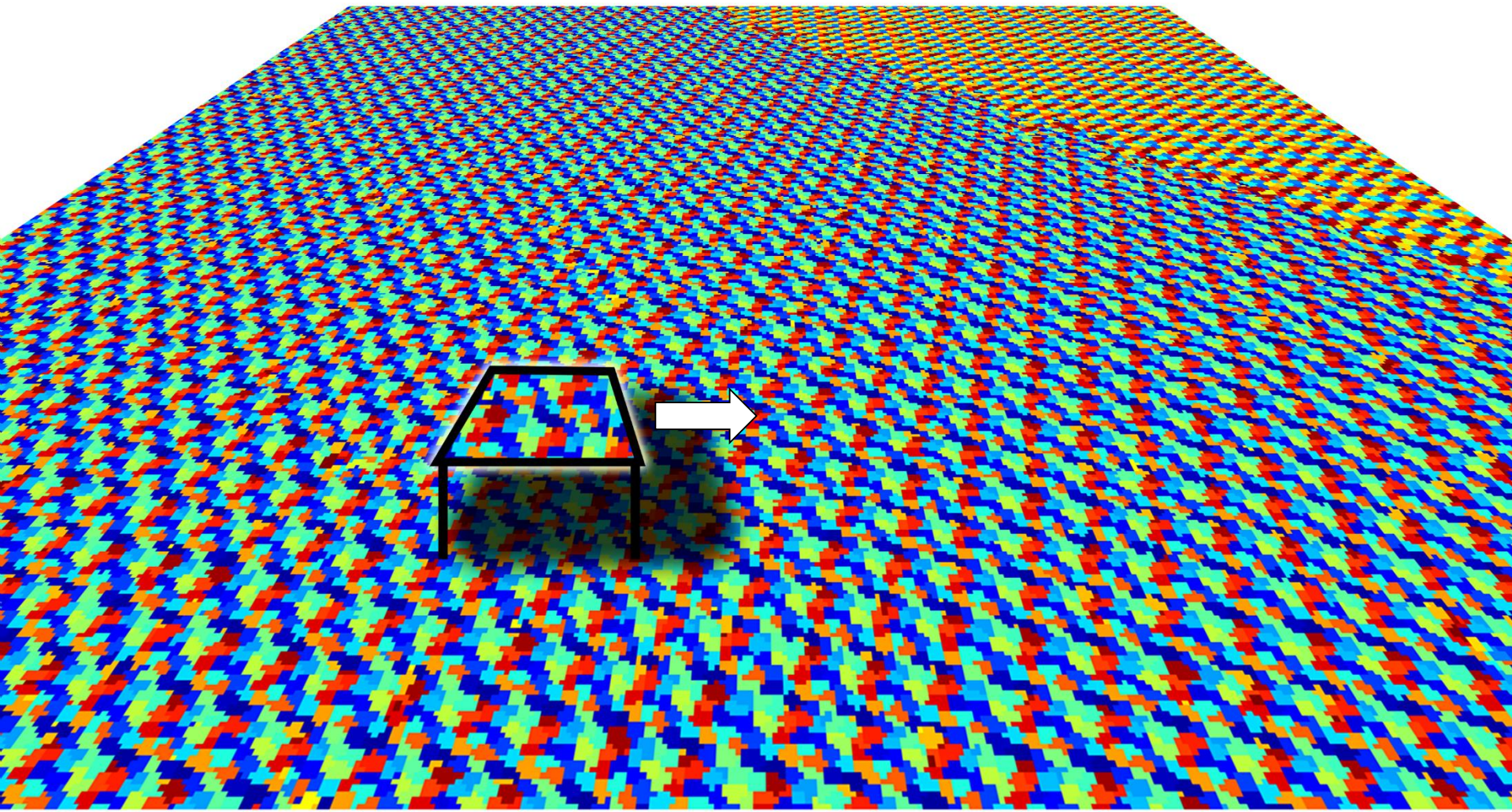
Motif Matching



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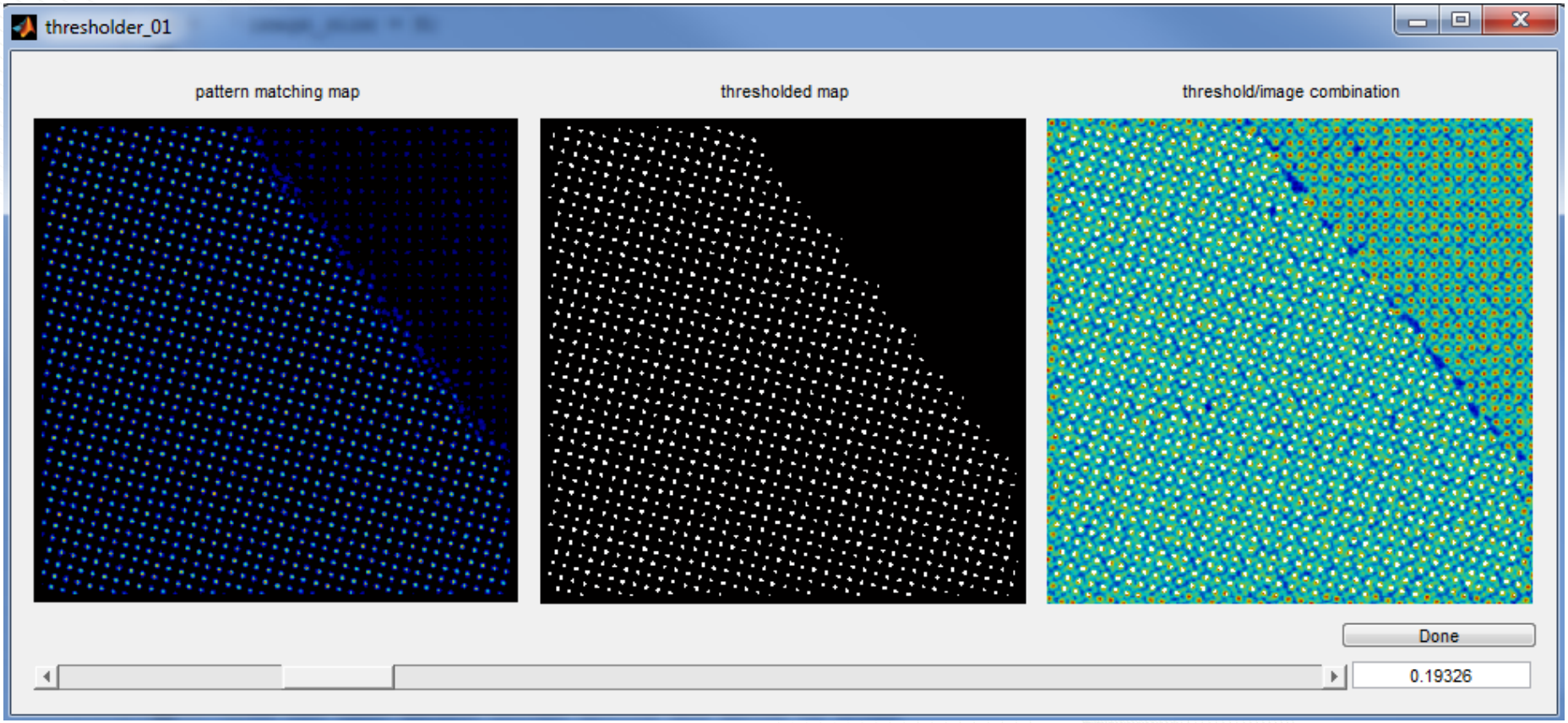
Motif Matching



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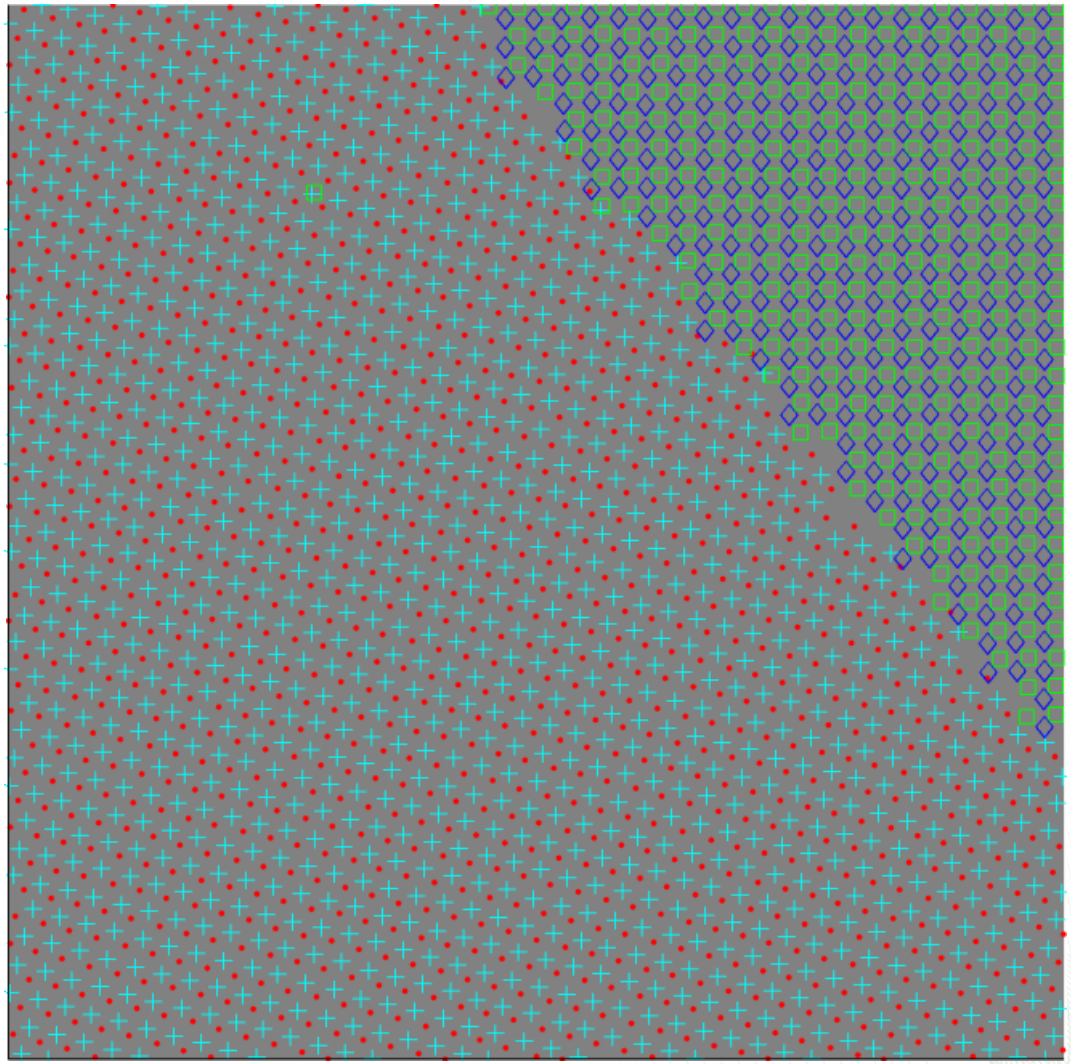
Sliding Window PCA + Clustering

After motif matching…



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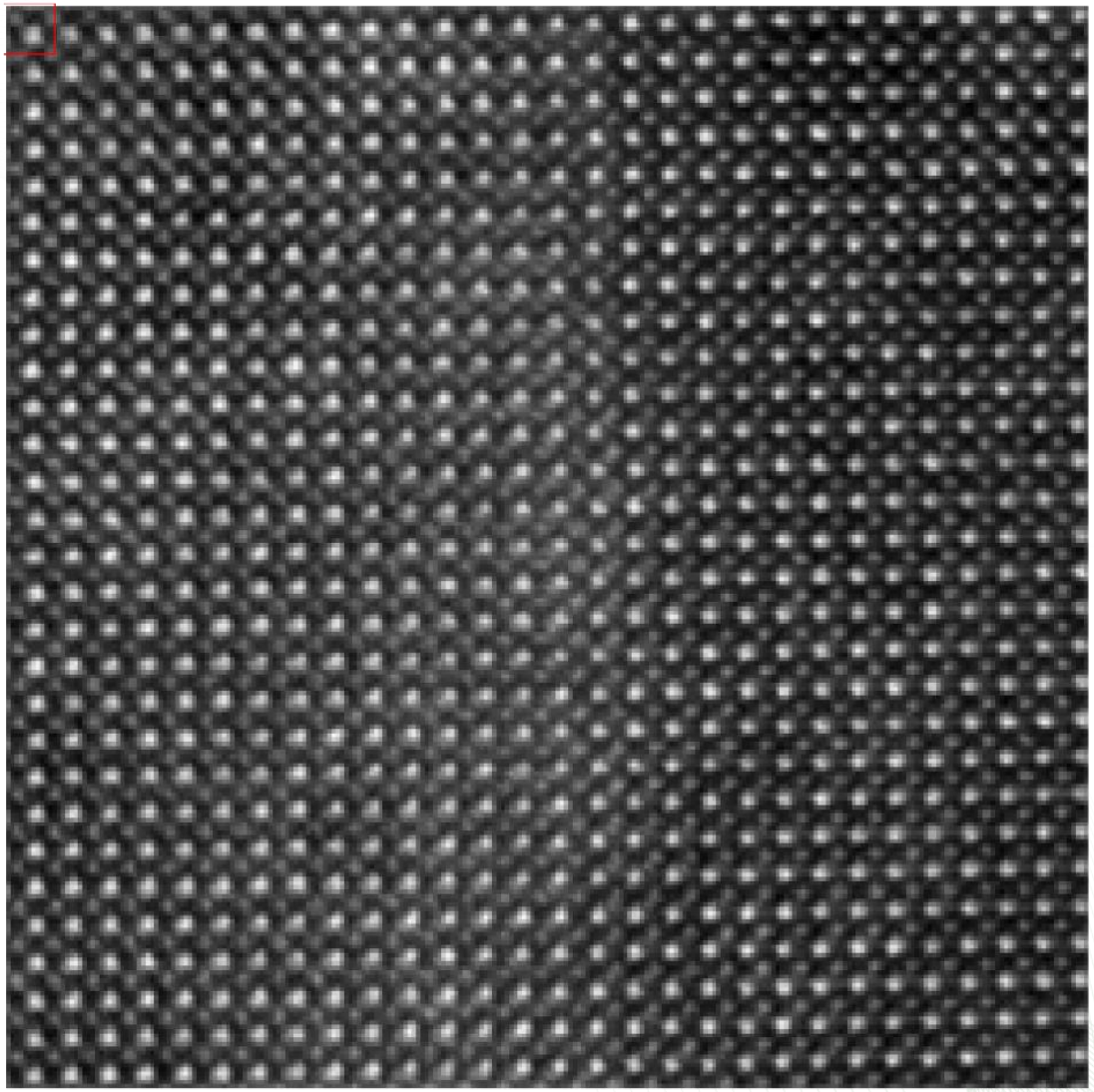
Sliding Window PCA + Clustering

original image



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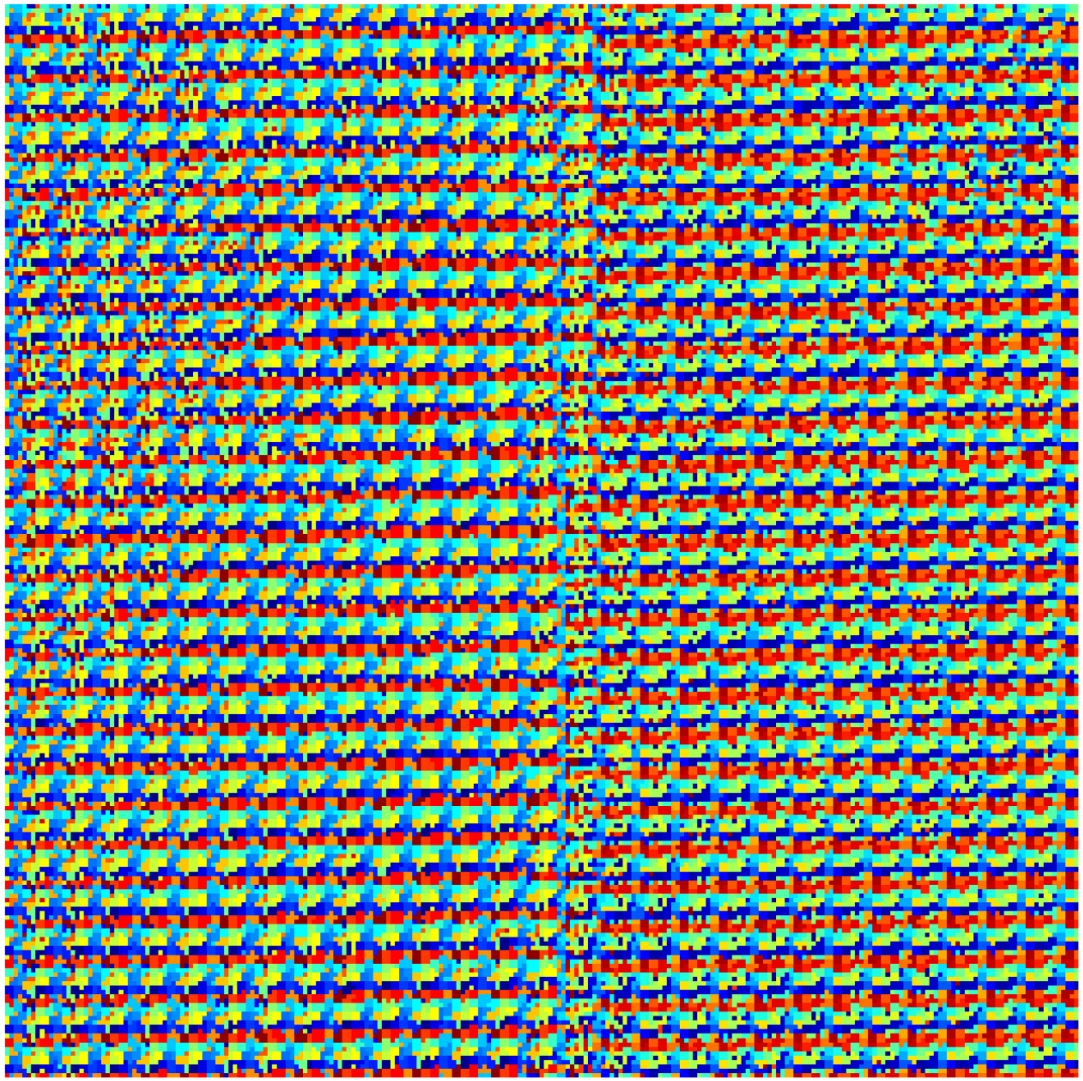
Sliding Window PCA + Clustering

Clustering of the first 32 PC's

36 Clusters



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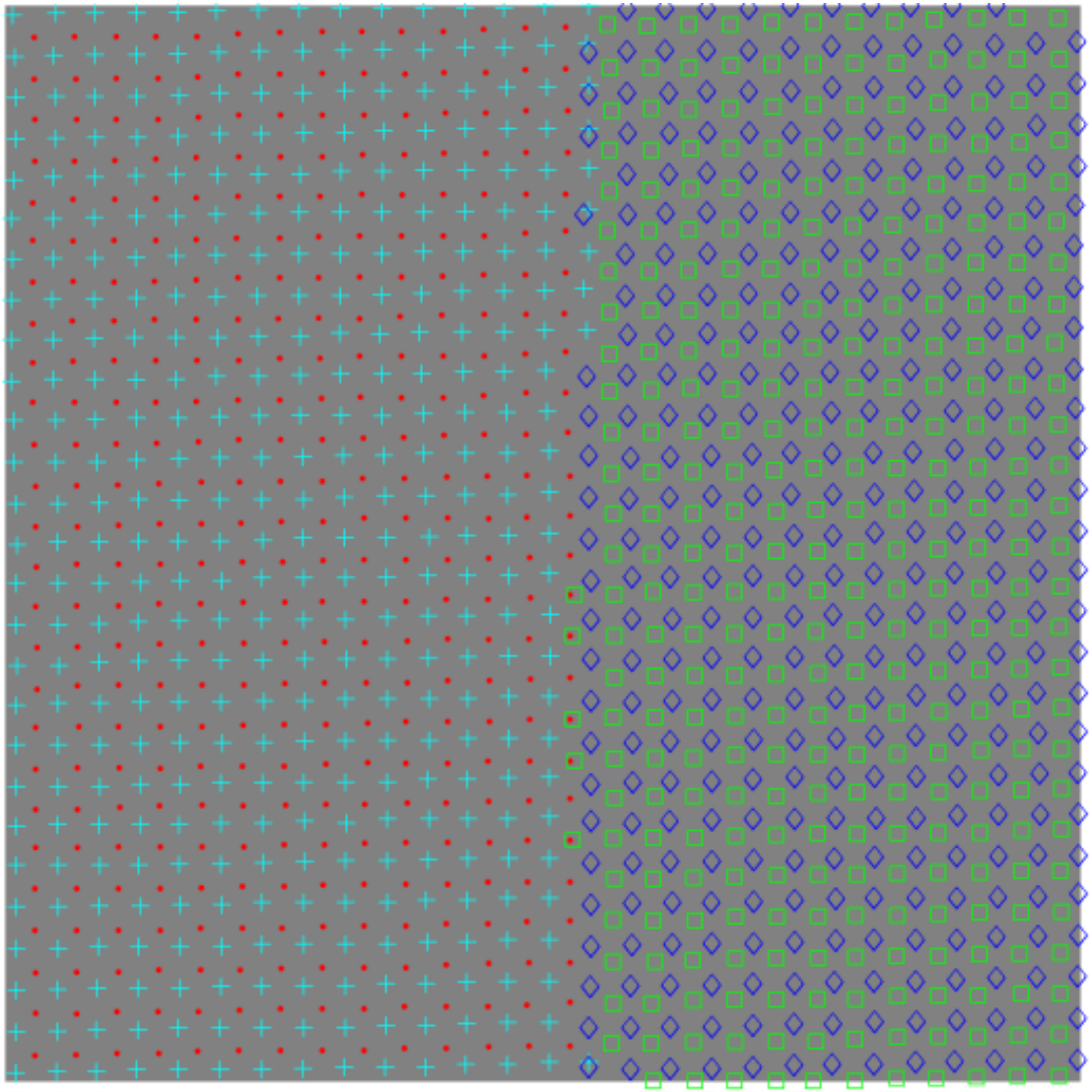
Sliding Window PCA + Clustering



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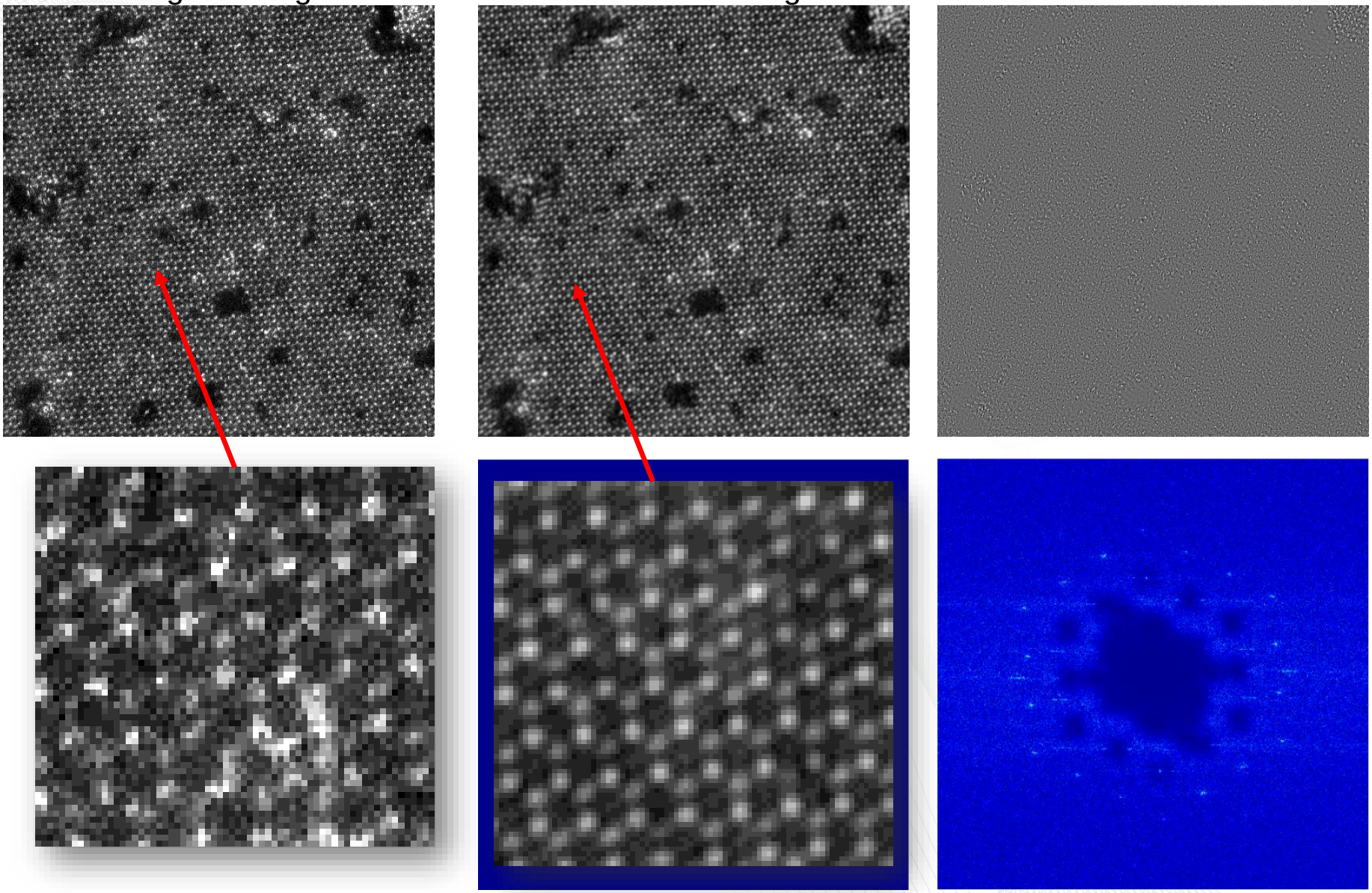
Sliding Window PCA + Clustering

Original image

Denoised image

Removed noise



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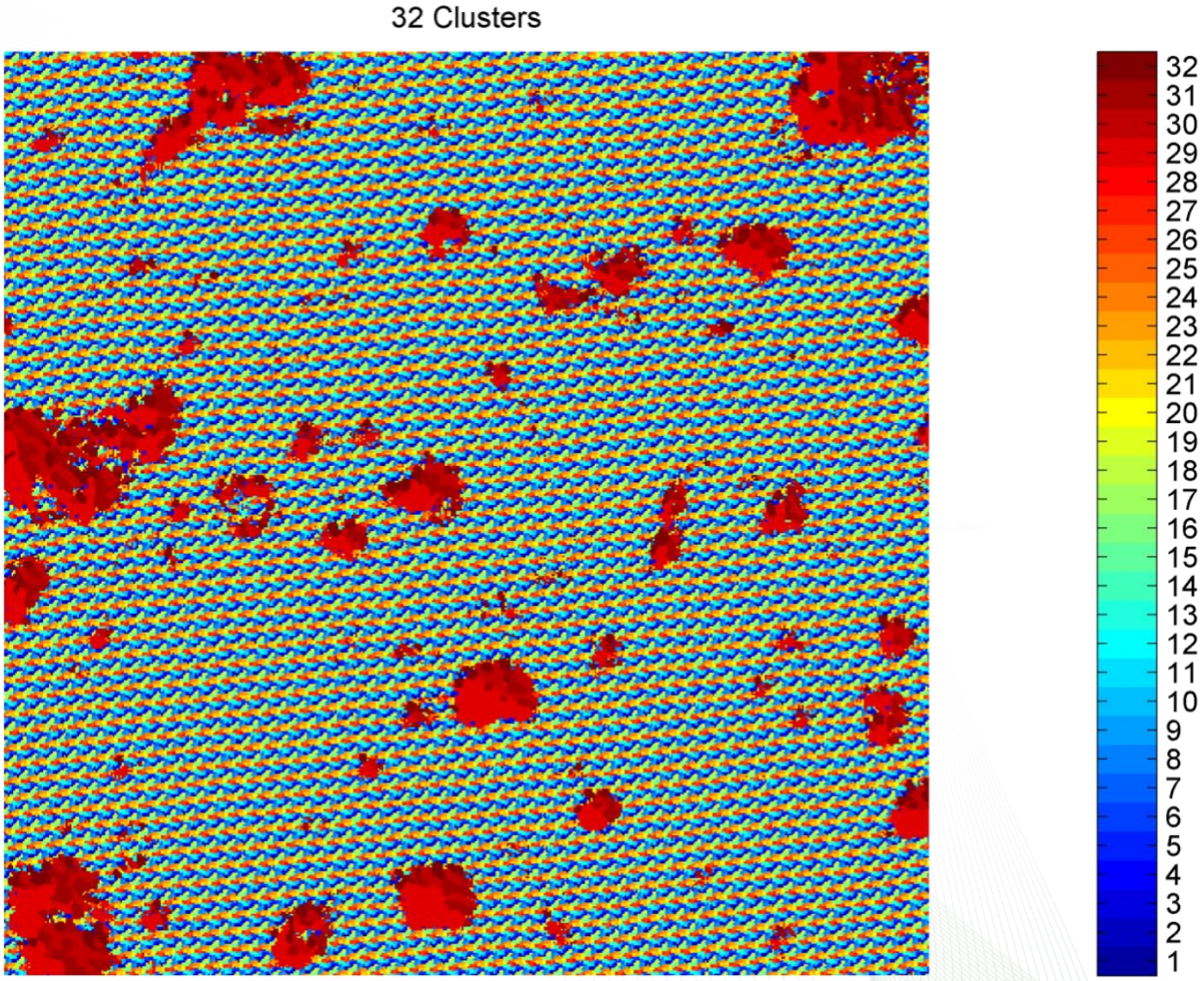
Sliding Window PCA + Clustering



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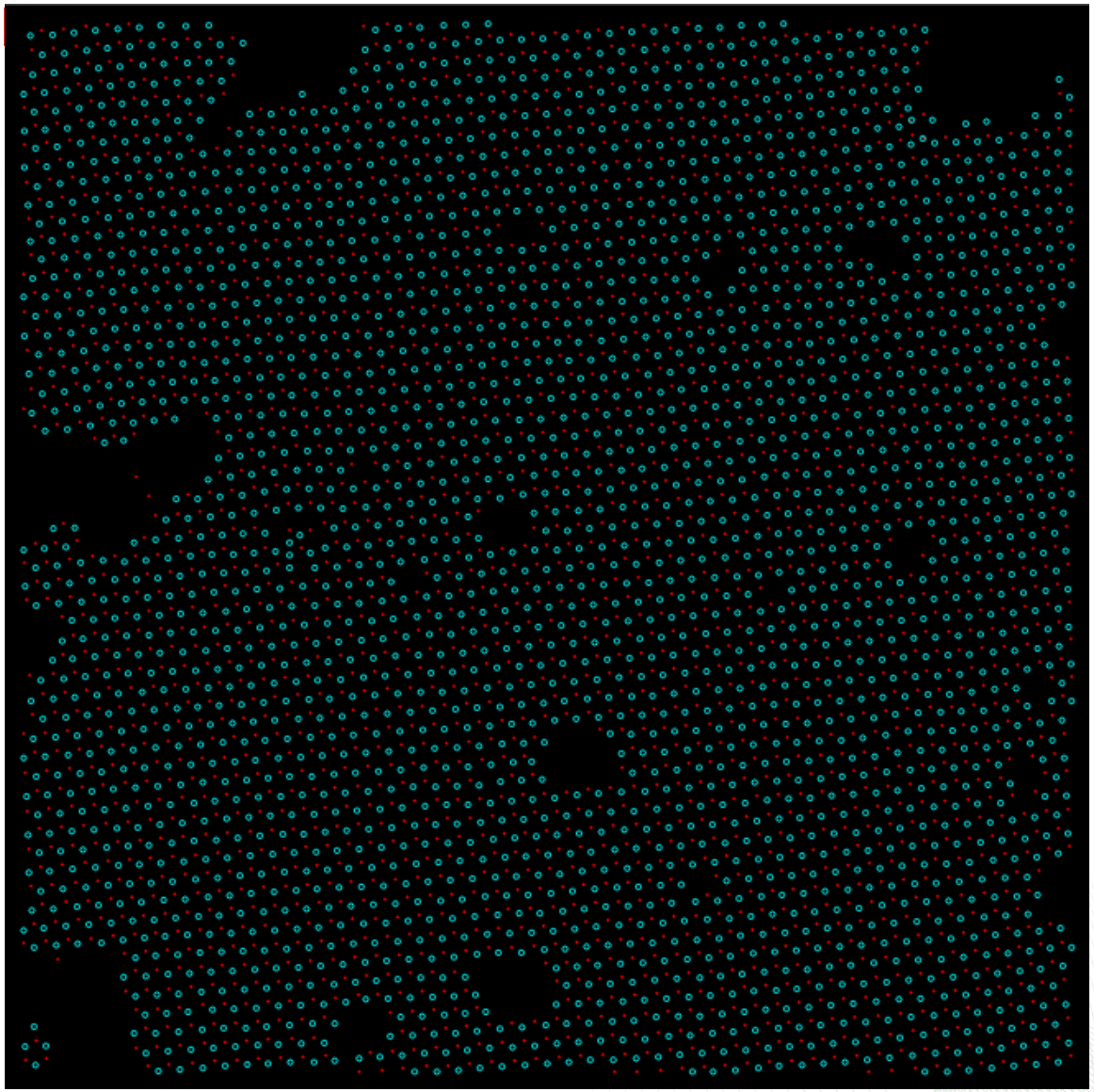
Sliding Window PCA + Clustering

Found atoms



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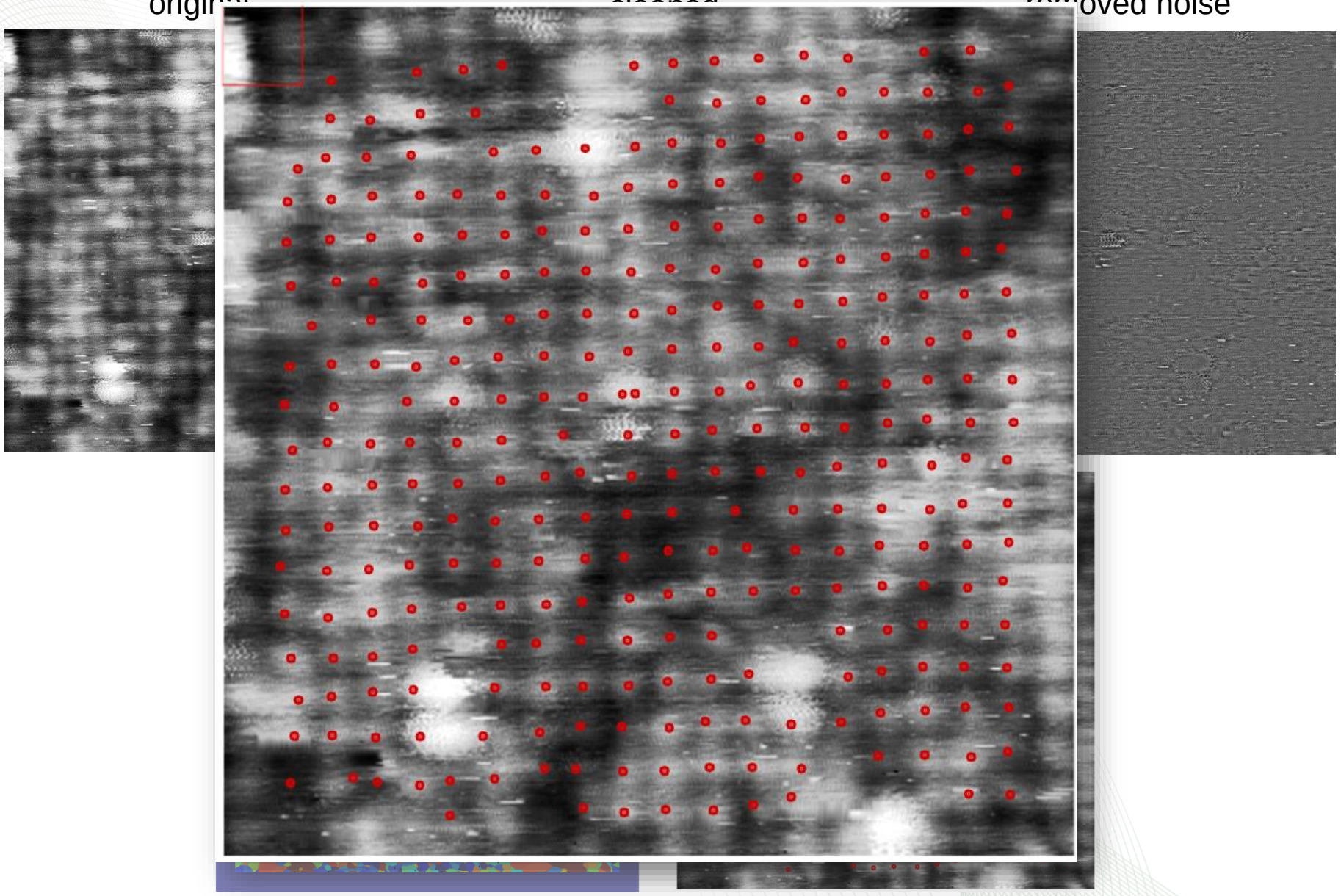
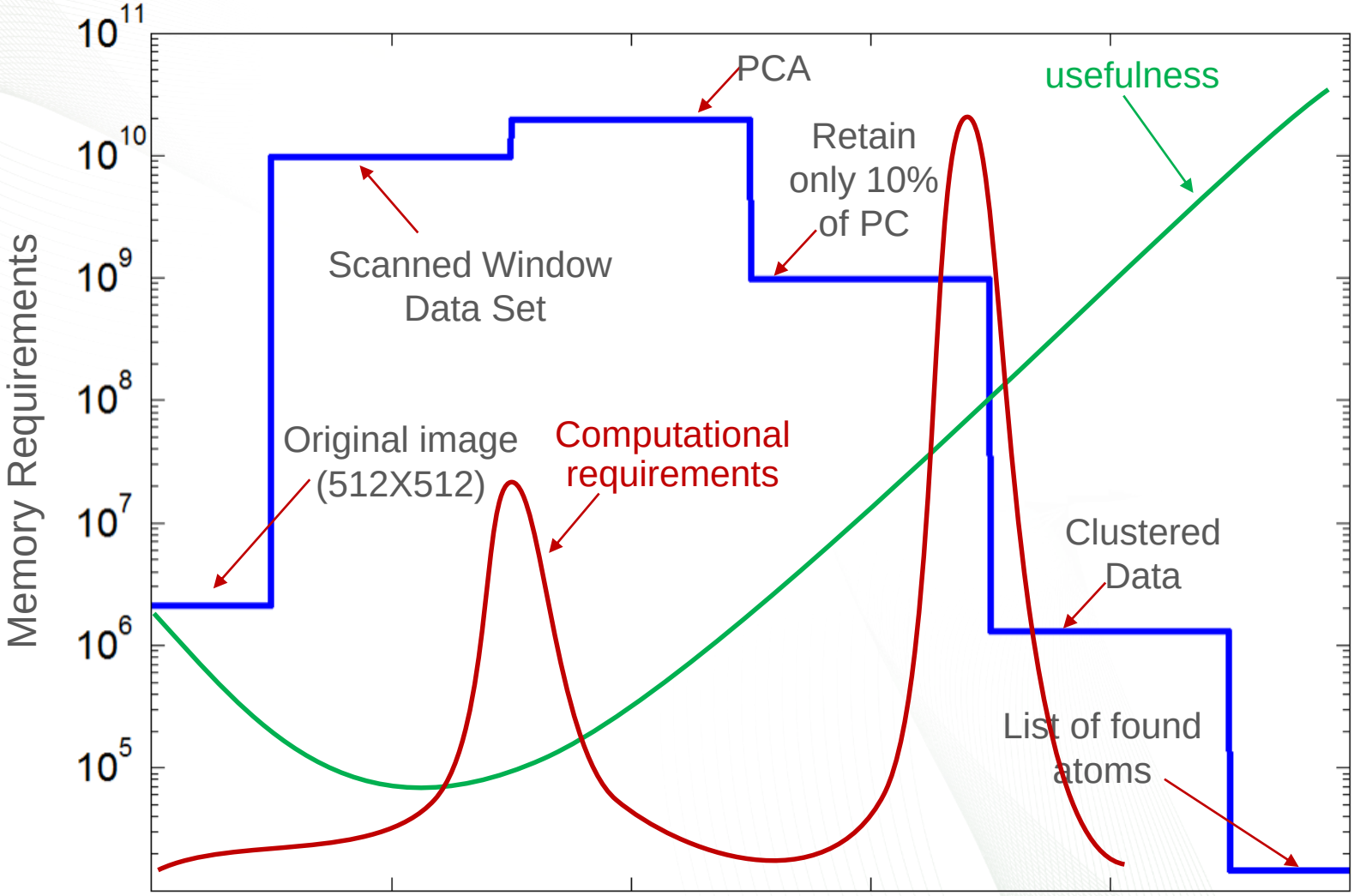
Sliding Window PCA + Clustering

original

removed noise



Sliding Window PCA + Clustering as Big Data



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Alternate atom finding
K-means on found atom positions

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Multivariate Analysis of 4D STEM Data

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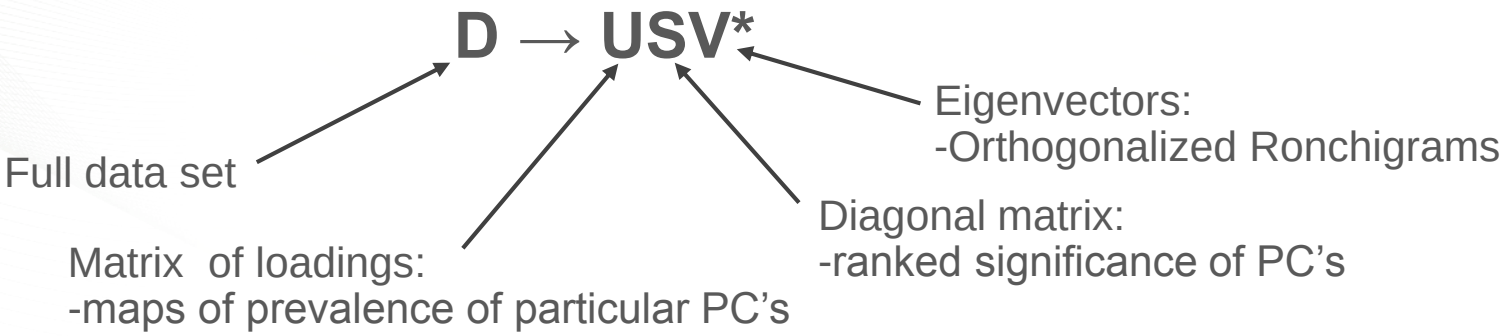
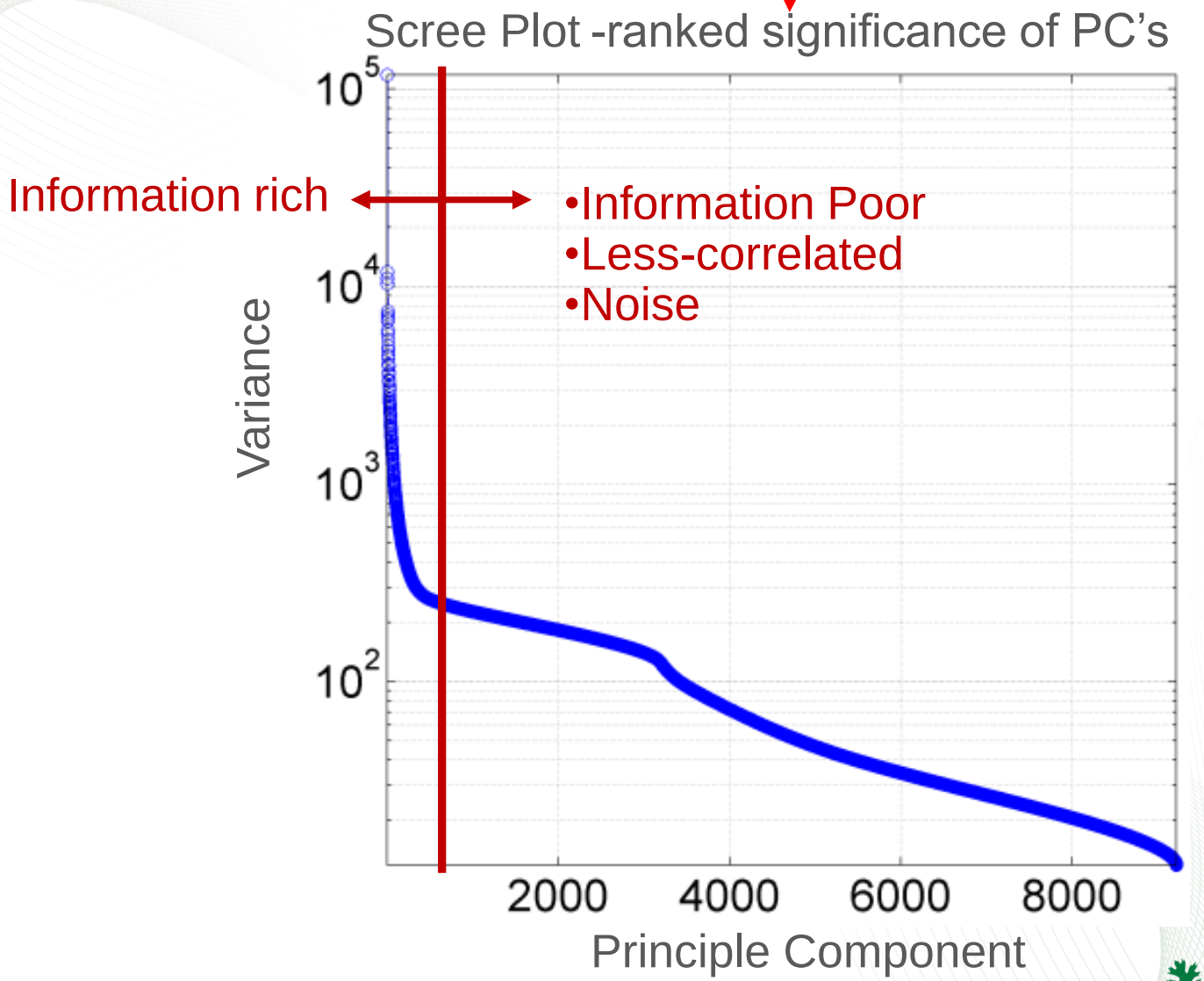
Principal Component Analysis (PCA)



- Compares every individual observable with every other observable
- Find the most common behavior
- Find the next most information rich (orthogonal) variation on the above behavior
- Find the next most information rich (orthogonal) variation on the above behavior
- … loop

Principal Component Analysis (PCA)

$D \rightarrow USV^*$



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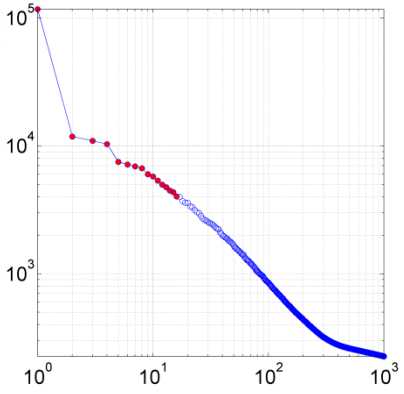
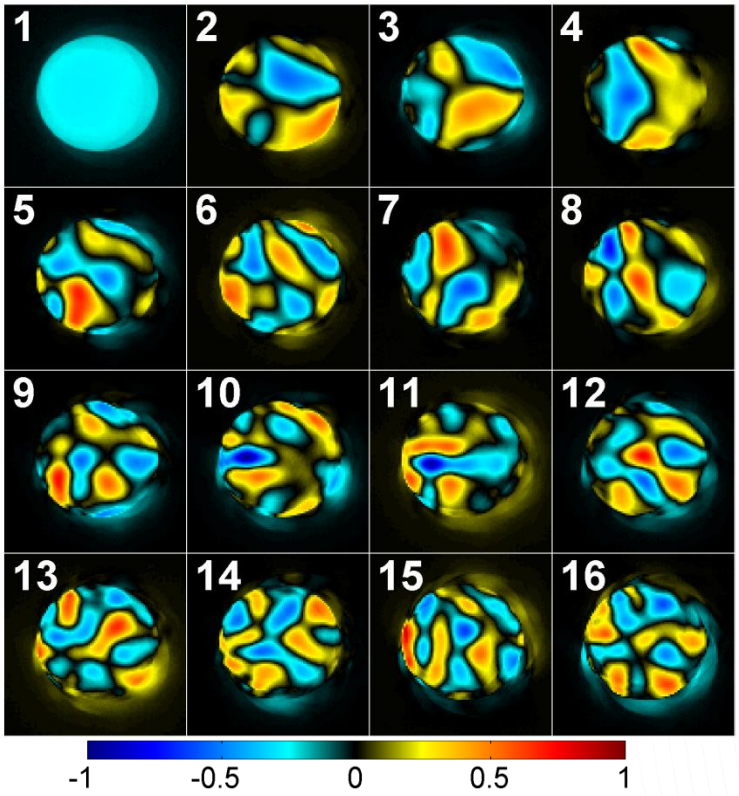
Principal Component Analysis (PCA)

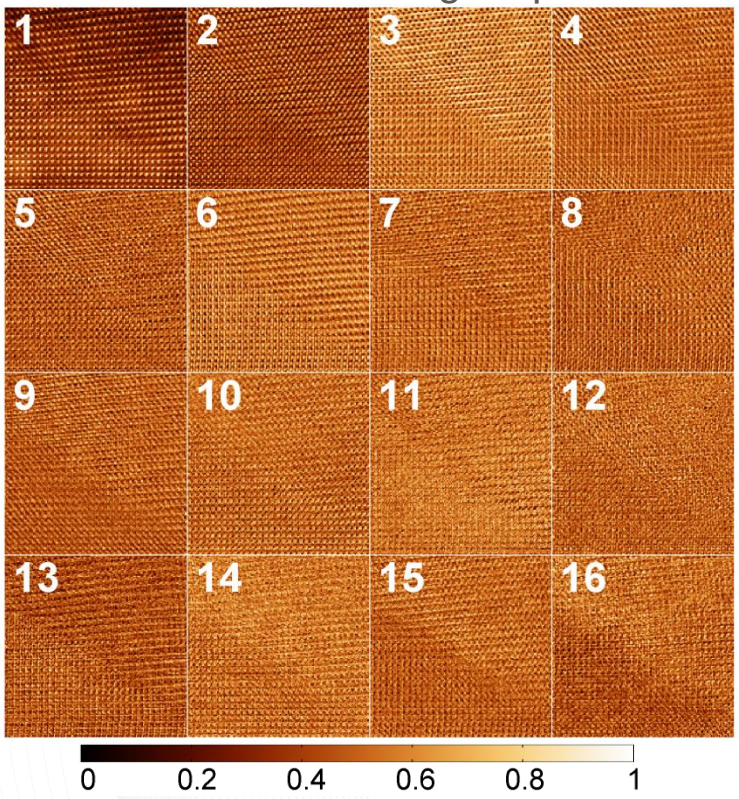
Scree Plot



First 16 eigenvectors



First 16 loading maps



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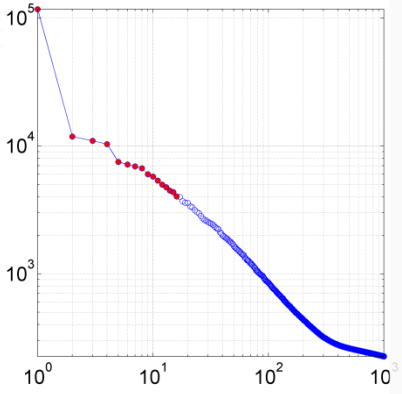
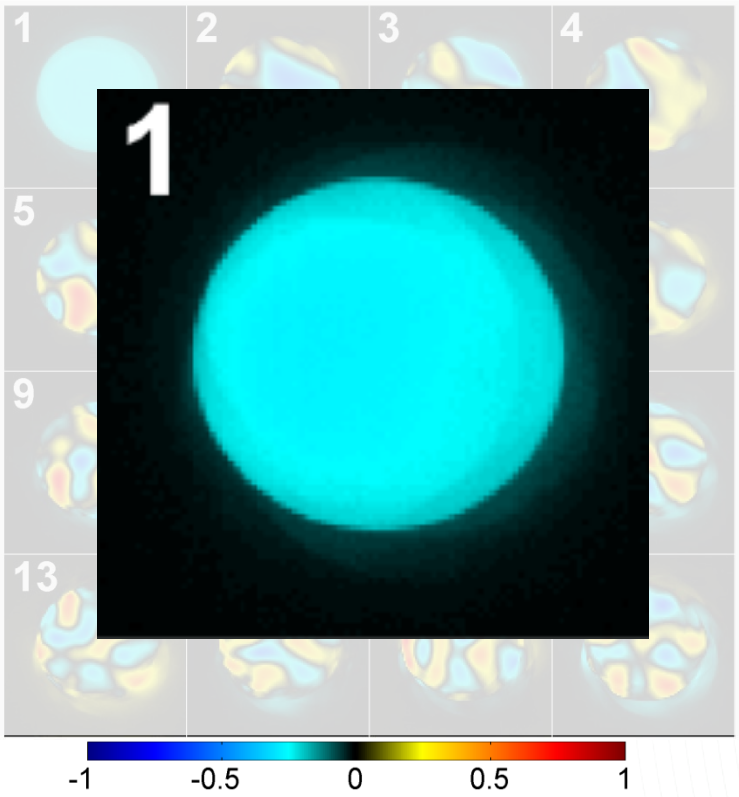
Principal Component Analysis (PCA)

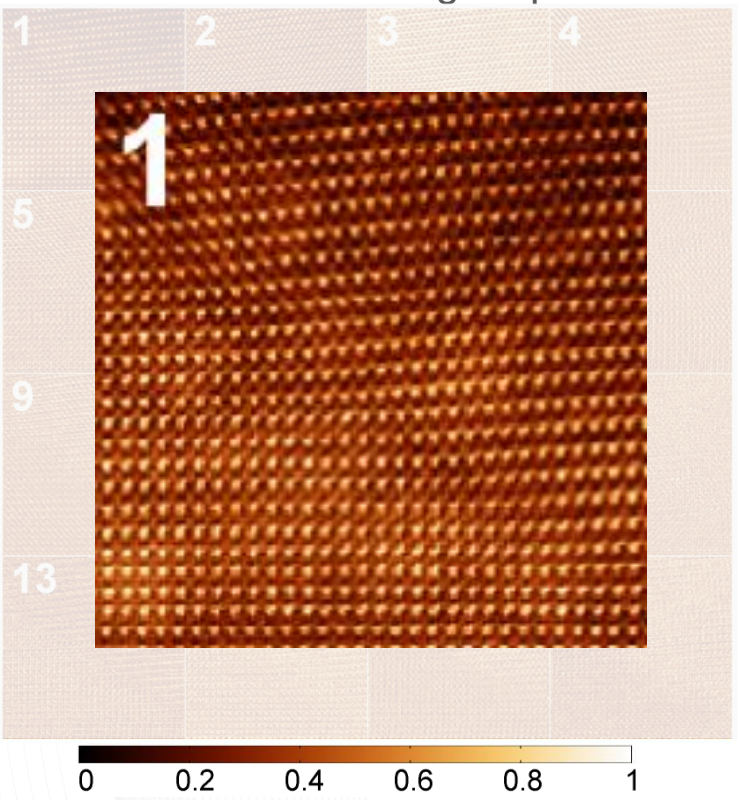
Scree Plot



First 16 eigenvectors



First 16 loading maps



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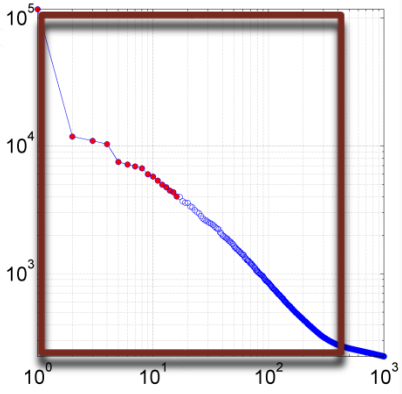
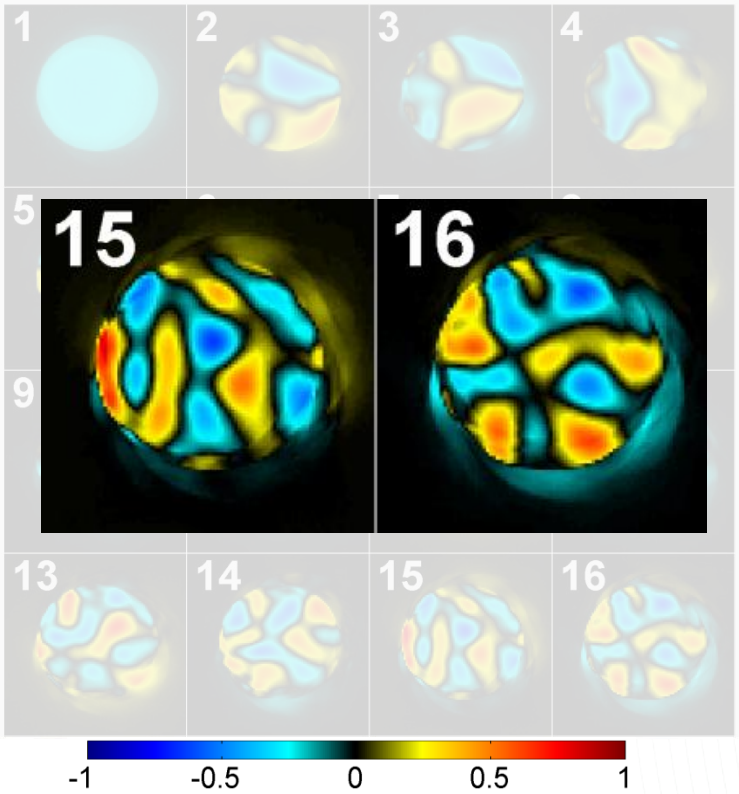
Principal Component Analysis (PCA)

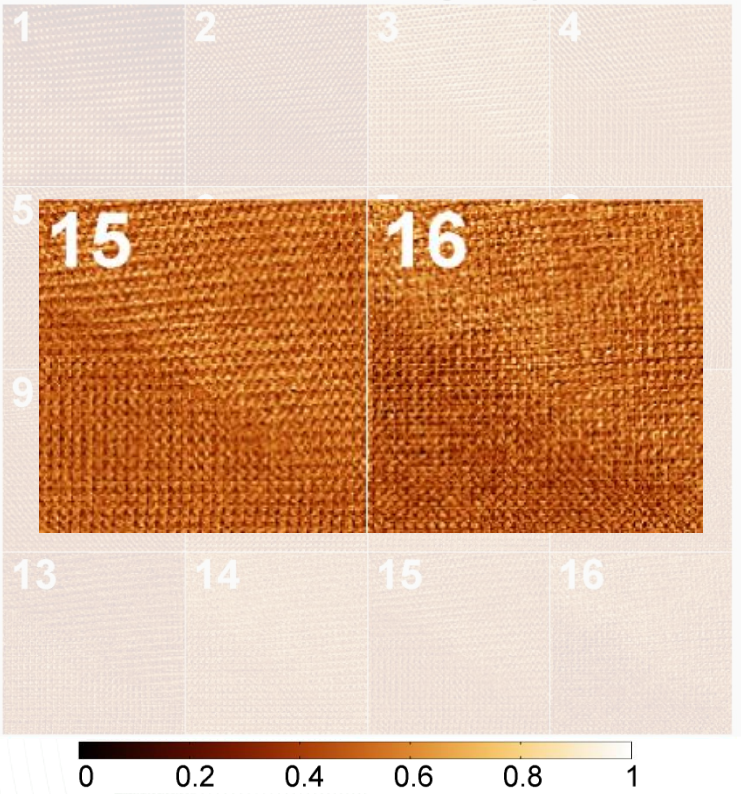
Scree Plot



First 16 eigenvectors



First 16 loading maps



PCA typically fails at: elucidating underlying physics

PCA typically succeeds at: - being fast and efficient
- de-noising
- data compressio

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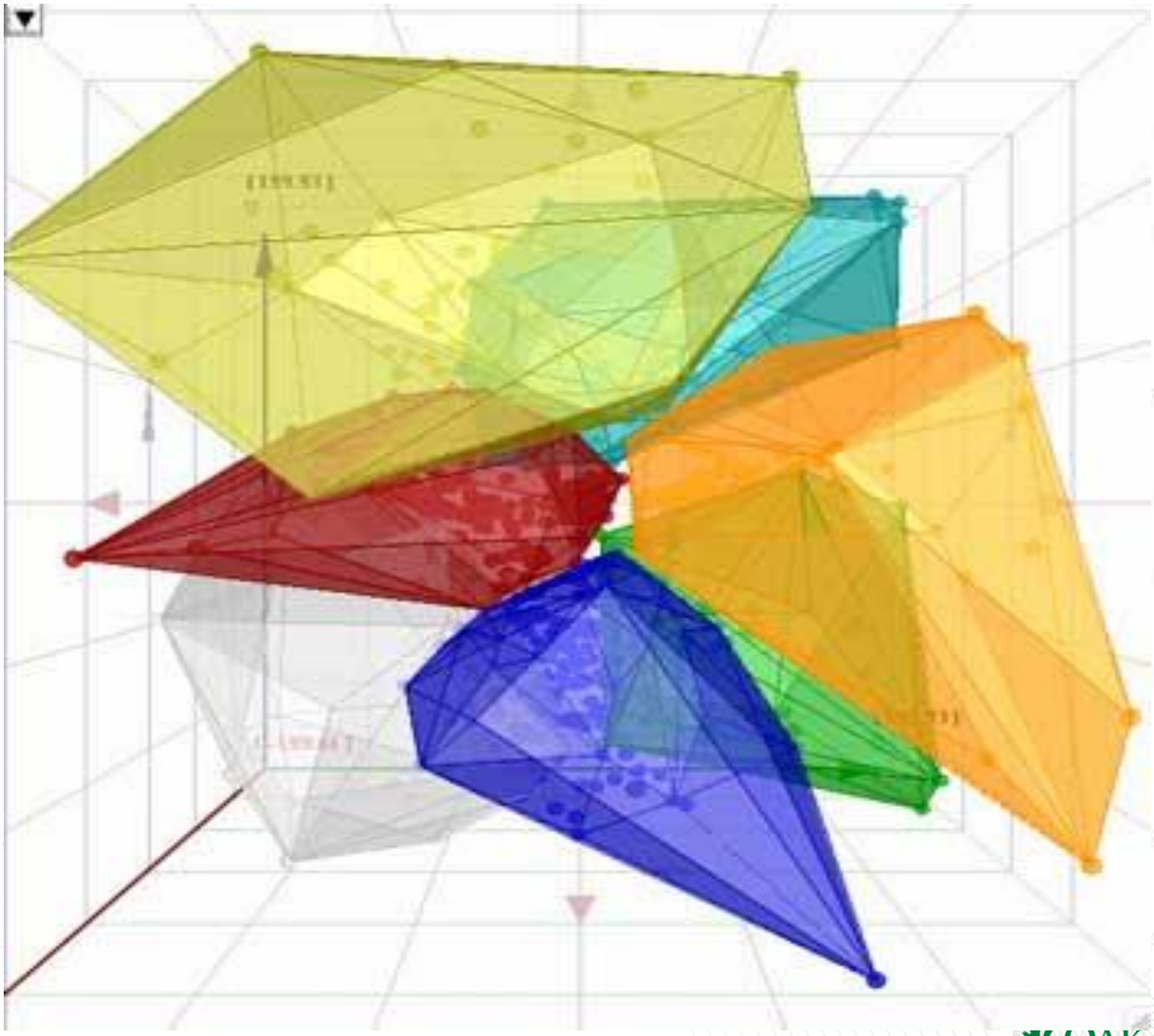
Cluster analysis

Group observables by “distance” to one another



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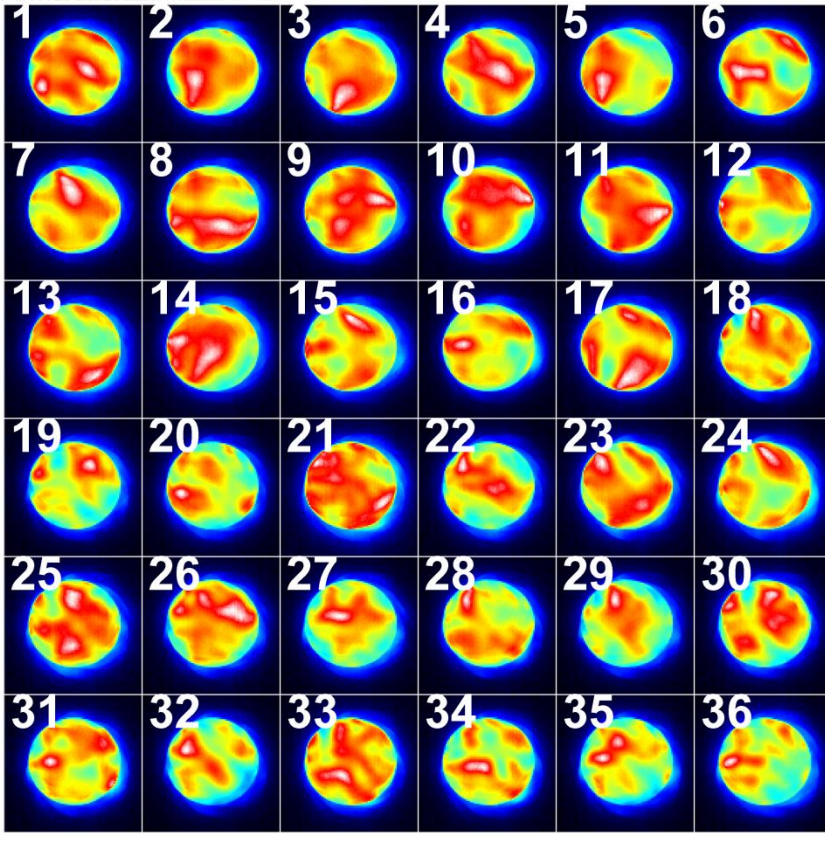
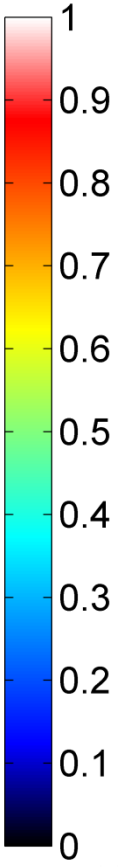
Cluster analysis

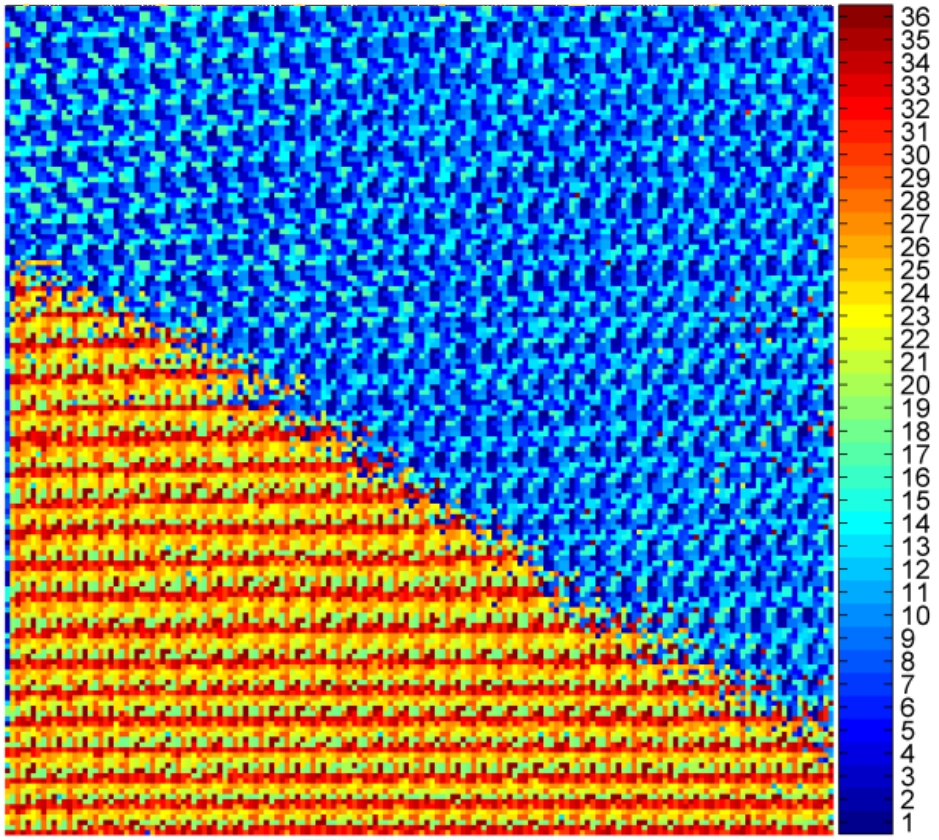
K-means clustering: 36 Clusters

Ronchigram corresponding to each cluster





Cluster Locations



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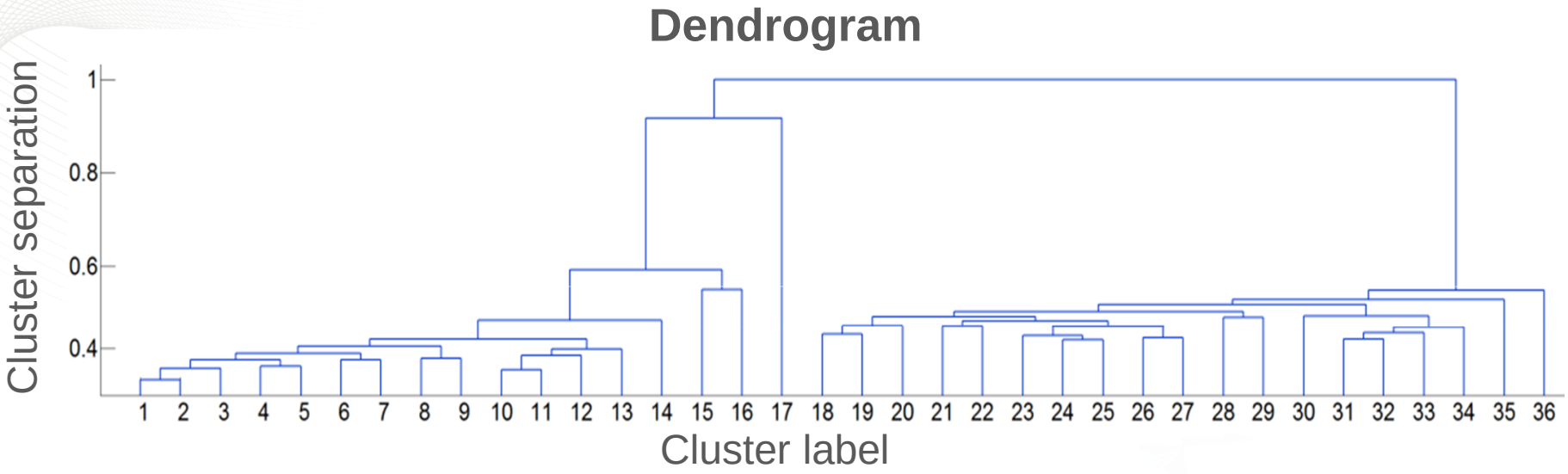
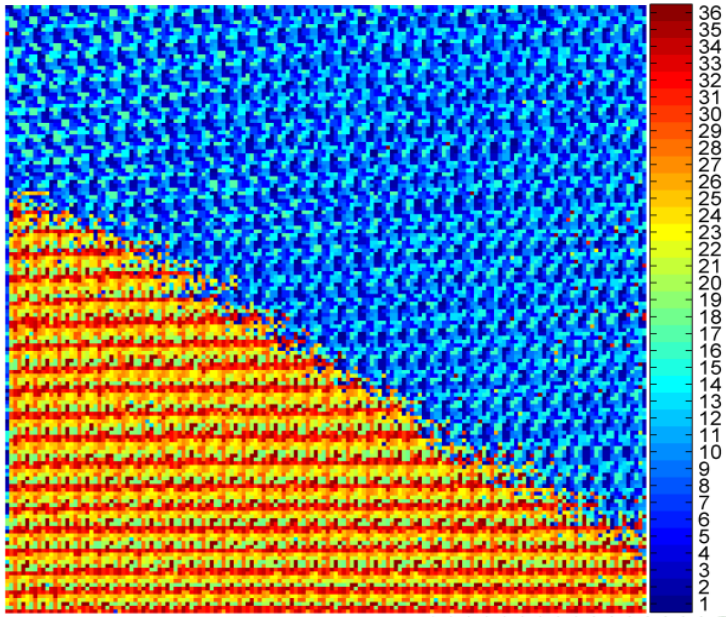
Cluster analysis

How many clusters is the right number of clusters?





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Cluster analysis

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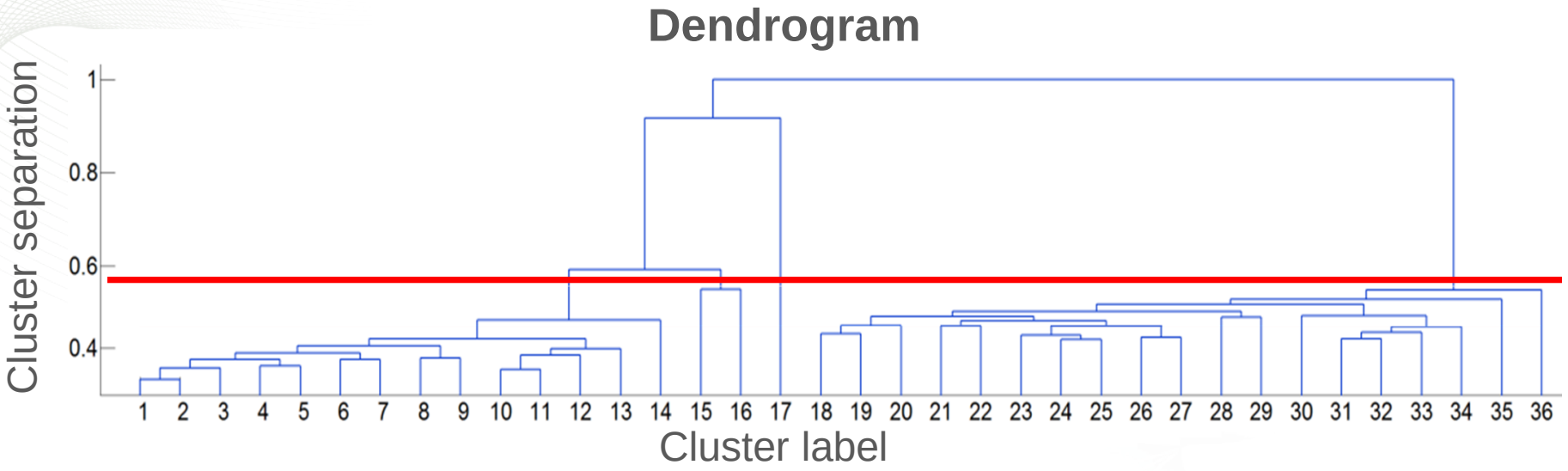

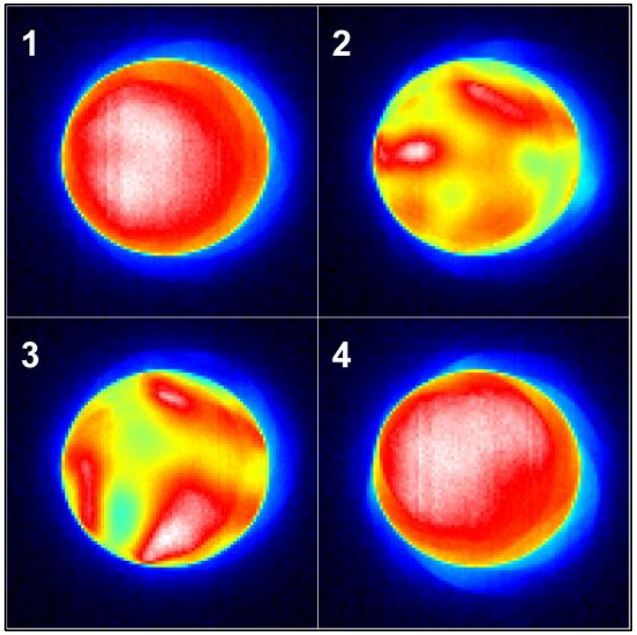

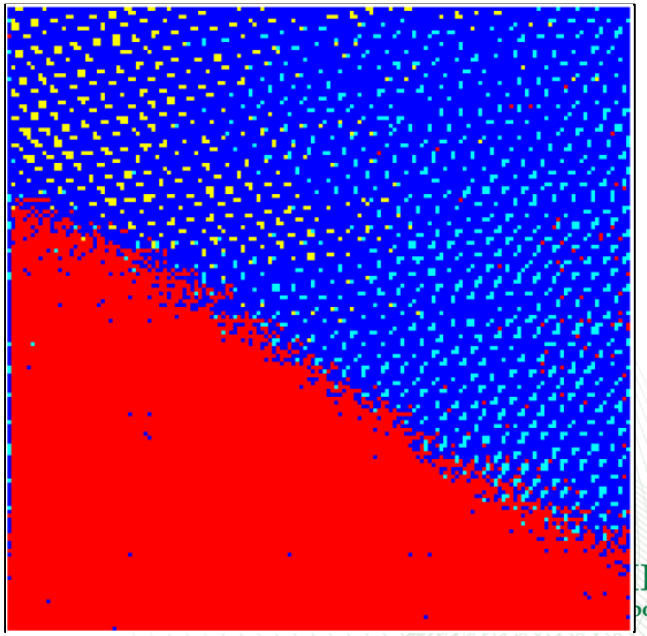

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- Scientific user facility
- 2 Page Proposal
- sjesse@ornl.gov