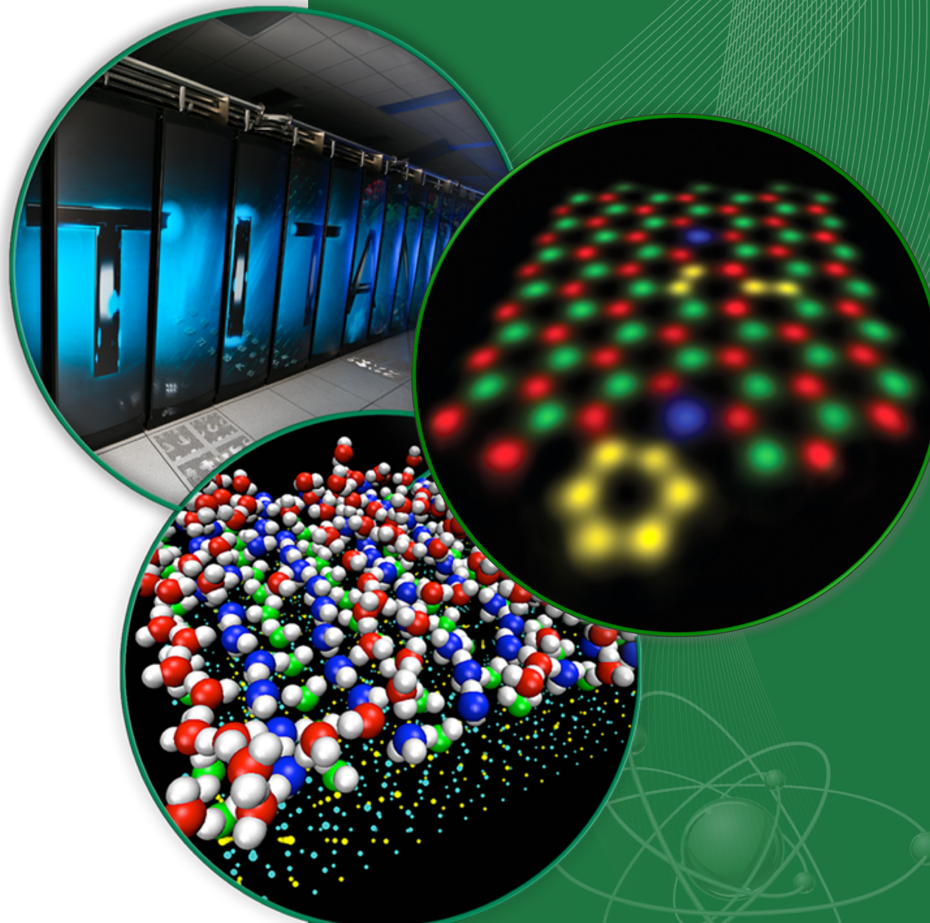
Spectral Unmixing Methods



Rama Vasudevan

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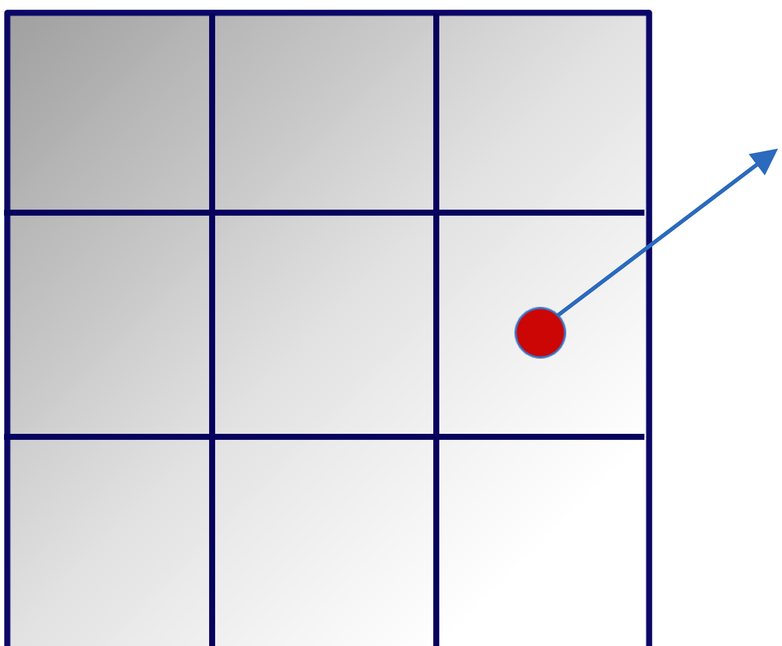
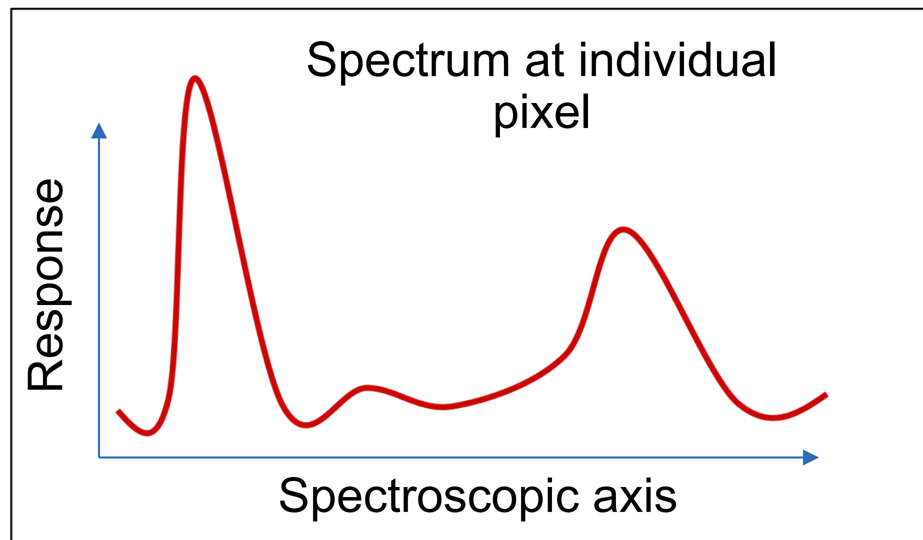
Spectral Data

- Many imaging modalities have spectroscopy components
- By capturing spectra across an image, it allows us to correlate features of the spectra with specific regions of the sample

Image (MxN pixels)





M (rows) x N (columns) x P (spectral points)

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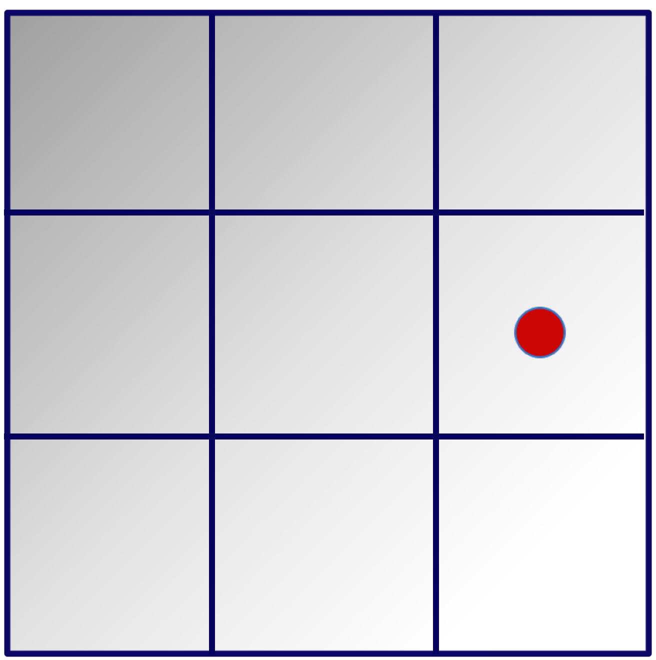
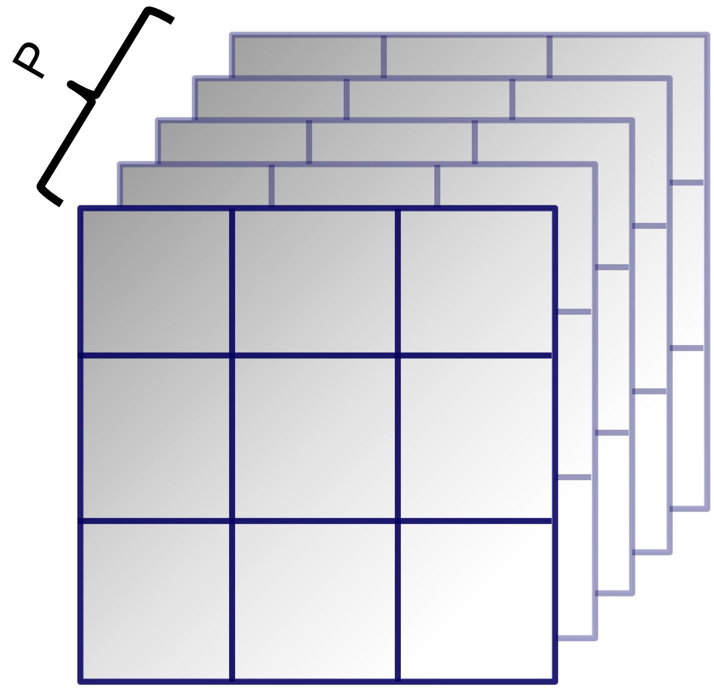




(Repeat MxN matrix P times to make 3D cube)

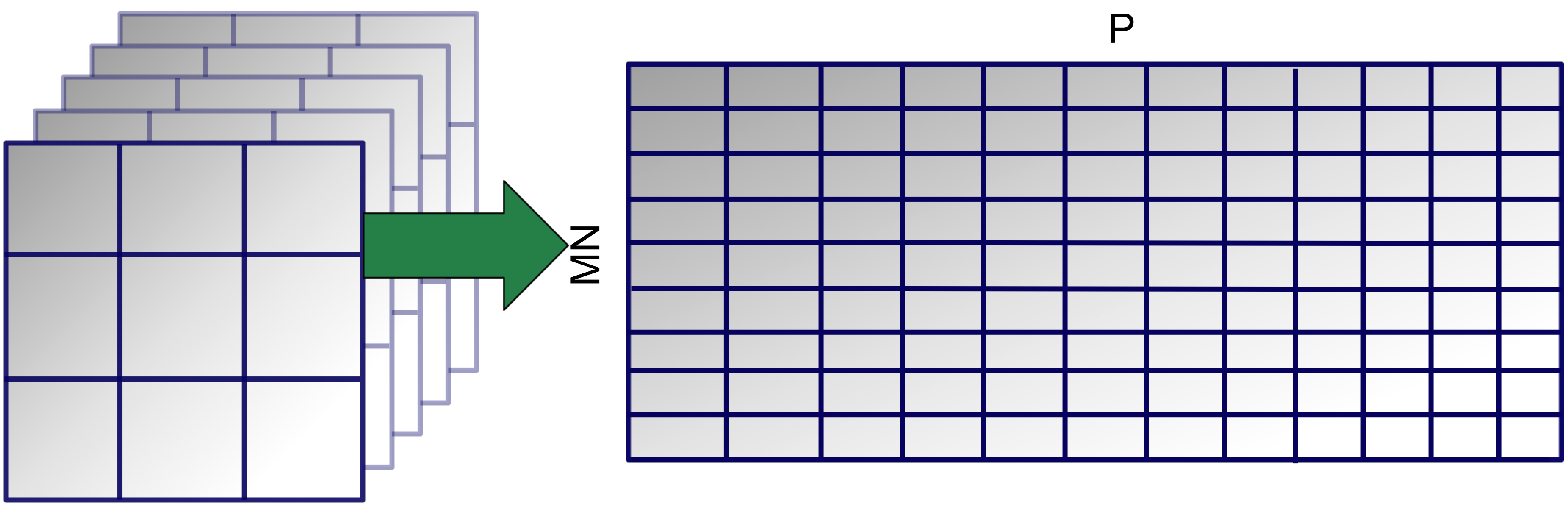
Spectral Data

- Examples include EELS, micro Raman imaging, force-distance curve maps in AFM, Scanning tunneling spectroscopy, etc.
- Usually, the 3D matrix is converted to a 2D matrix

M (rows) x N (columns) x P (spectral points)

= (MN) x P

Pixels x spectral points



Matrix Factorization

- We now have a 2D matrix (call it **X**) of size (MN,P)
- If **X** is ‘small’ (e.g., (10,10)) we can comprehend it easily. But if the size of X is (2500, 32), then this becomes more difficult
- The number of spectral points **P** is often termed the “number of dimensions”.
- To see trends in our data, we want to visualize them in some manner. But the 3D data cube is big, so what can we do?

→ **Matrix Factorization**

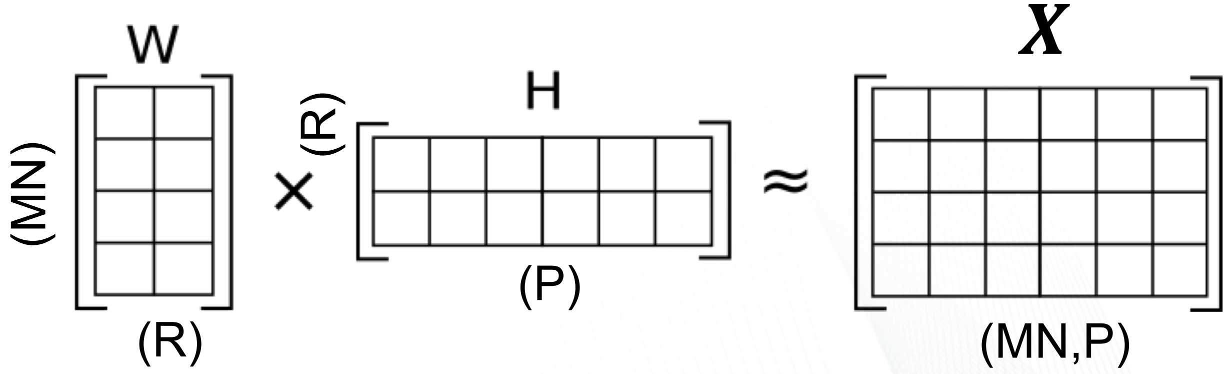
Dimensionality Reduction

- The reason it is difficult to visualize is because there are too many spectral points *P* per pixel. What we need is to reduce the dimensionality, while preserving most of the data structure.
- What if we could write our matrix **X** (size MN,P) as

$$\boldsymbol{X} \approx \boldsymbol{W}\boldsymbol{H}$$

Where W is size (MN,R)
H is size (R,P)

R <P



Dimensionality Reduction

- The reason it is difficult to visualize is because there are too many spectral points *P* per pixel. What we need is to reduce the dimensionality, while preserving most of the data structure.
- Alternative viewpoint: Represent the spectrum at pixel z by a linear expansion

$$f(z_i, s) = c_0(z_i)f_0(s) + c_1(z_i)f_1(s) + \ \ldots + c_n(z)f_n(s)$$

$$f(z, s) = \sum_{i=1}^{MN} c_i(z_i)f_i(s)$$

The task boils down to determining the functions $f_n(s)$, and determining the coefficients c_n

Dimensionality Reduction

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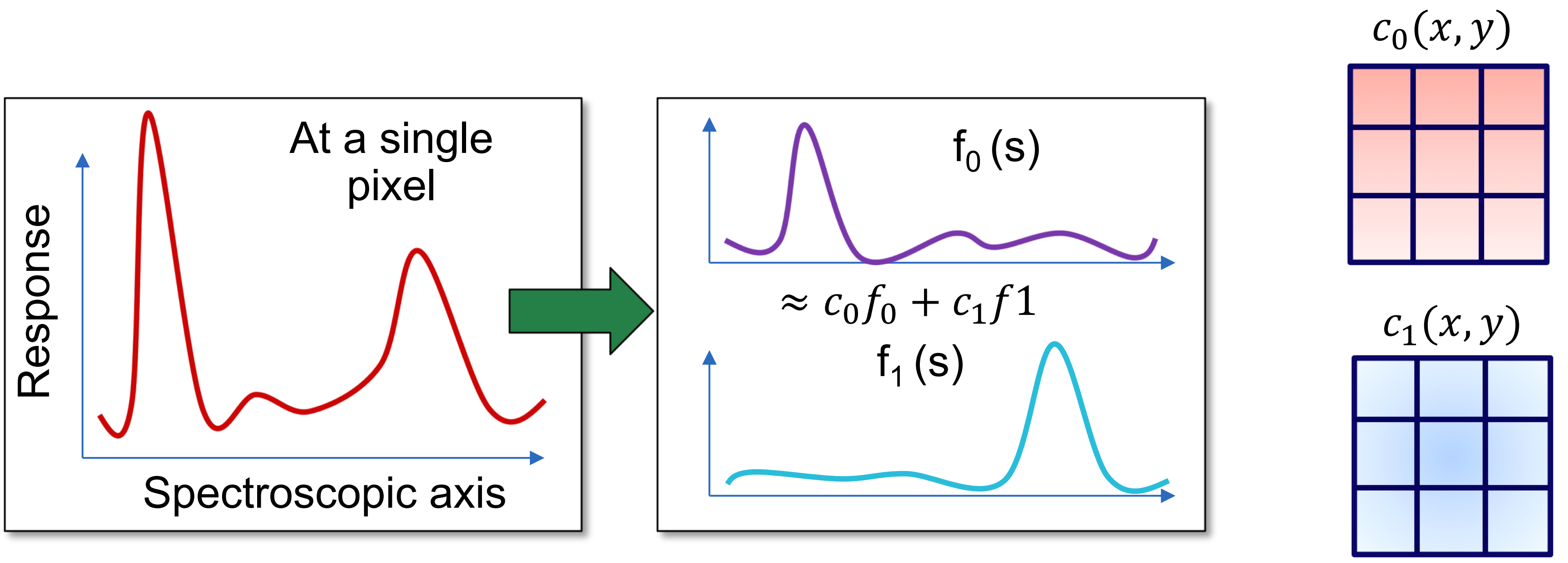


Segmenting based on phases

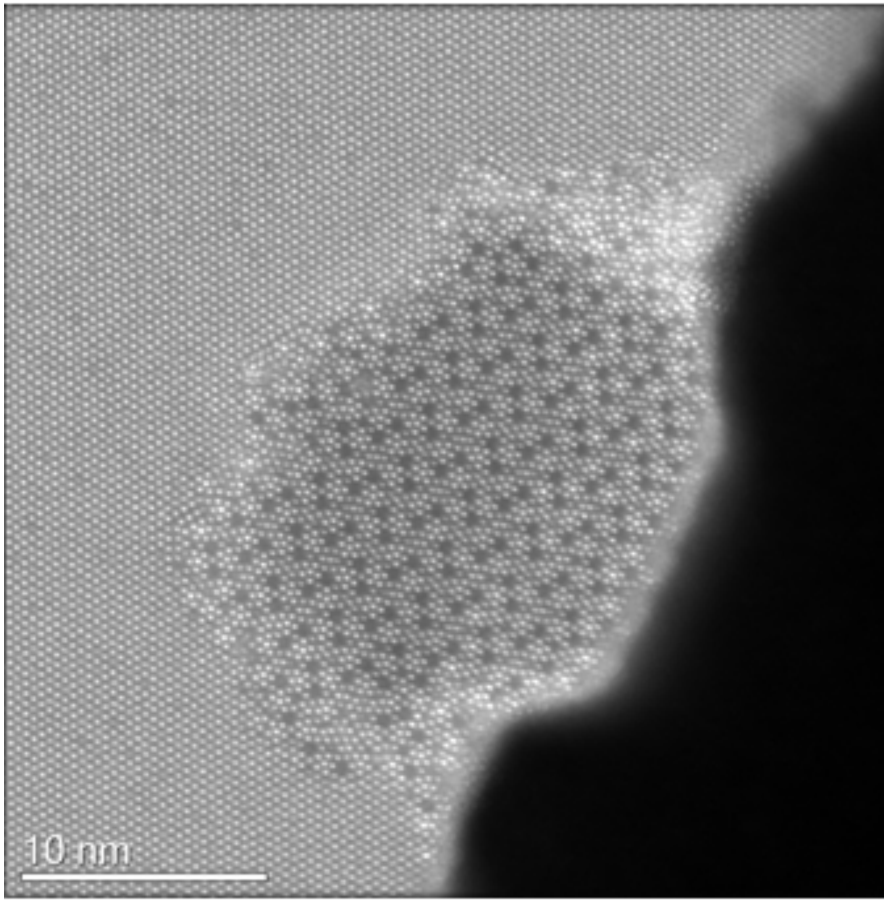
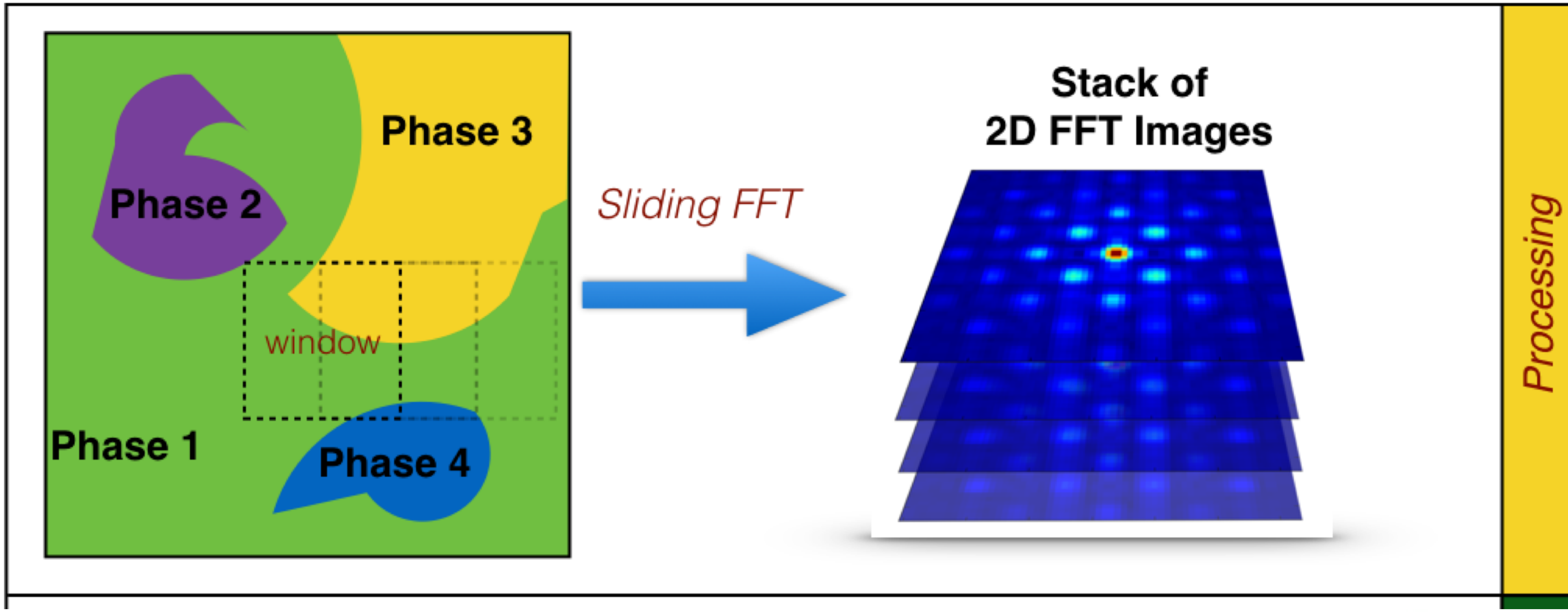


Image courtesy of
A. Borisevich (ORNL)
and
Q. He
(ORNL/Manchester)

How can we segment this image based on the phases present?

Sliding Window Method



Now, we can try to do spectral unmixing on the 2D stack of FFT images

Spectral Unmixing: N-FINDR

- Spectra for a given pixel is assumed to be a linear combination of the end-member spectra (+ Gaussian noise). The mixing proportions sum to 1

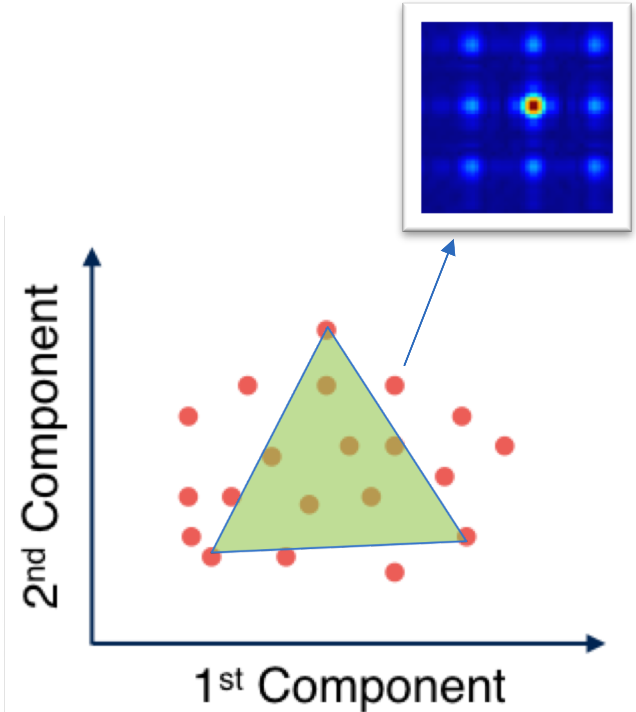
Physics constraint

$$p_{ij} = \sum_k e_{ik} c_{kj} + \varepsilon \qquad\qquad \sum_k c_{kj} = 1$$

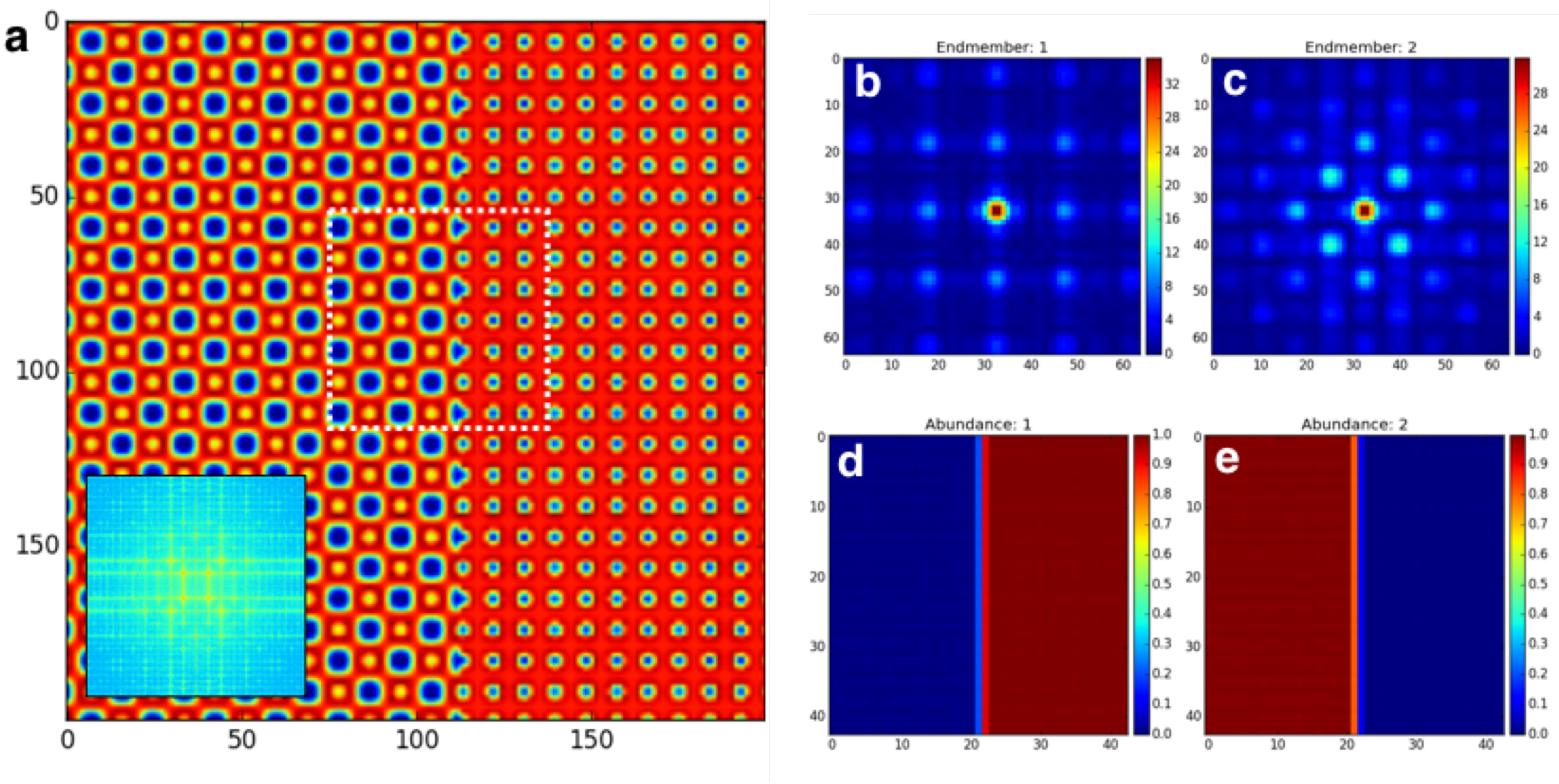
- Let E be the matrix of end-members (here, 3).

$$\boldsymbol{E} = \begin{bmatrix} 1 & 1 & 1 \\ \overrightarrow{e_1} & \overrightarrow{e_2} & \overrightarrow{e_3} \end{bmatrix} \qquad V\left(\frac{\mathbf{1}}{(\boldsymbol{l}-1)!}\right)|\det(E)|$$

- Iteratively select endmembers, accepting the new selection if the volume increases



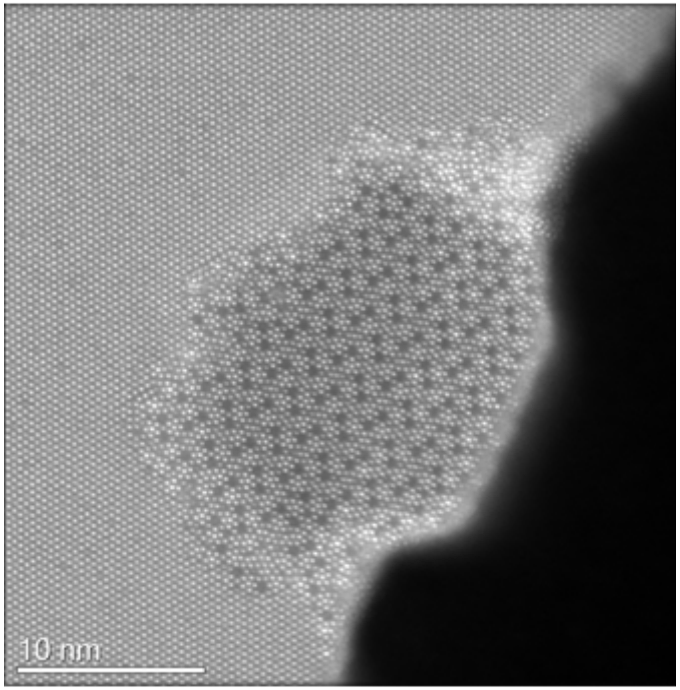
Ideal test case



Spectral Unmixing: Notebook

Let’s try out various unmixing methods including N-FINDR on the STEM image shown below

Open the notebook on spectral unmixing



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