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Microstructure in materials data and analytics

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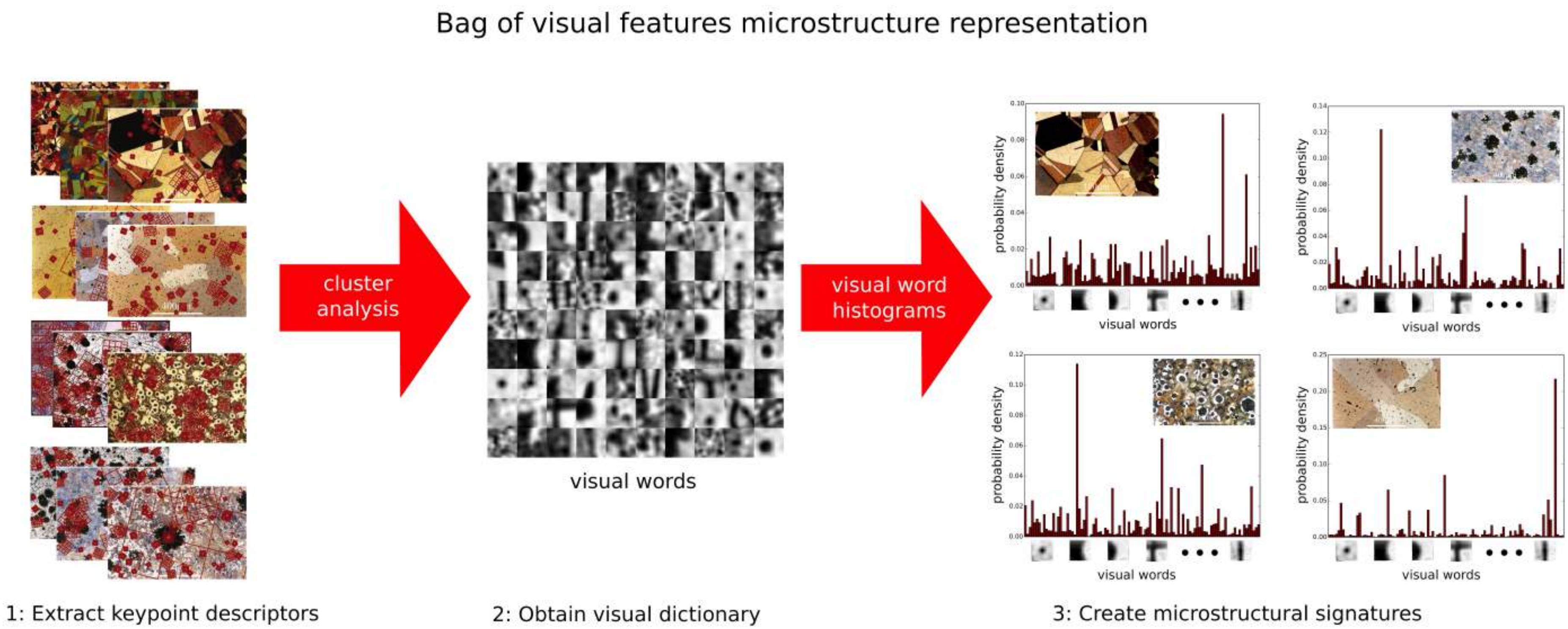
- Microstructural images are key components for materials data and analytics approaches.
- We should represent them as we see them: not as materials data, but as image data.
- Data science unlocks new applications of microstructural data.

A computer vision system for microstructural representation

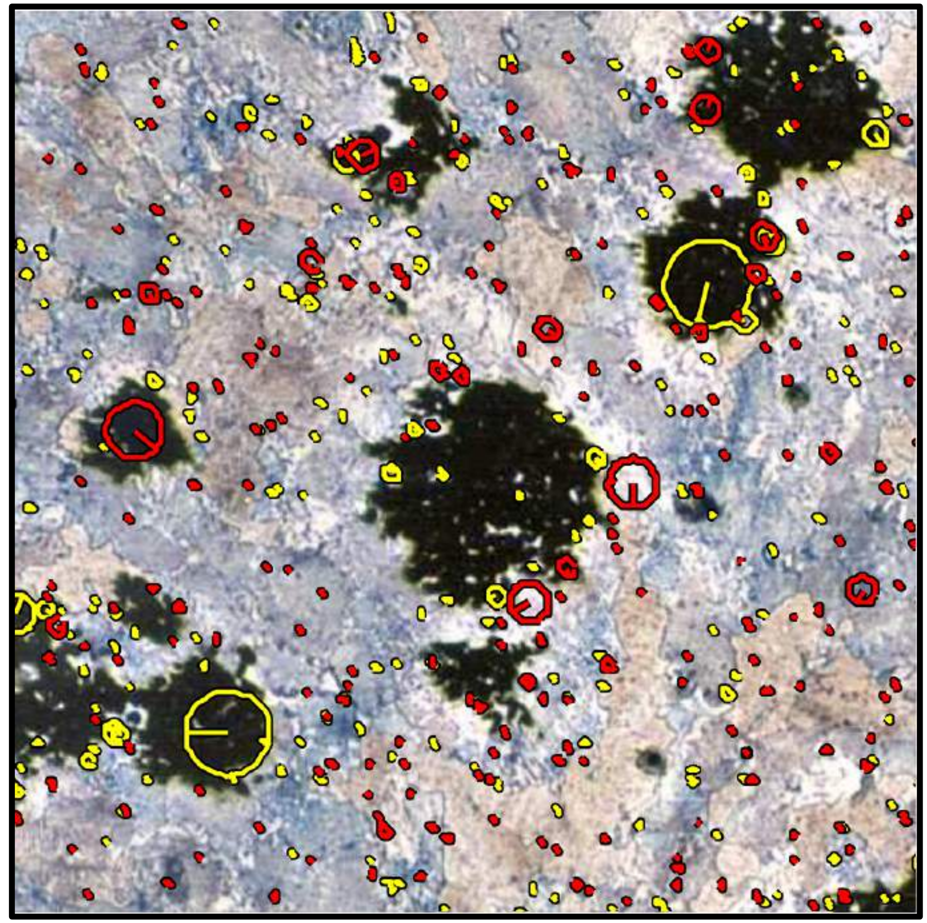
- Using machine vision and machine learning techniques, we automatically harvest, store, and compare microstructural image data.



DeCost, Brian L., and Elizabeth A. Holm. *Comp. Mater. Sci.* **110** (2015): 126-133.

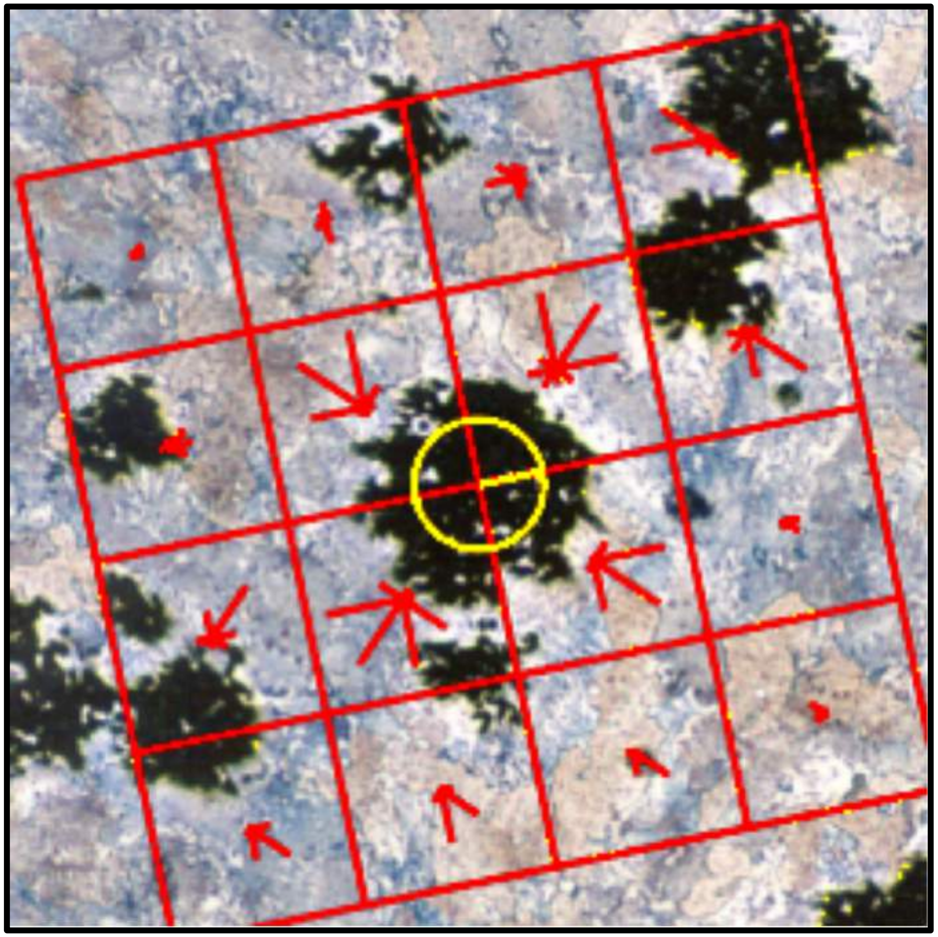
Extract keypoint descriptors

- Apply contrast-gradient detectors to identify features
  - Difference of Gaussians (blobs - red)
  - Harris-Laplace (corners - yellow)



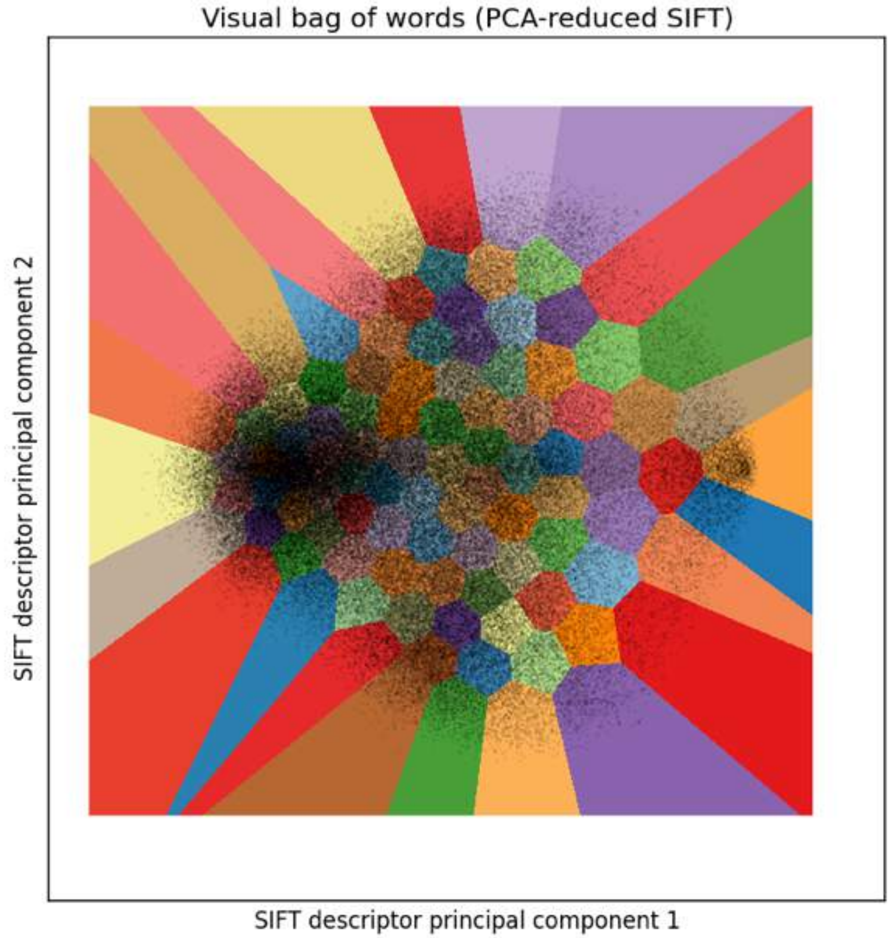
Characterize keypoint descriptors as vectors

- SIFT: Scale Invariant Feature Transform
  - spatially resolved histogram of oriented intensity gradient values
  - rotation and scale invariant local feature descriptor
  - 128 element vector



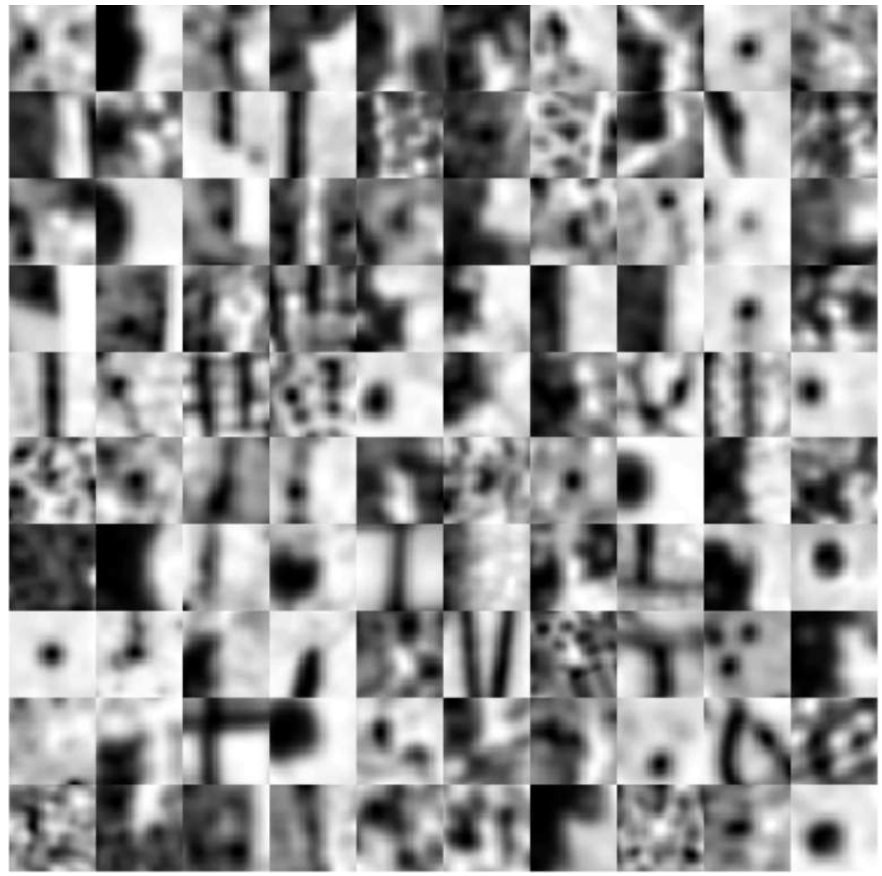
Create a visual dictionary

- Determine *N* most frequent "visual words" via *k*-means cluster analysis
  - Locate the centroids of the *N* best clusters
  - Voronoi partition the 128-D space using cluster centroids as cell centers



Create a visual dictionary

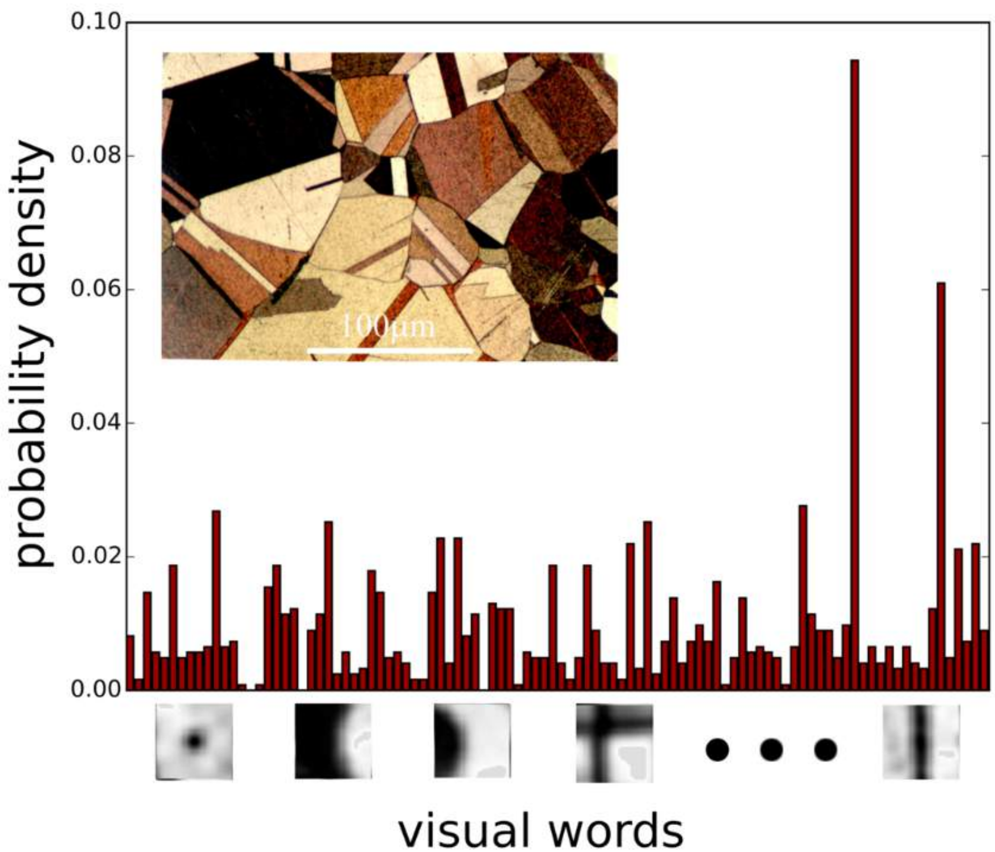
- Visual words can be represented by image patches, corresponding to their centroid feature, i.e. a metafeature
  - particles
  - corners
  - flat boundaries
  - edges
  - speckled textures
  - etc.



100 most frequent visual words in the Cambridge Micrograph Library

Determine "microstructural fingerprints"

- The histogram of visual words generates a unique microstructural identifier, the "microstructural fingerprint."

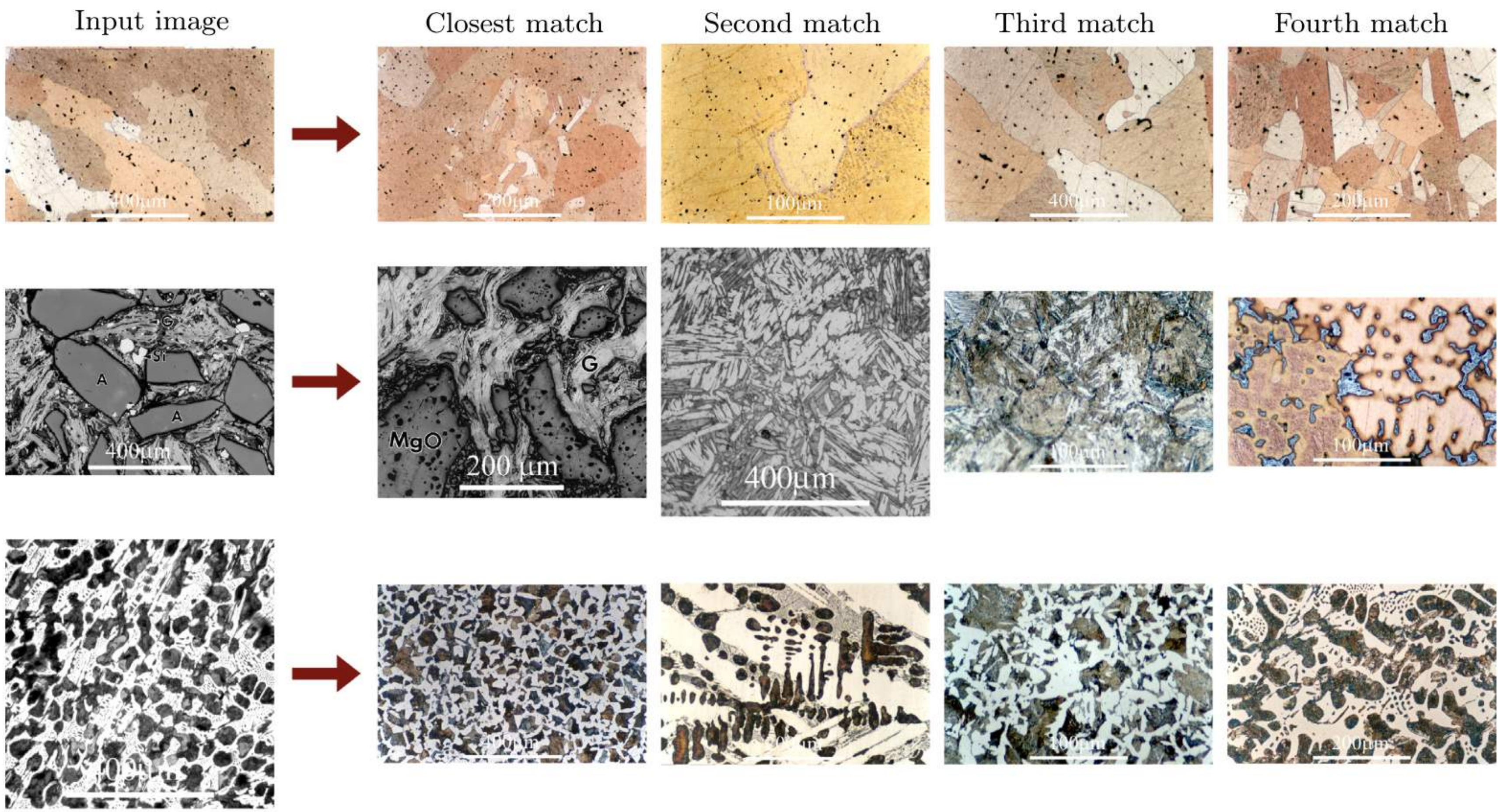


Now that the visual content of a microstructure is captured in a vector representation, what can we do with it?

- Search
- Sort
- Scan
- Specify
- Systematize
- Science

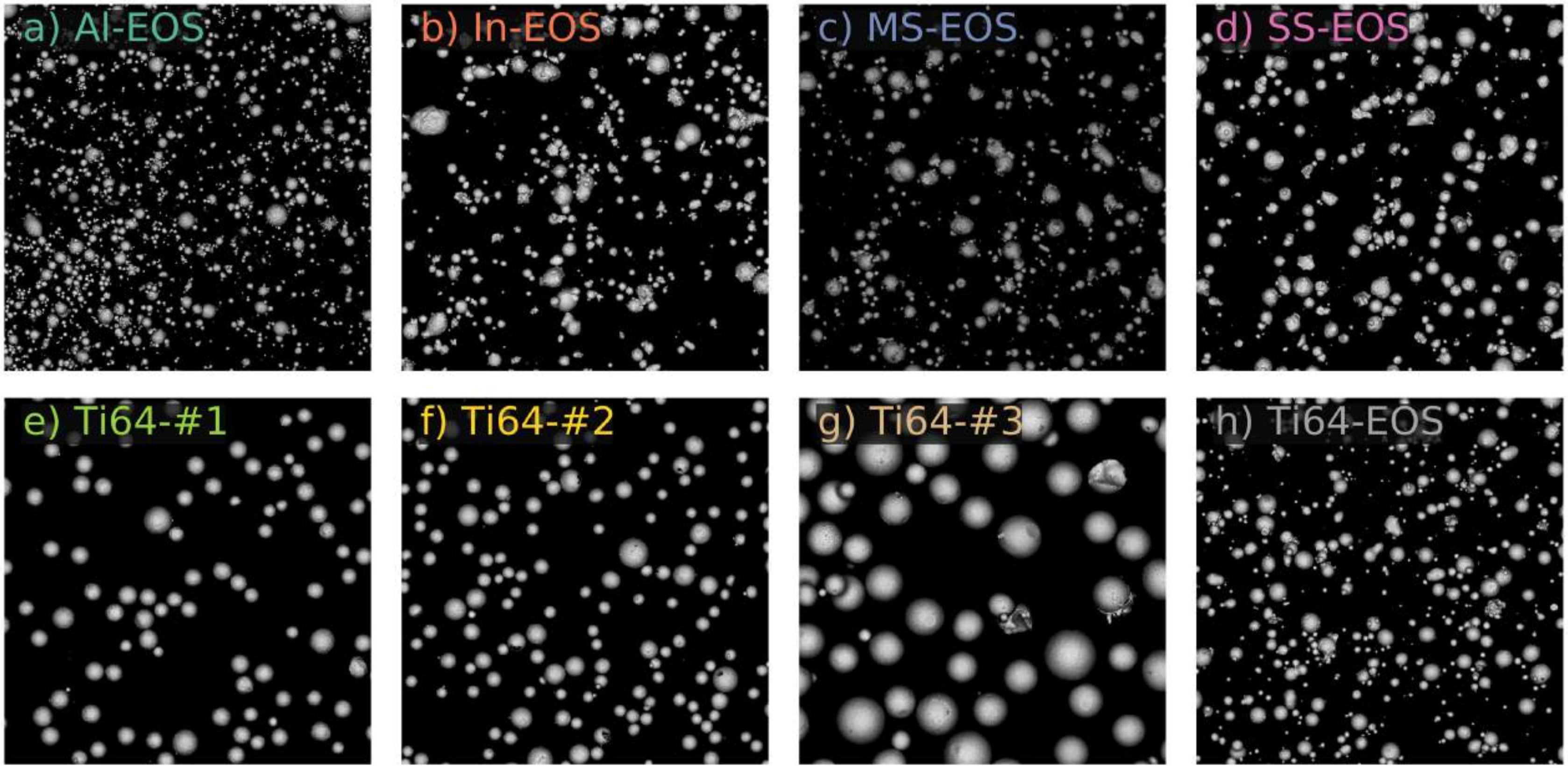
Visual search of the DoitPOMS database

- Histogram similarity can form the basis for a visual search:



Sorting powders for AM

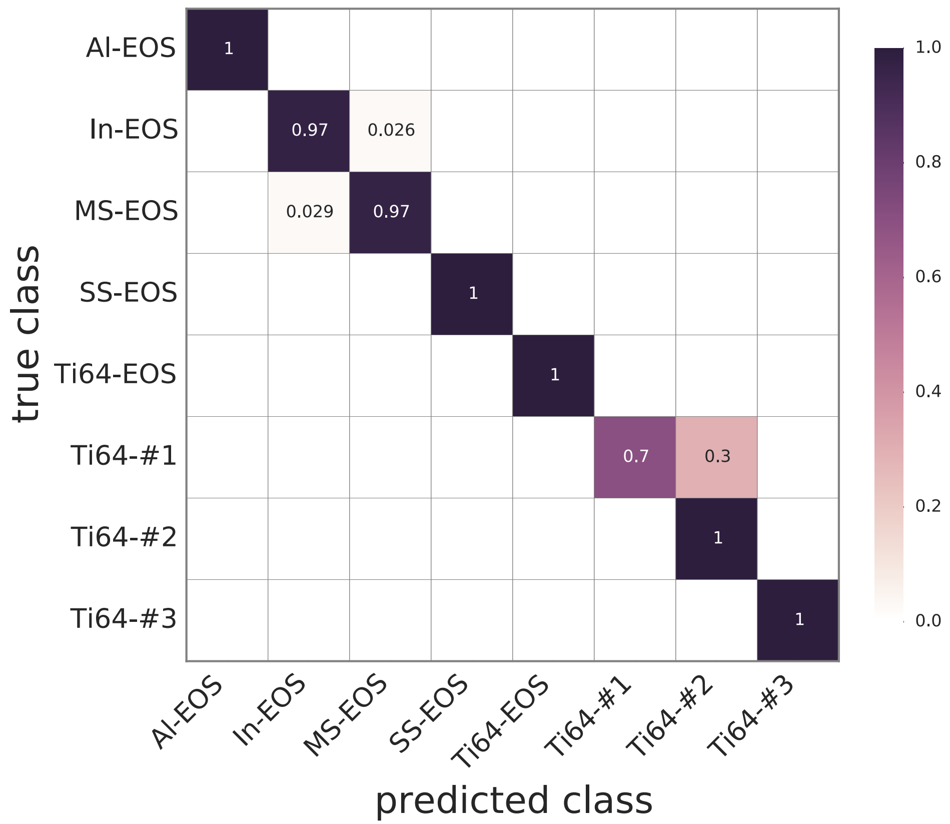
- Additive manufacturing process control and component quality depend on characteristics of the powder feedstock.
- Can our system classify different powders from SEM images?



courtesy of A. D. Rollett, R. Cunningham, H. Jain

Powder classification results

- The machine vision system classifies powders with **~95%** accuracy



•System trained on ~24 images in each class, and tested on ~12 previously unseen images.

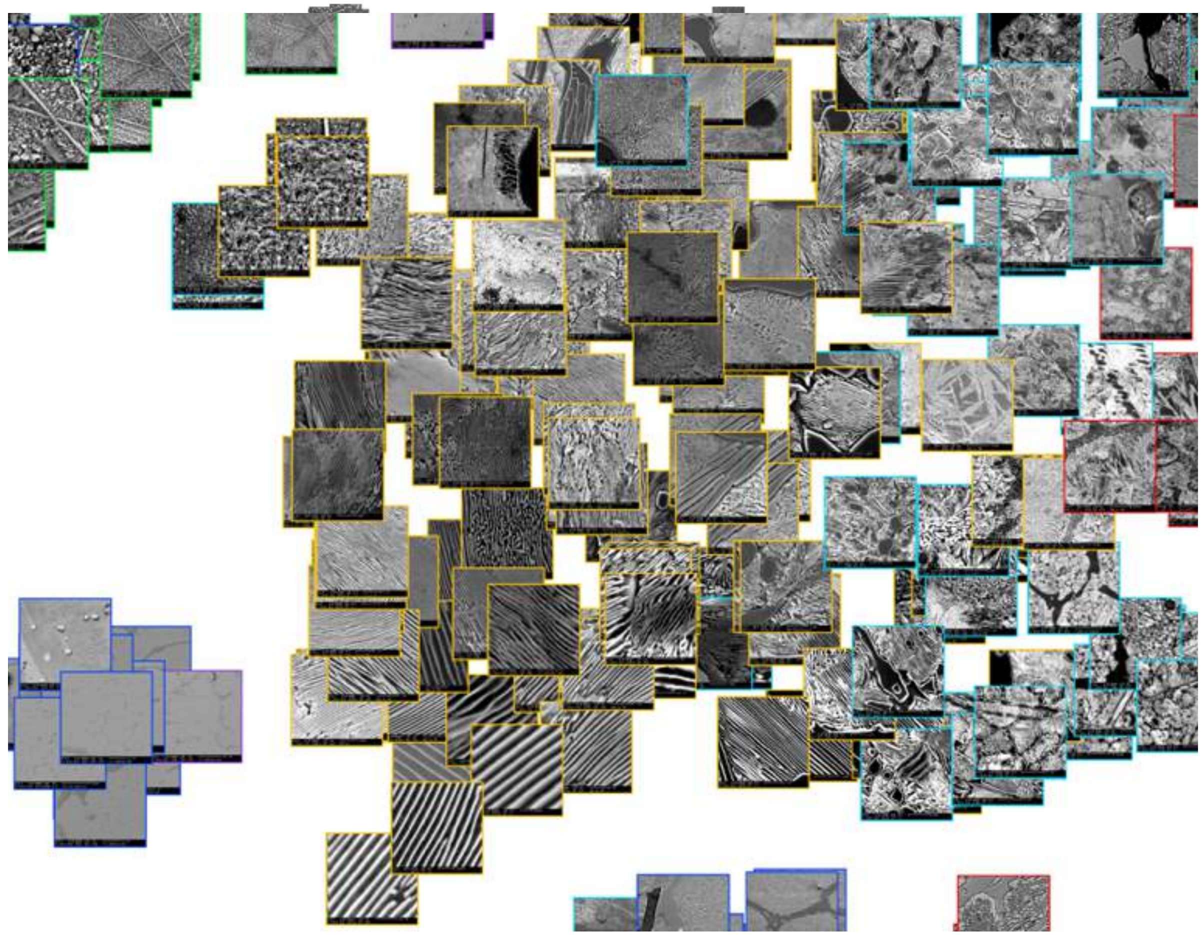
The machine vision system is as accurate as segmentation and measurement (and more accurate than the human eye).

Scaning through images

- Visually clustering images enables efficient exploration of the data set

t-SNE map of 894 high-carbon steel micrographs

(box colors represent processing conditions)

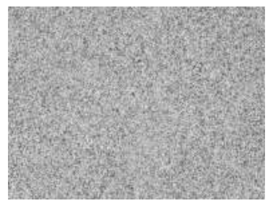


Dataset courtesy of Matt Hecht, Prof. Yoosuf Picard, Prof. Bryan Webler of CMU

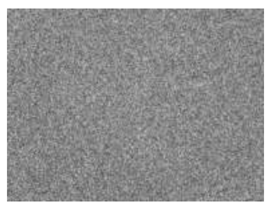
Specify microstructural appearance

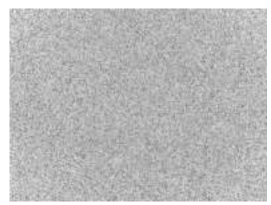
- It can be difficult to create a specification for microstructure: What must be measured? What subjective decisions must be made?
- A vision representation contains both qualitative and quantitative information for an entirely objective comparison

This is the desired microstructure:

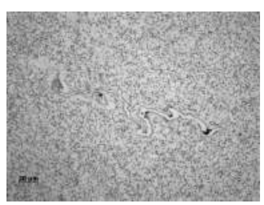


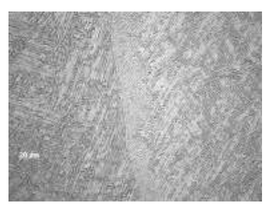
These are also OK:

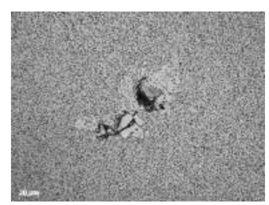




These are not:



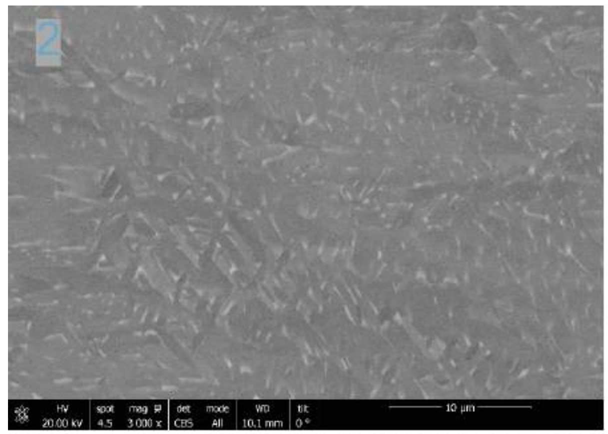




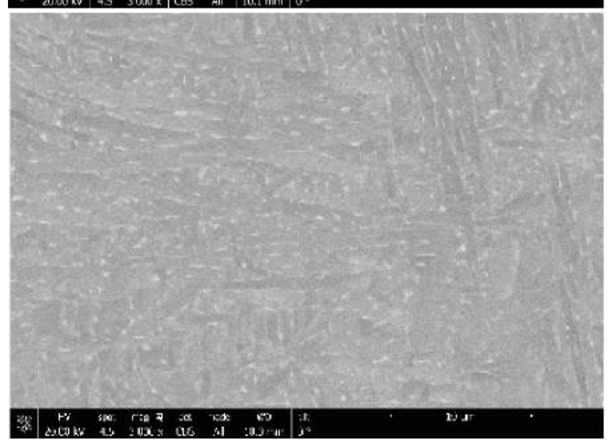
Systematize images

- How do we decide what image “represents” the material?
- We can find the image closest to the cluster center of images of that material. This is an objective definition of “most representative.”

The representative microstructure of a Ti64 AM build:



The least representative microstrucure



Images courtesy of E. Schwalback, AFRL

Conclusions

- Microstructural images are key components for materials data and analytics approaches.
- We should represent them as we see them: not as materials data, but as image data.
- Data science unlocks new applications of microstructural data: search, sort, scan, specify, systematize
- Next steps:
  - Bigger and more datasets!
  - Link metadata to image data = Science!