Multivariate Methods Applied to 4D STEM data

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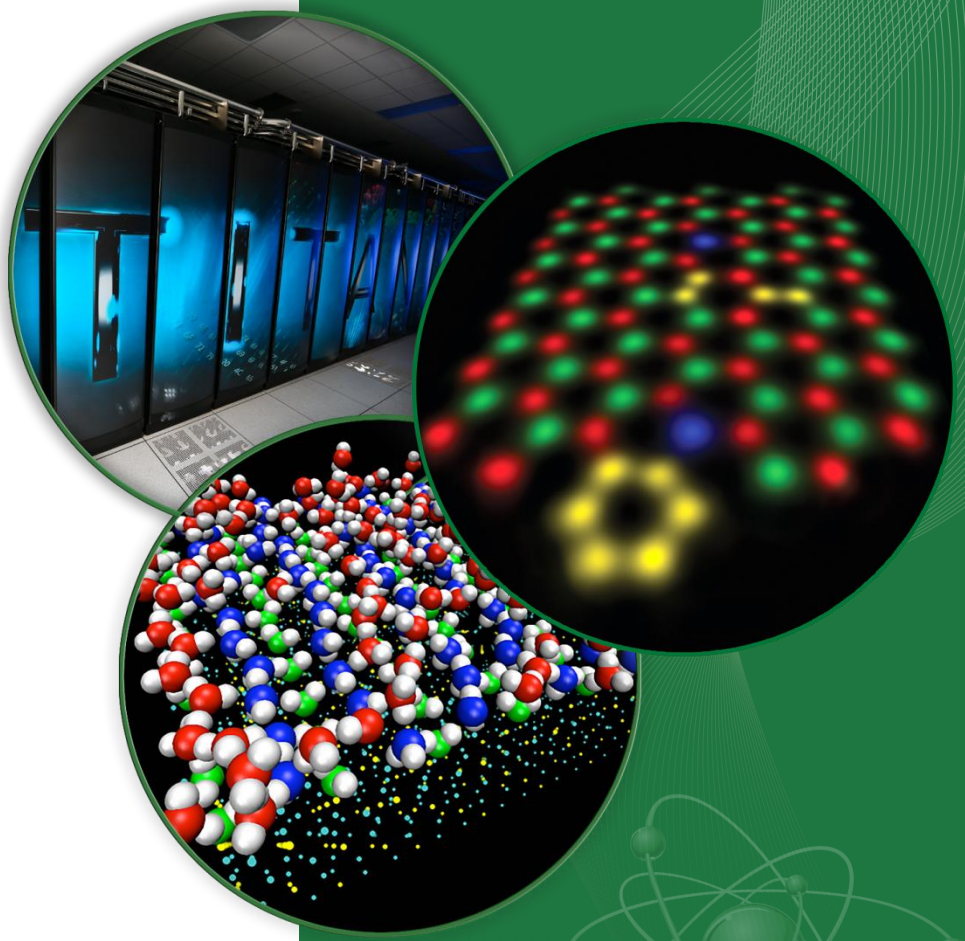

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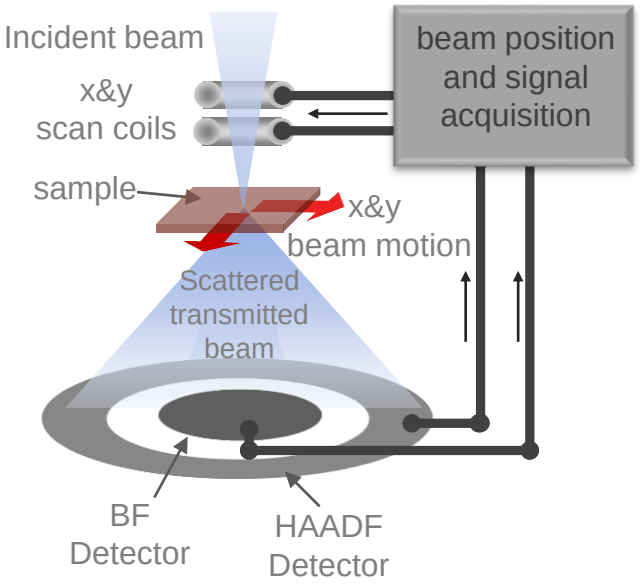
Introduction

- The standard STEM configuration is exquisitely tuned to capture material structure (in projection)
- However, the transmitted electrons carry far more information than is captured by monolithic detectors



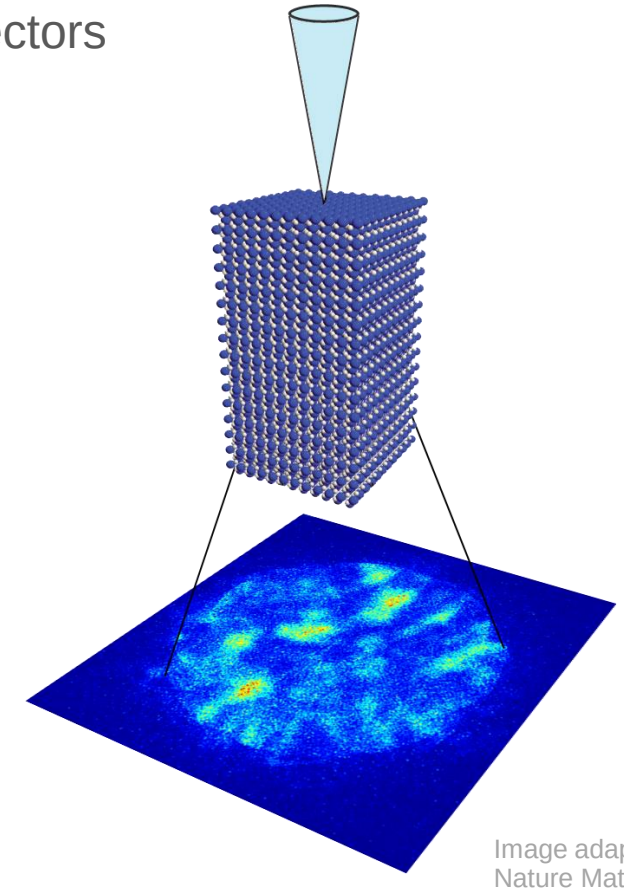


Image adapted from:
Nature Materials 10, 270–271 (2011)

Introduction

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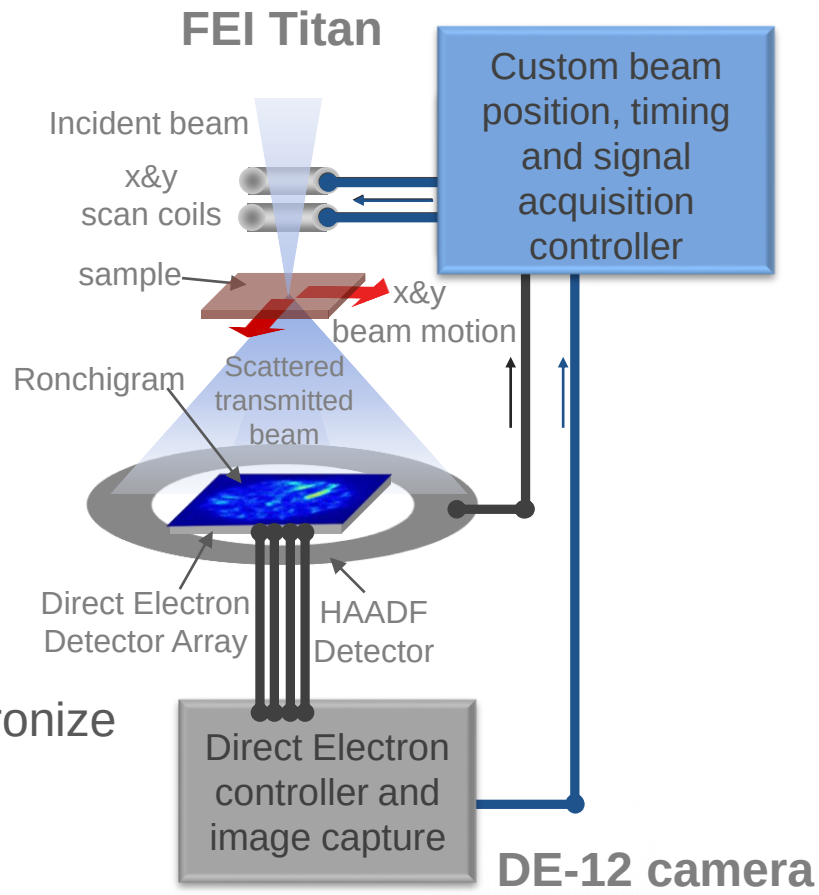
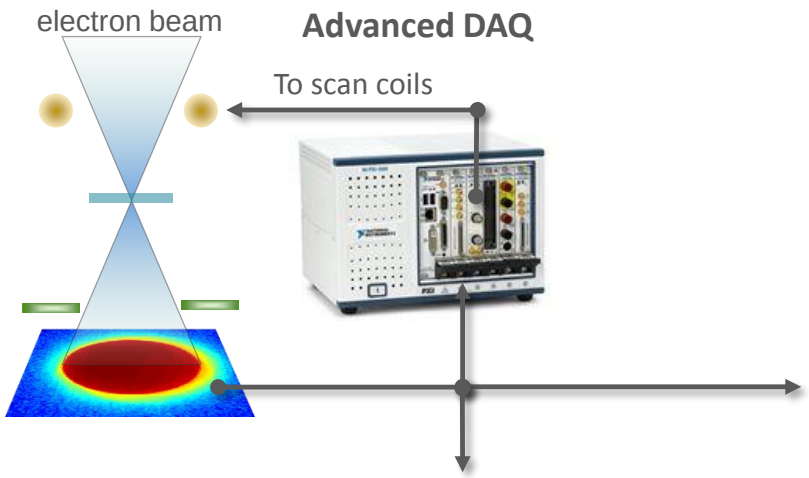
- However, the transmitted electrons carry far more information than is captured by monolithic detectors
- Recent advances in detectors has enabled rapid and sensitive capture of Ronchigrams
- Developed FPGA based controller to synchronize beam positioning with Ronchigram capture enabling:
  - Ronchigram capture at ~400 frames/sec
  - 192X192 pixels per image with 384X384 pixels per Ronchigram
  - 4-dimensional data set (4 GB)



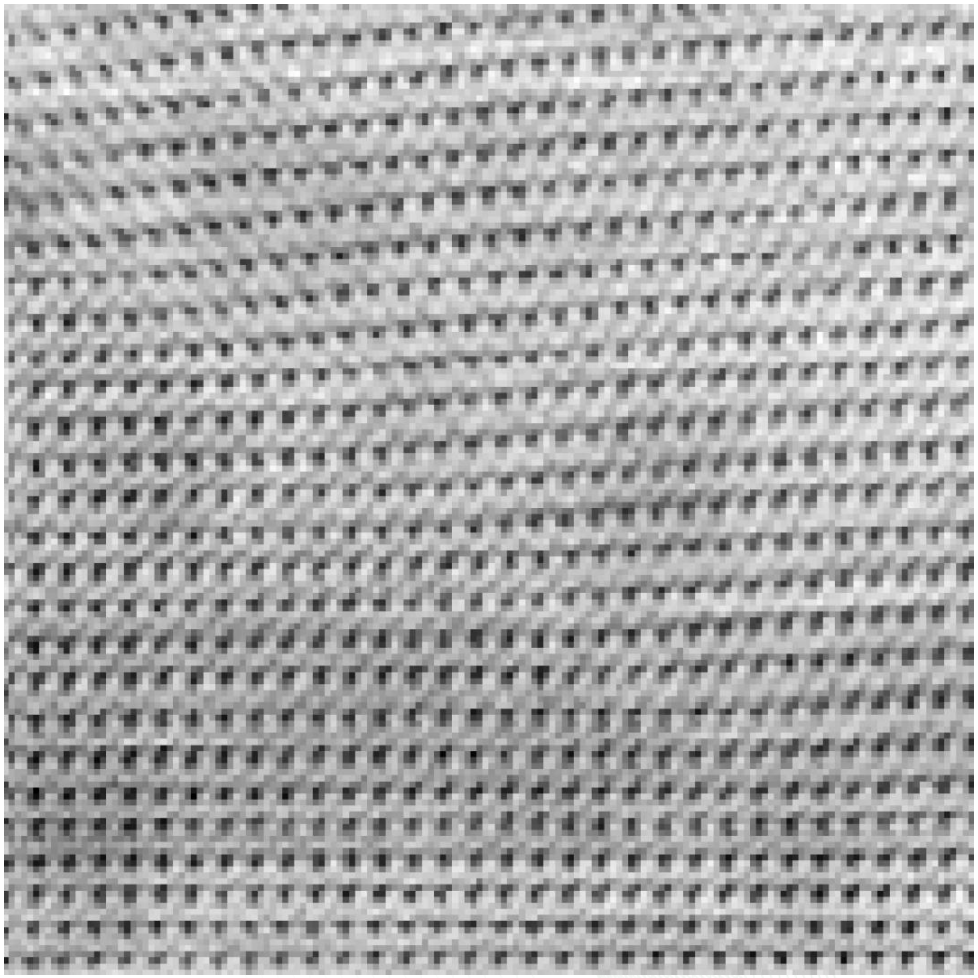
How can we explore this data to yield new and useful information?

Ptychography Data Capture



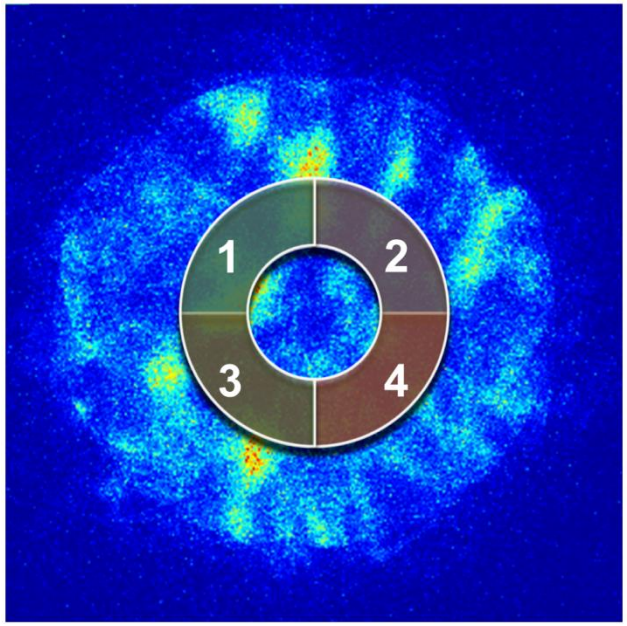
Bismuth Ferrite (Ferroelectric) Domain Boundary

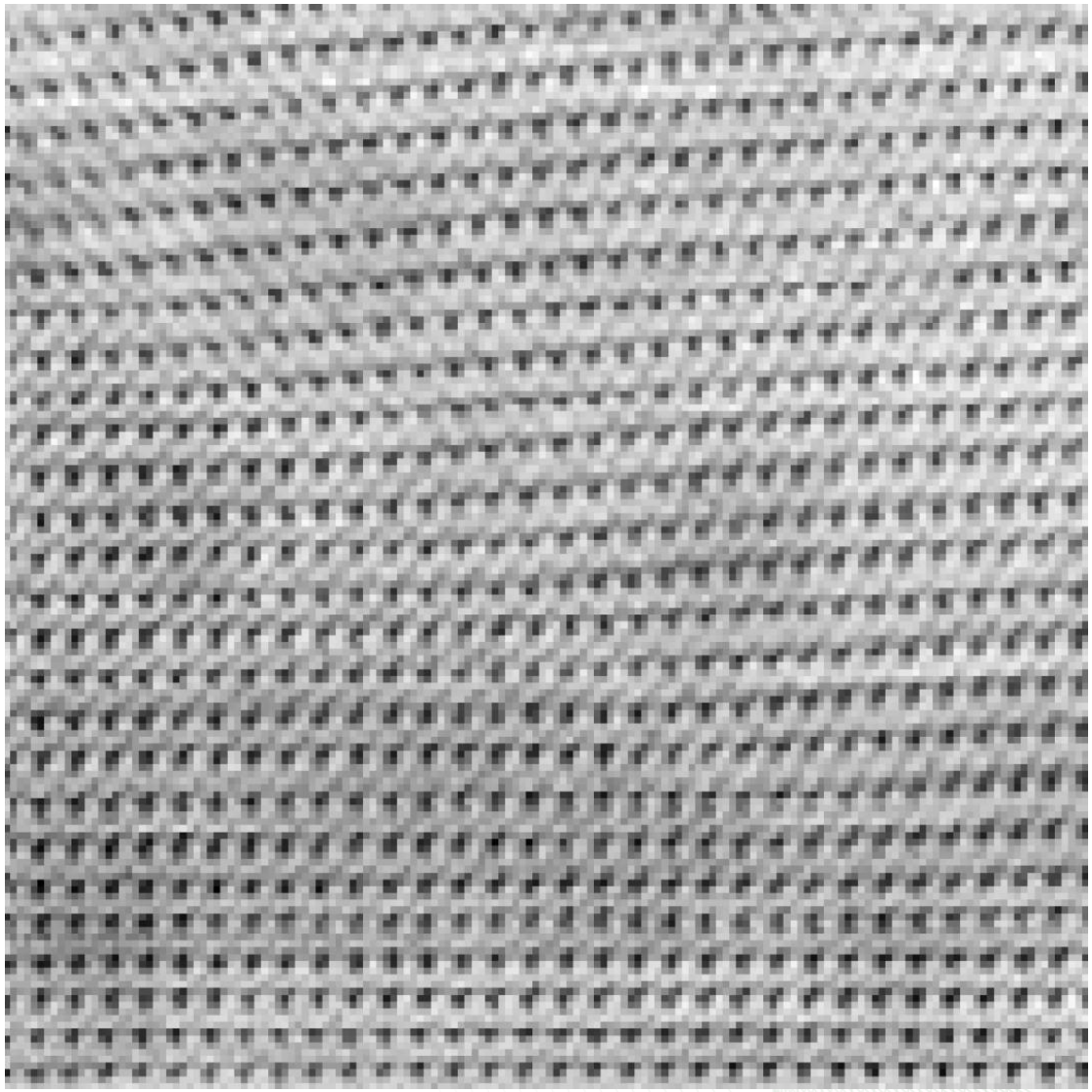
Average intensity of each Ronchigram ~ BF image



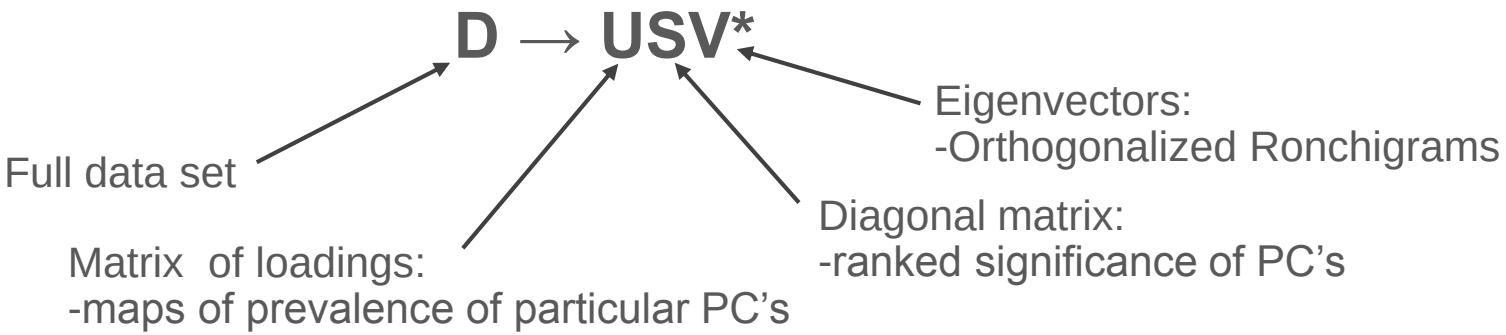
Arbitrary Detector Shape

We can simulate arbitrary and optimal detectors after the data has been captured





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
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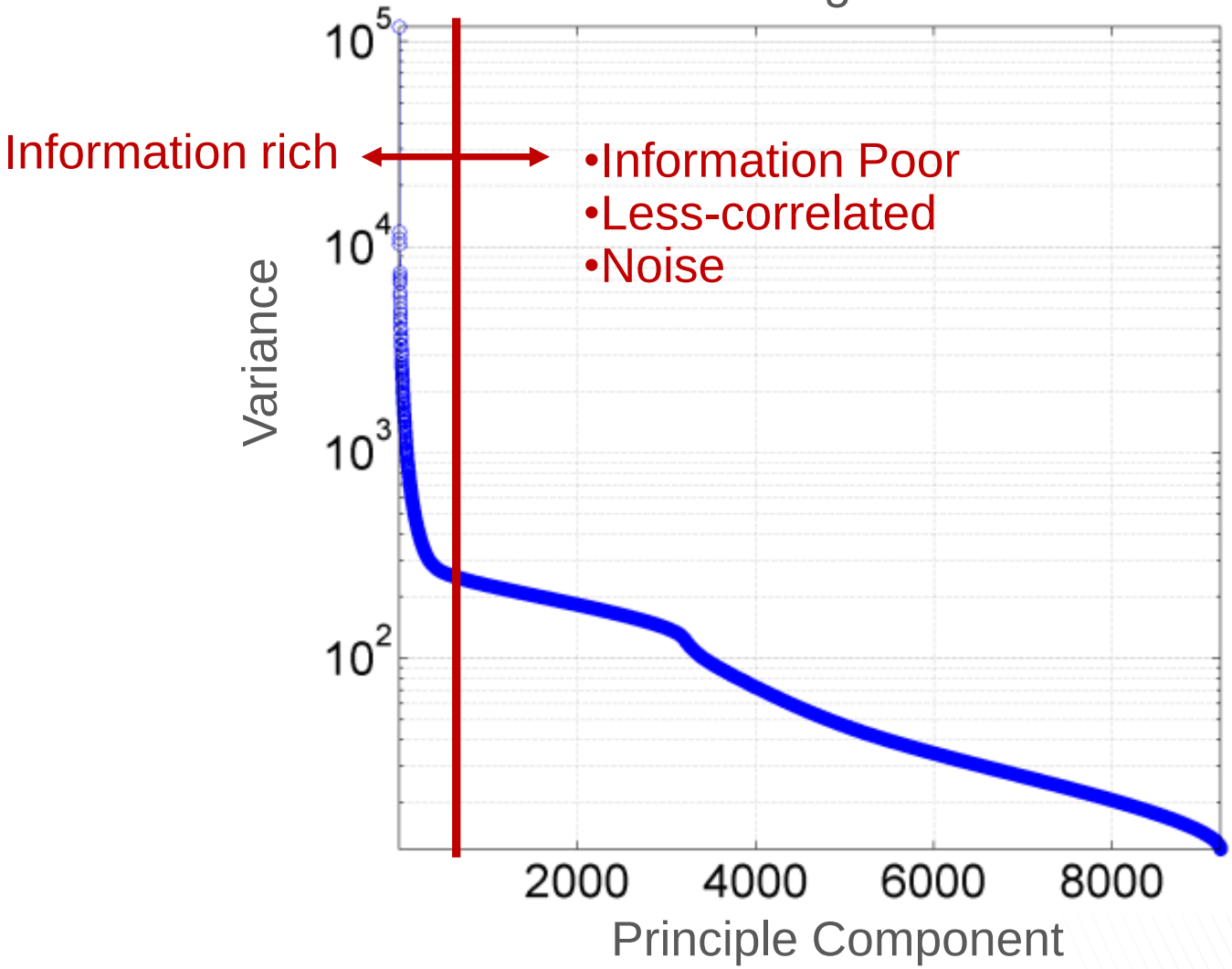
- … loop

Principal Component Analysis (PCA)

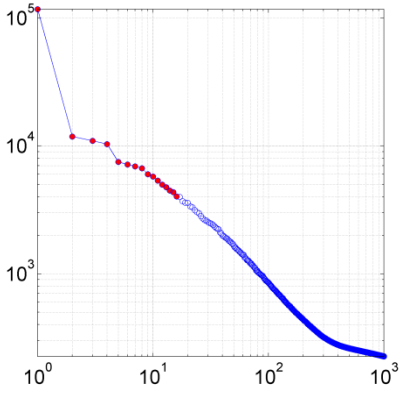
$D \rightarrow USV^*$

Scree Plot -ranked significance of PC's

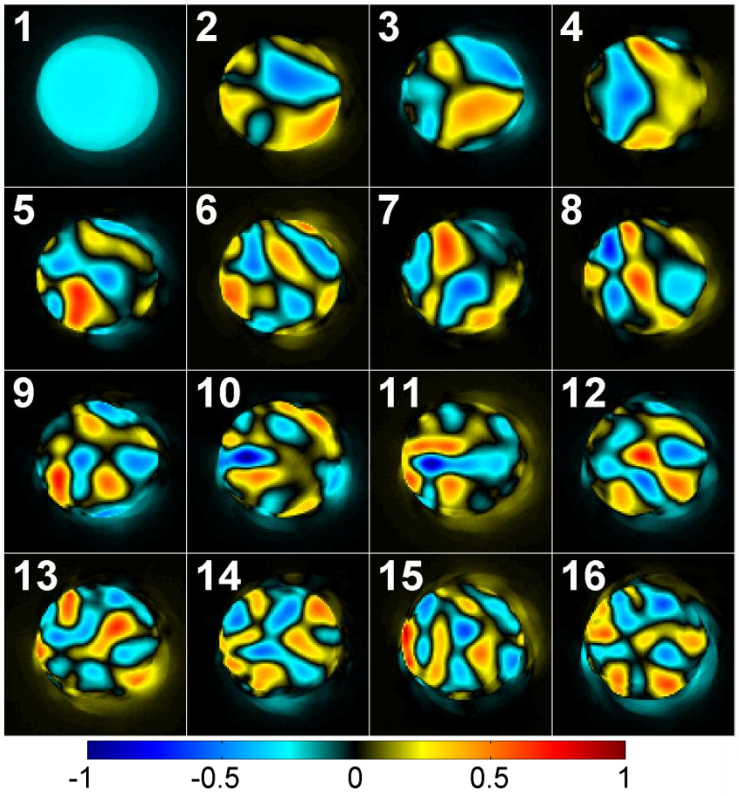


Principal Component Analysis (PCA)

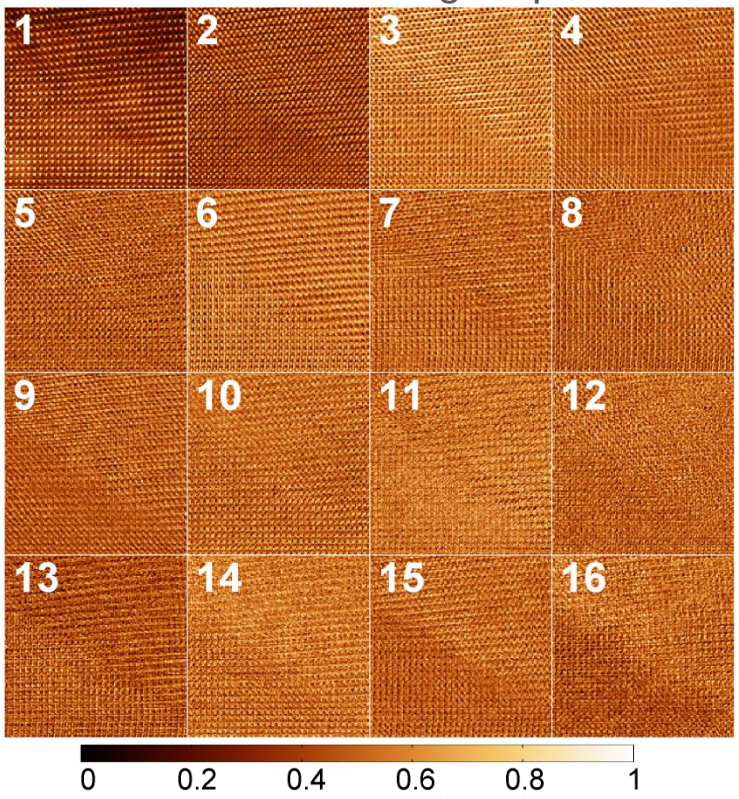
Scree Plot



First 16 eigenvectors



First 16 loading maps



Principal Component Analysis (PCA)

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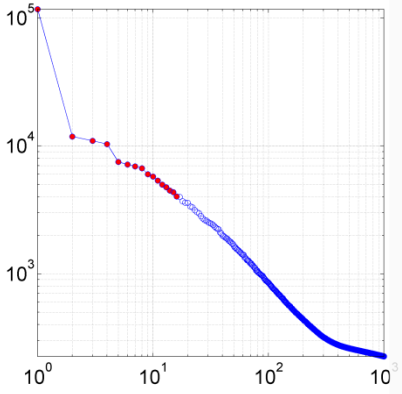

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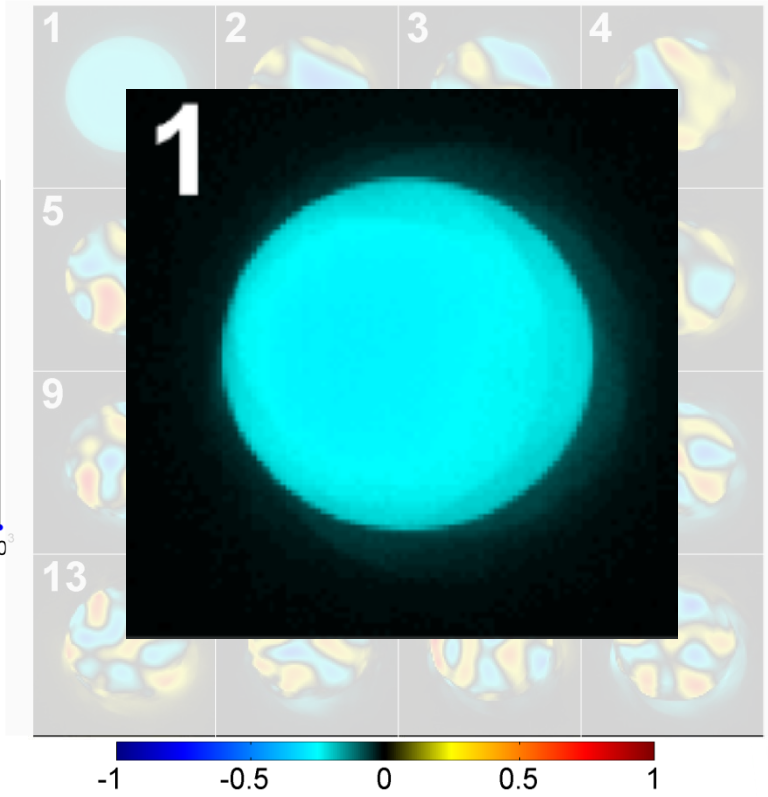

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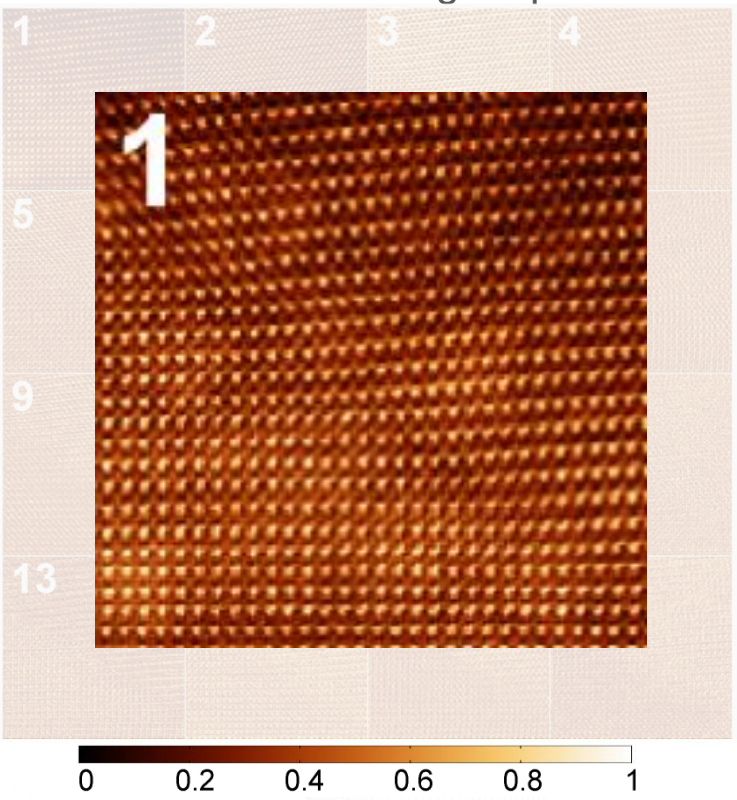

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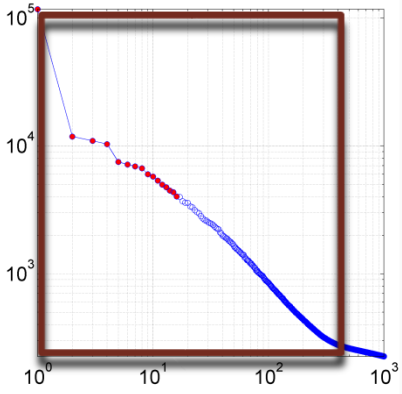

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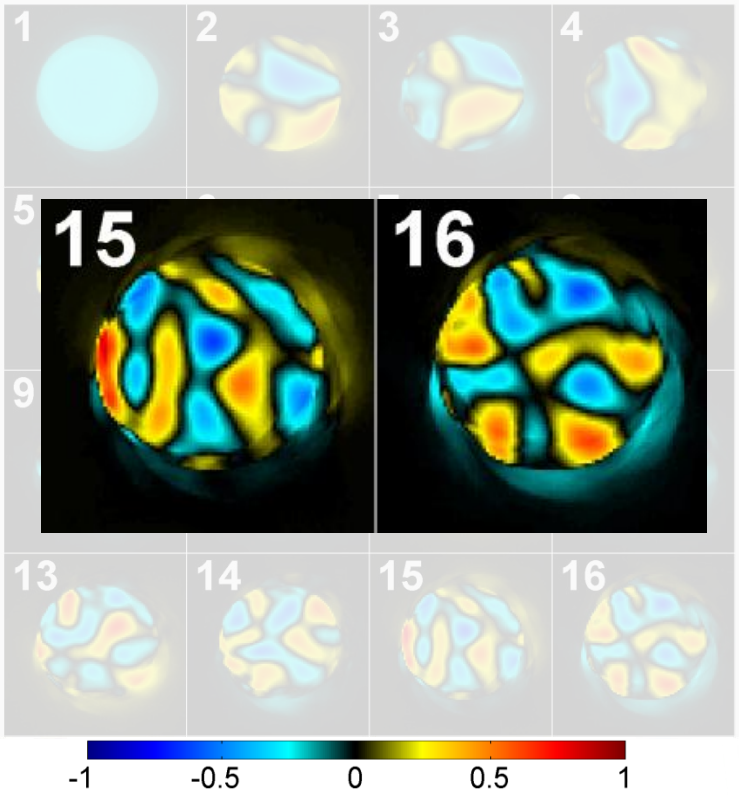

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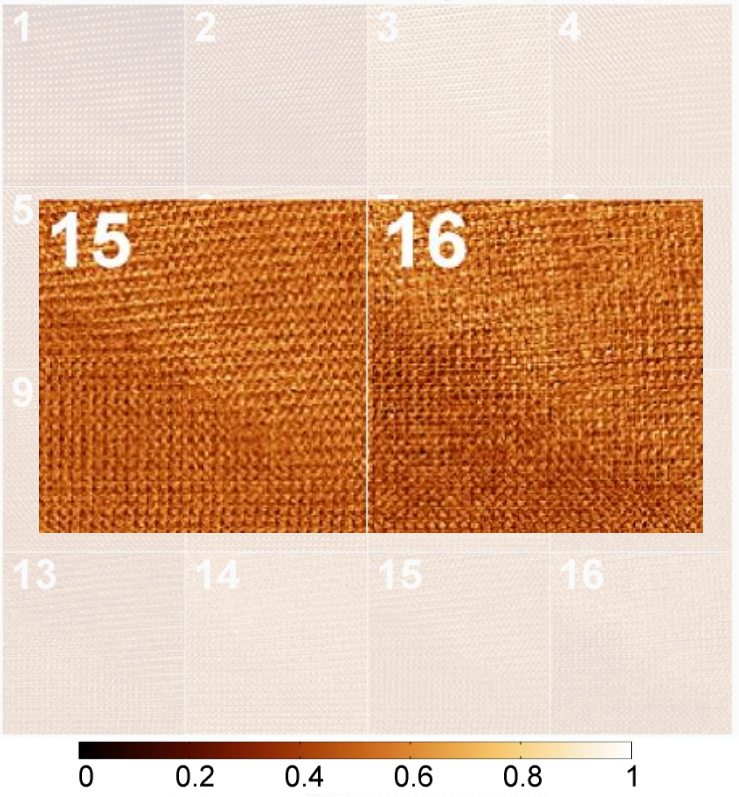
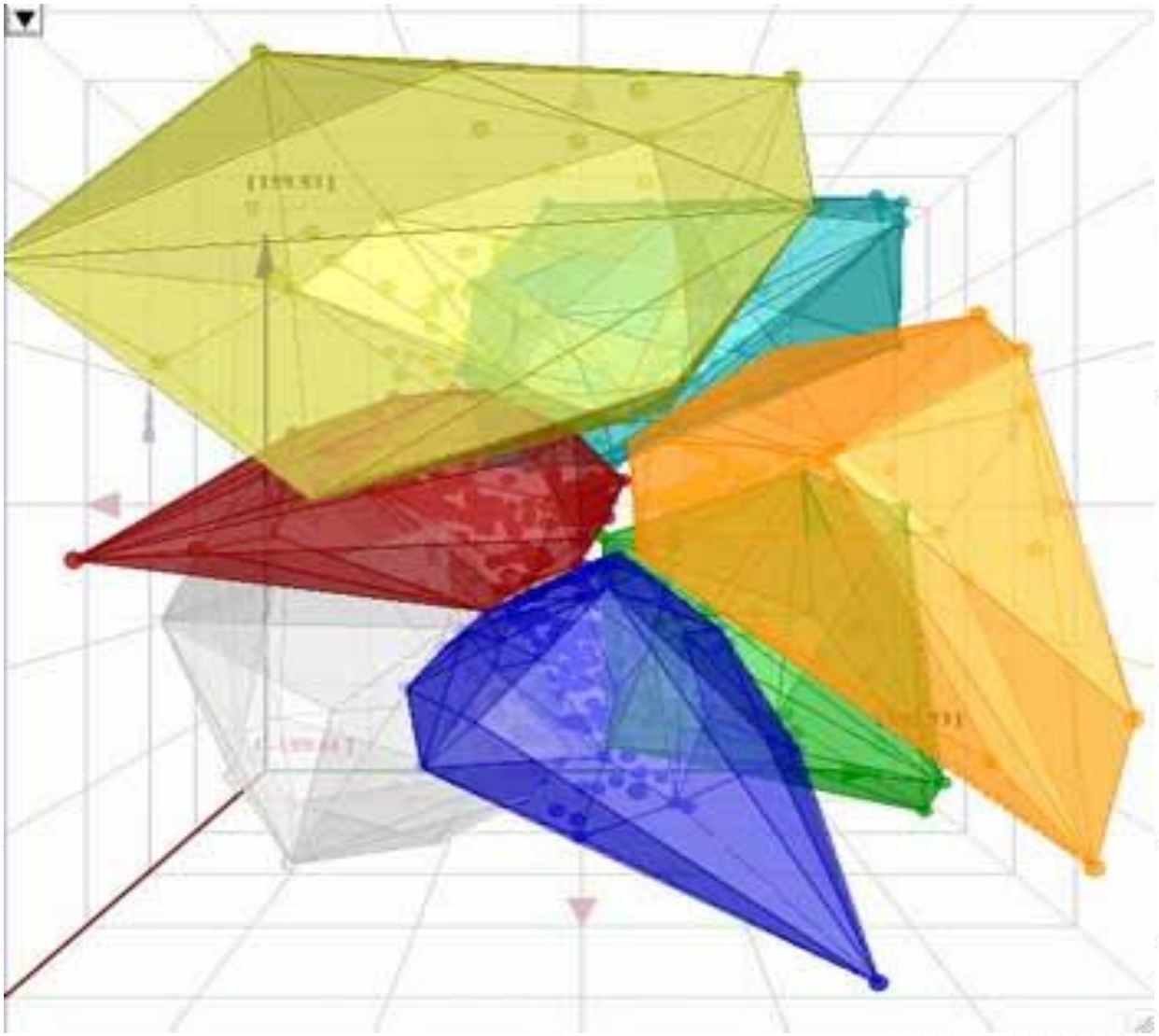


PCA typically fails at: elucidating underlying physics

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

Cluster analysis

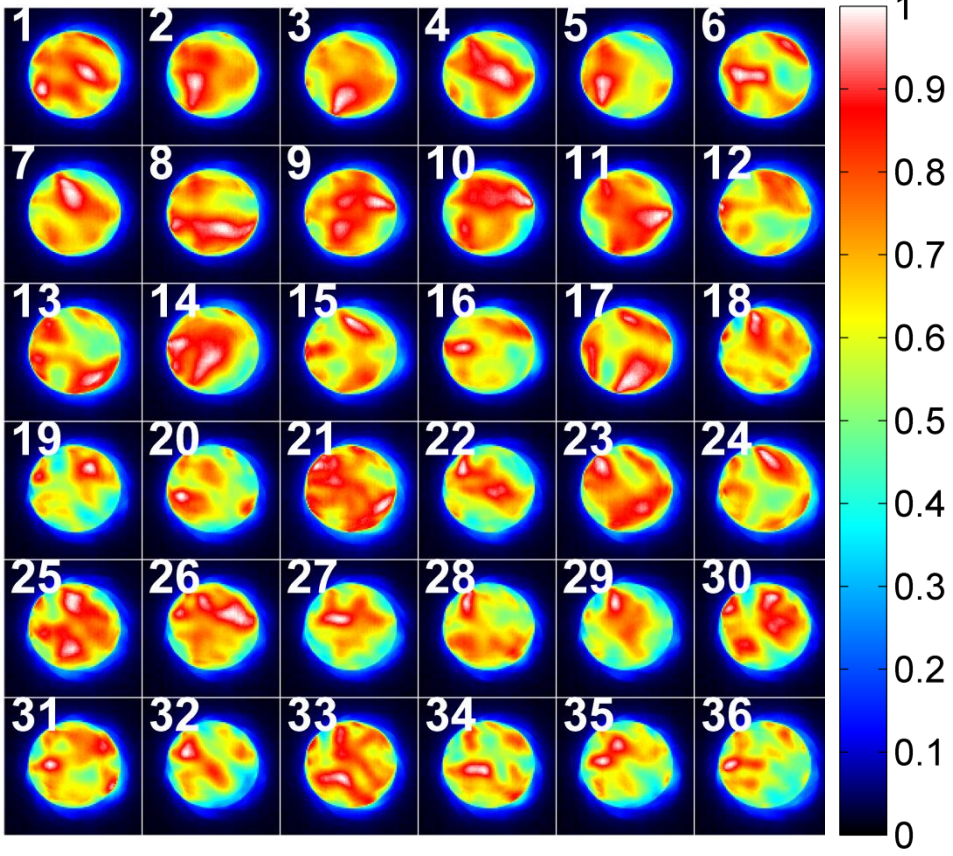
Group observables by “distance” to one another



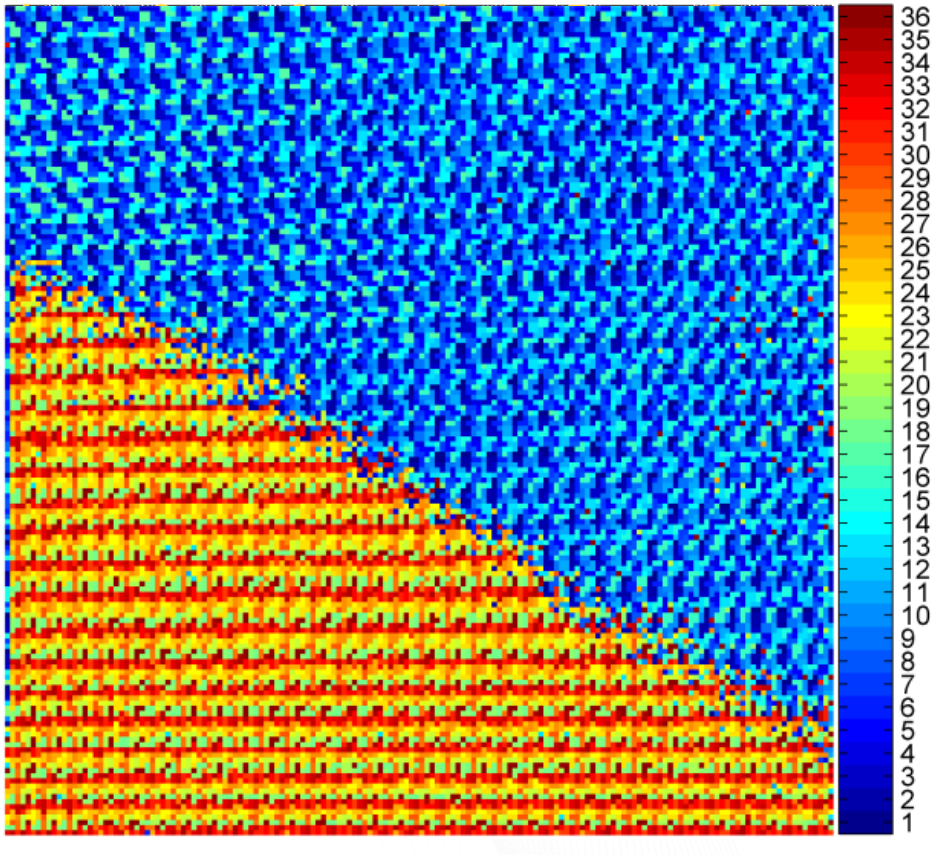
Cluster analysis

K-means clustering: 36 Clusters

Ronchigram corresponding to each cluster

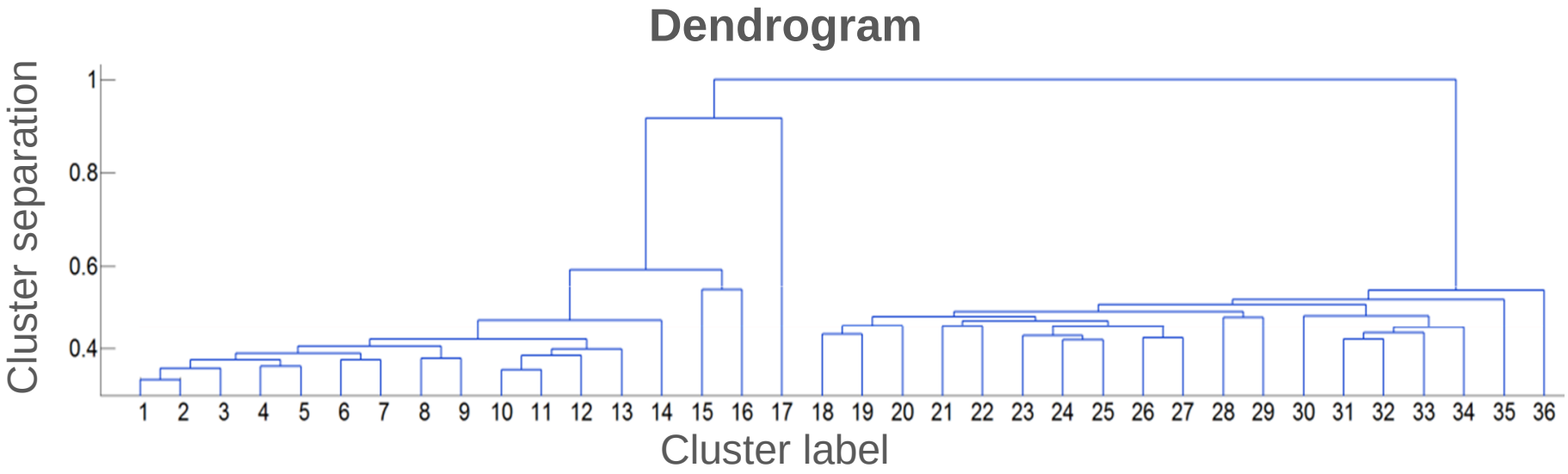


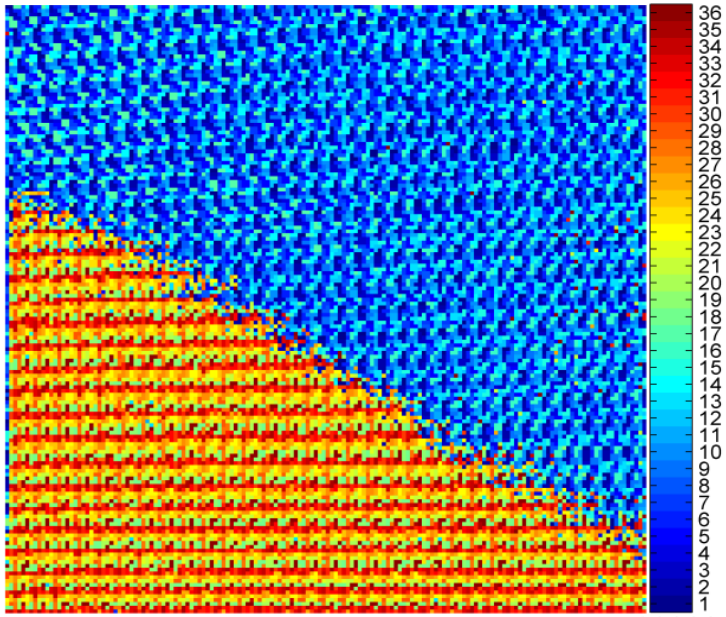
Cluster Locations



Cluster analysis

How many clusters is the right number of clusters?





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