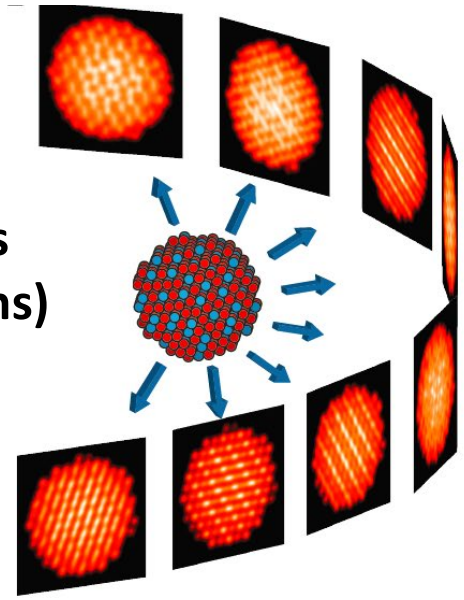
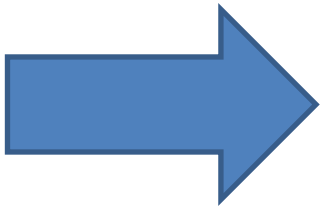
Artificial Neural Network for Electron Tomography Data Augmentation

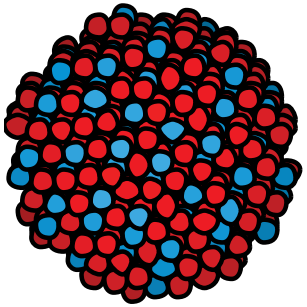
1. Basic Tomography Principles

Tomography

Tilt Series (projections)





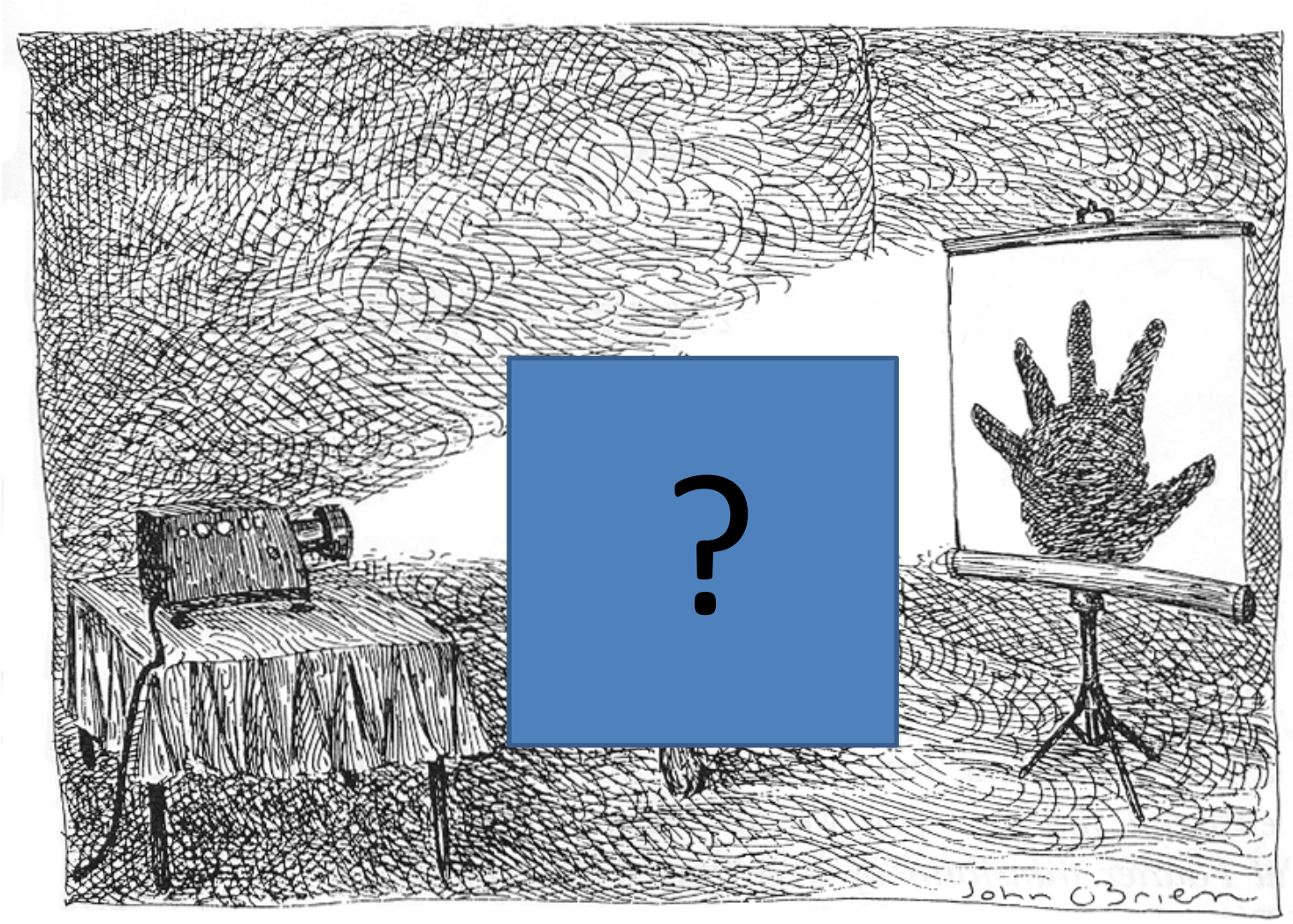


3D Object

Tomography is a method in which a higher dimensional structure is reconstructed from a series lower dimensional projections (usually by sampling the structure from many different directions).

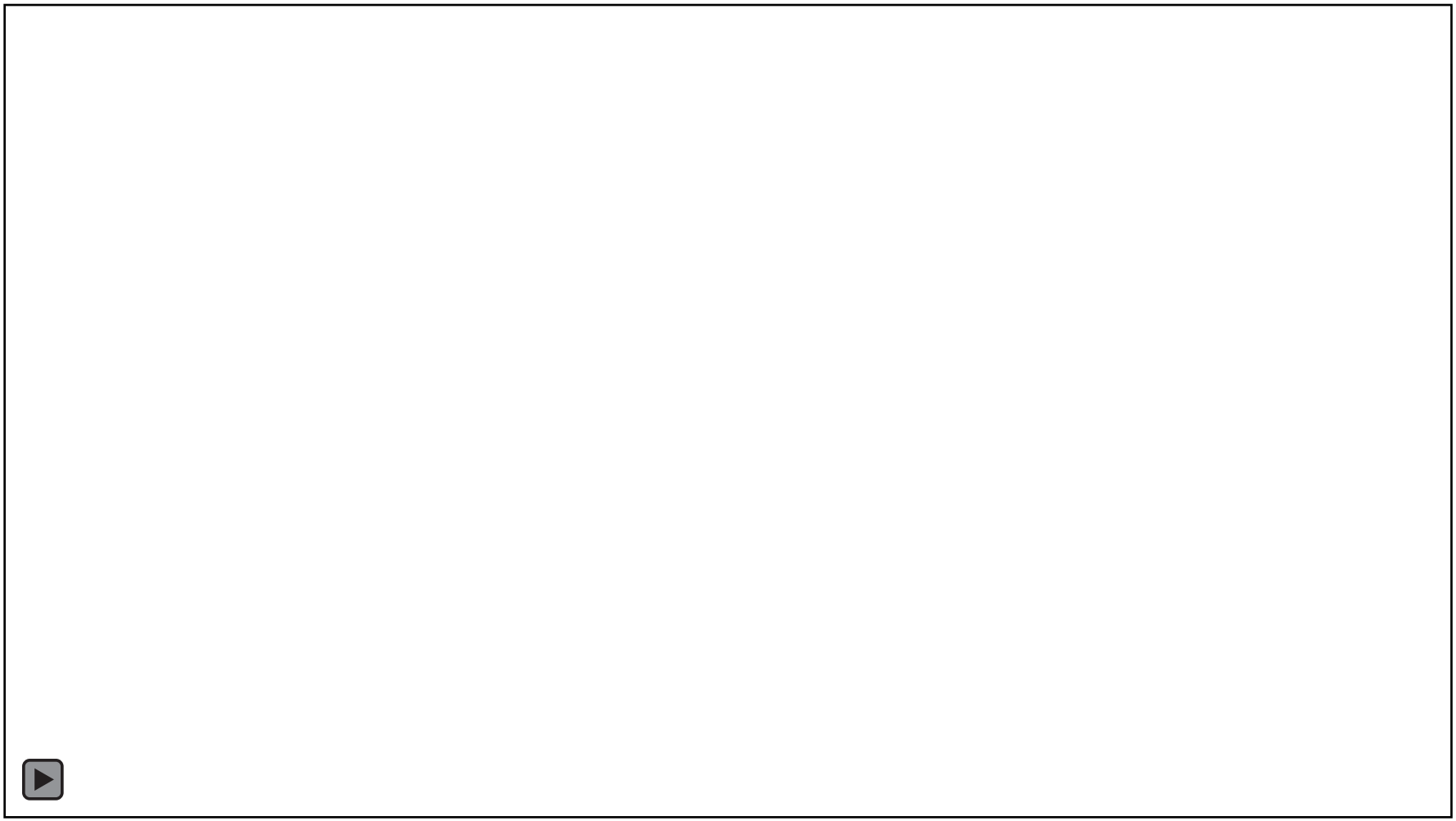
Physical phenomenon	Type of tomogram
X-rays	CT
radio-frequency waves	MRI
electrons	Electron tomography or 3D TEM
ions	atom probe

Why Tomography?



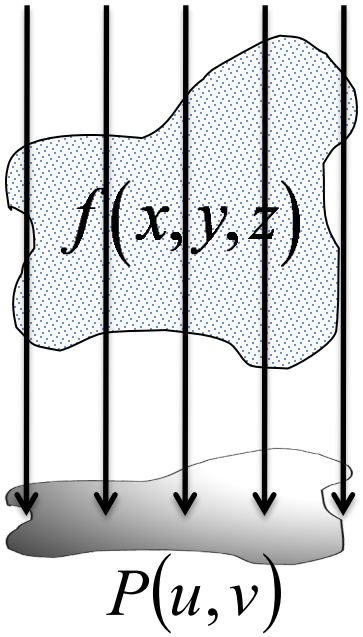
A single projection is usually insufficient to infer the structure of a general 3D object.
(New Yorkers Magazine, 1991)

Why Tomography?



Y. Yang et al., *Nature* **542**, 75-79 (2017).

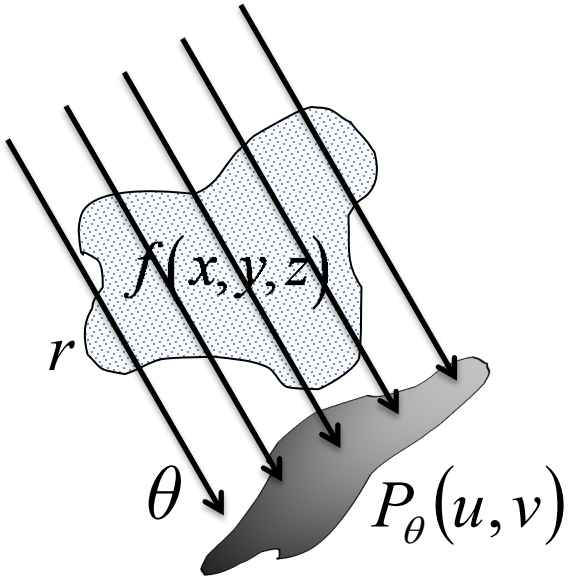
Projection



An object's density (or any other properties applicable) as a function $f(x,y,z)$

Projection is similar to summation along a given direction:

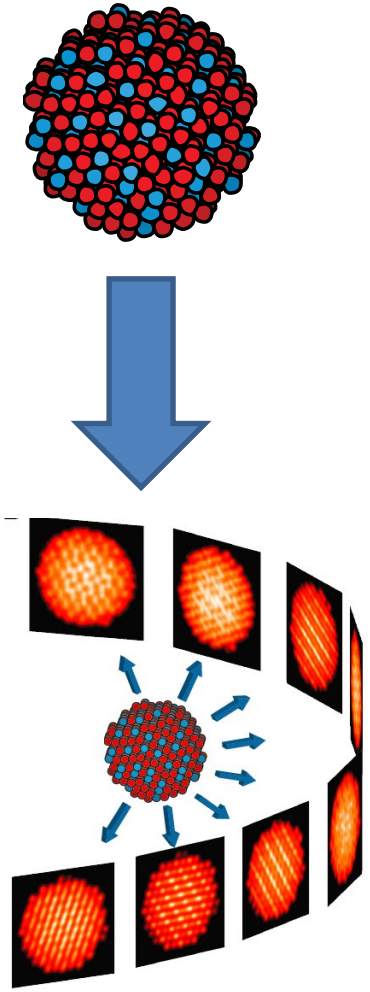
$$\int f(x,y,z)dz = \sum_z f(x,y,z) = P_0(u,v)$$



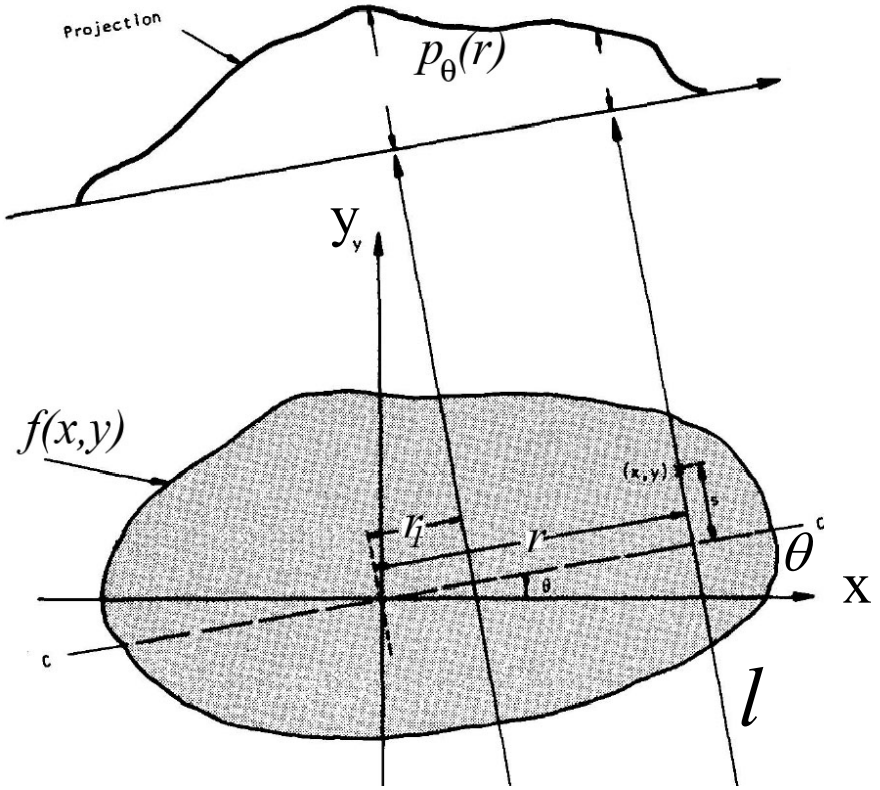
$$\int f(x,y,z)dr = \sum_r f(x,y,z) = P_\theta(u,v)$$

Figure courtesy of P. Ercius at NCEM
Lawrence Berkeley National Laboratory

The Radon Transform



$$x\cos\theta + y\sin\theta = r$$

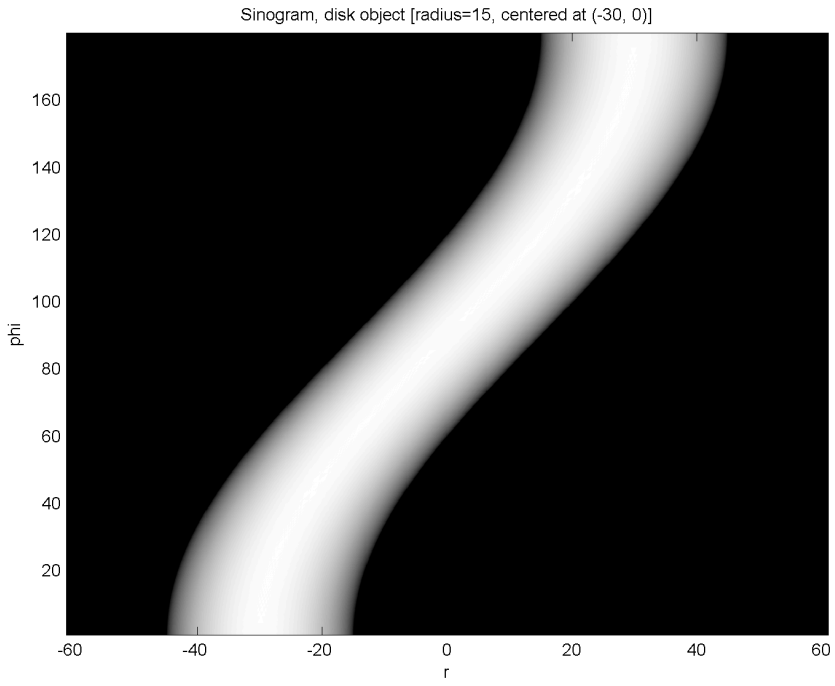


$$p_\theta(r) = \int_l f(x,y)\,dl$$

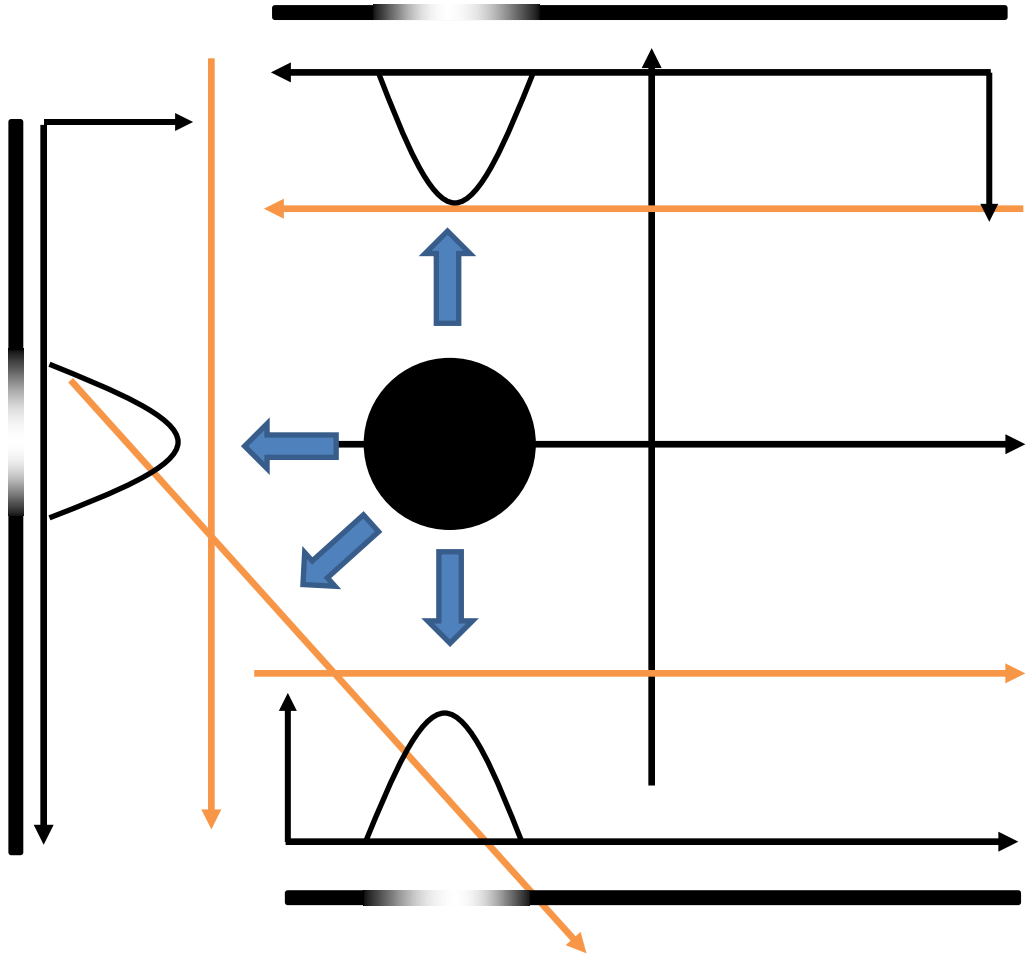
$$p_\theta(r) = \iint f(x,y)\,\delta(x\cos\theta + y\sin\theta - r)\,dx\,dy$$

$$= \Re\{f(x,y)\}$$

The Radon Transform



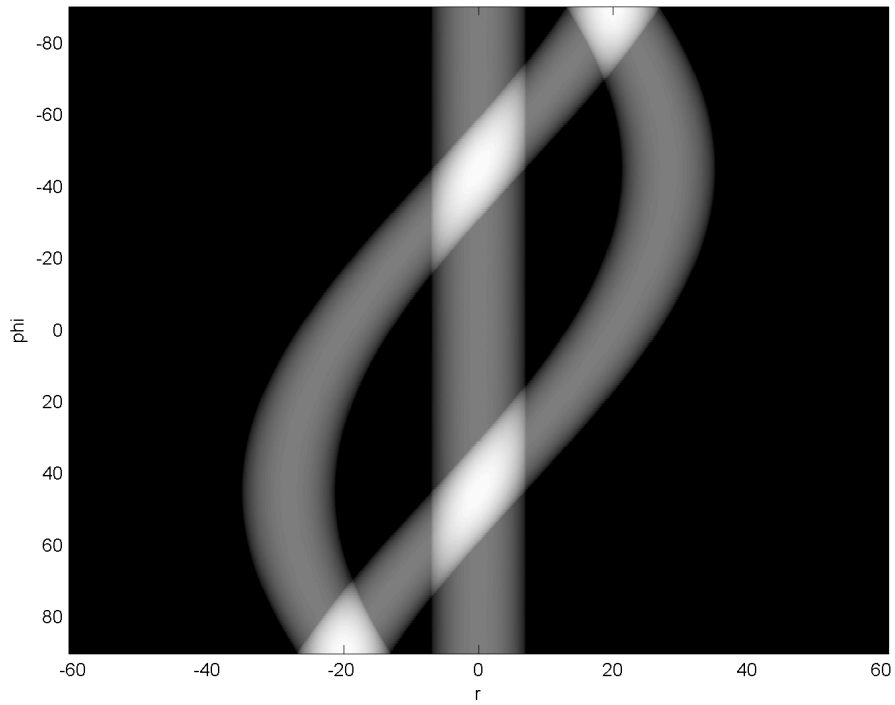
Sinogram



Radon transform relates an original object and its lower-dimensional projections.

The Radon Transform

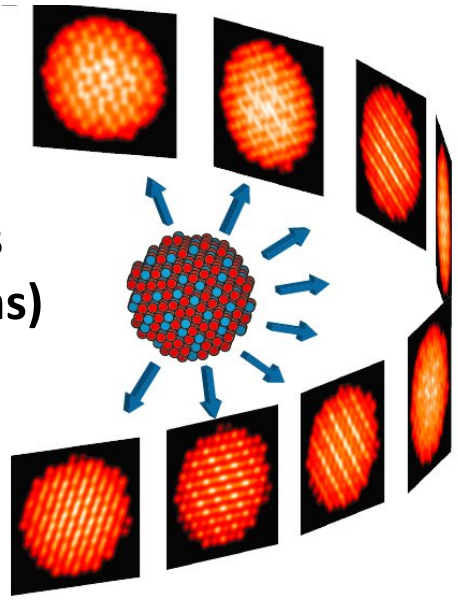
Sinogram



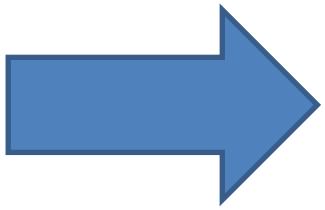
Radon transform ⇔Fourier Transform

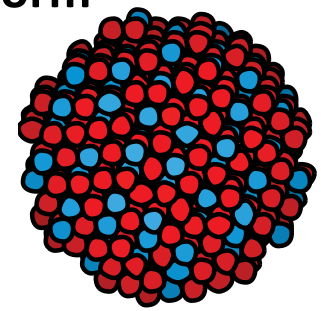
Tomography

Tilt Series (projections)



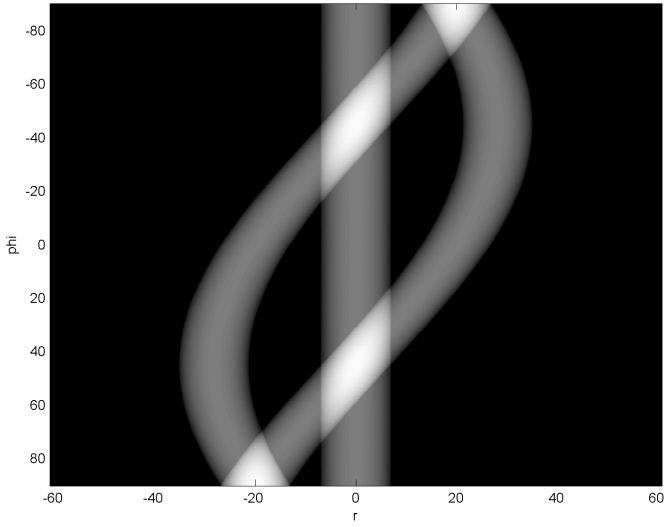
Inverse Radon Transform



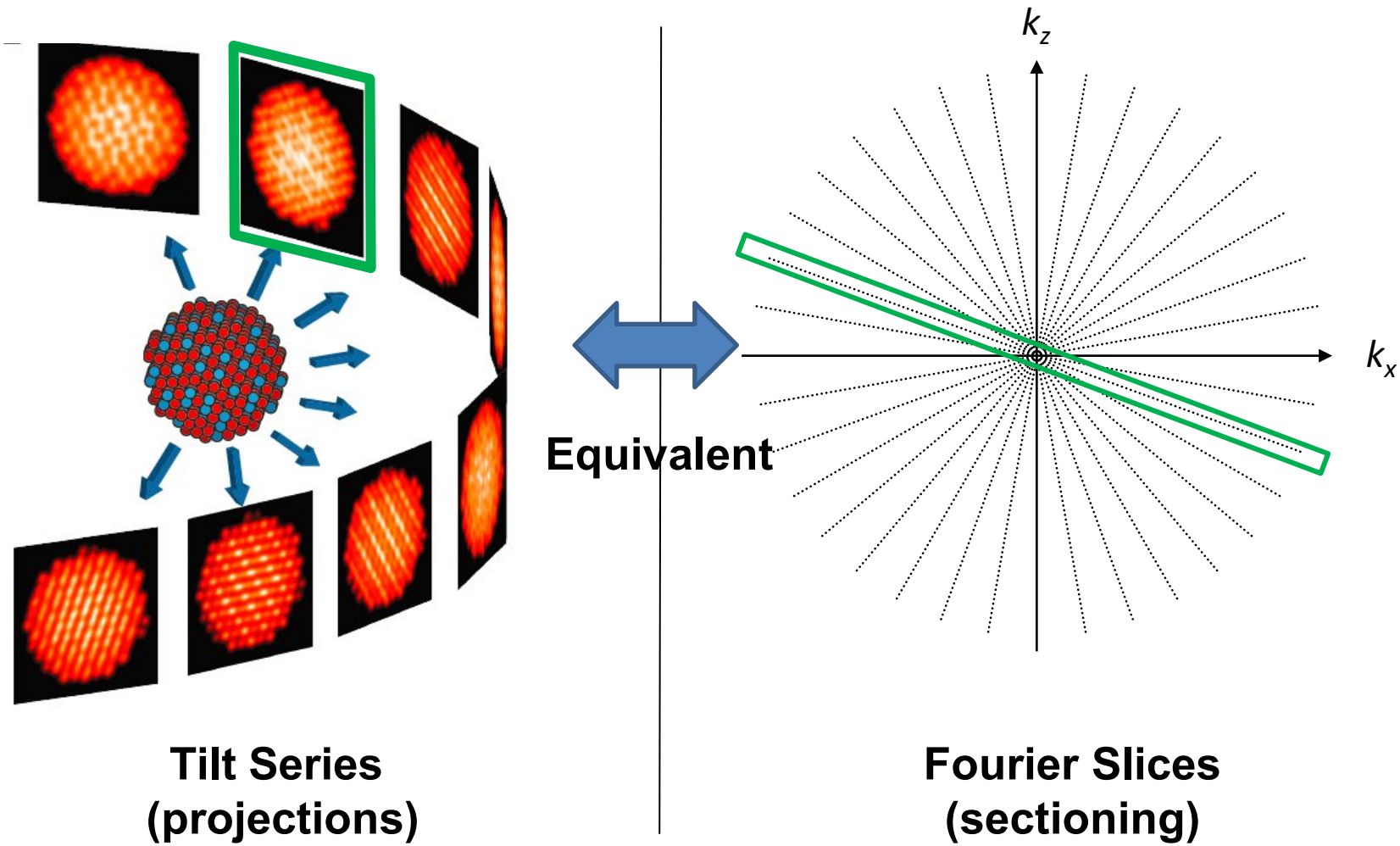


3D Object

Sinogram

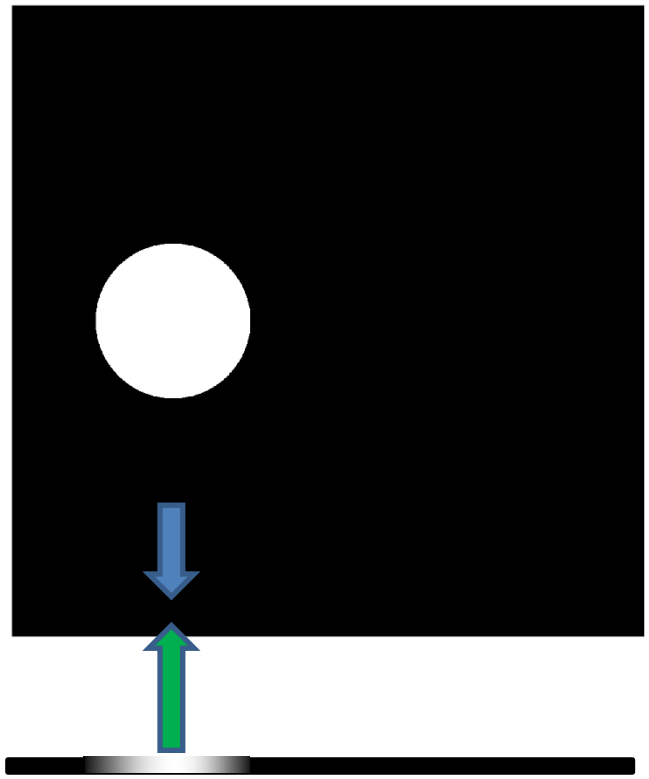


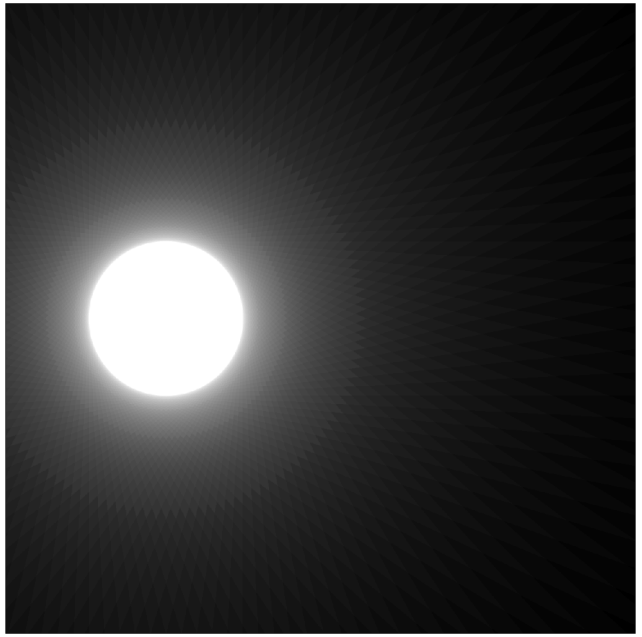
Fourier Slice Theorem



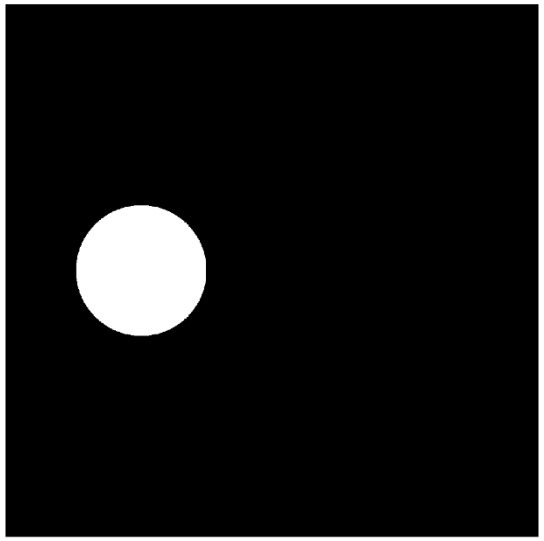
(Linear) Tomography Reconstruction

Backprojection: smearing each projection along the projection direction

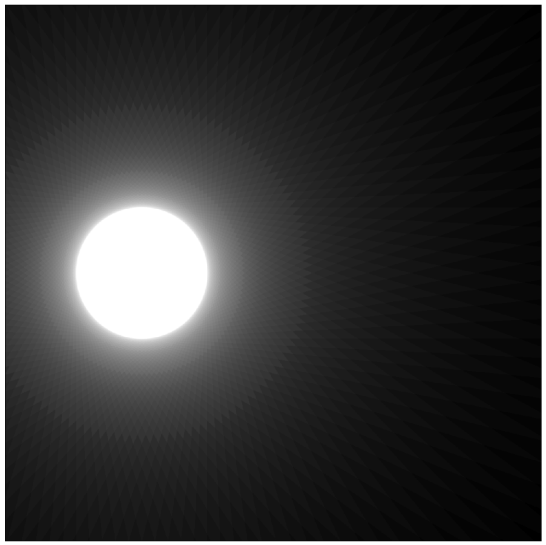




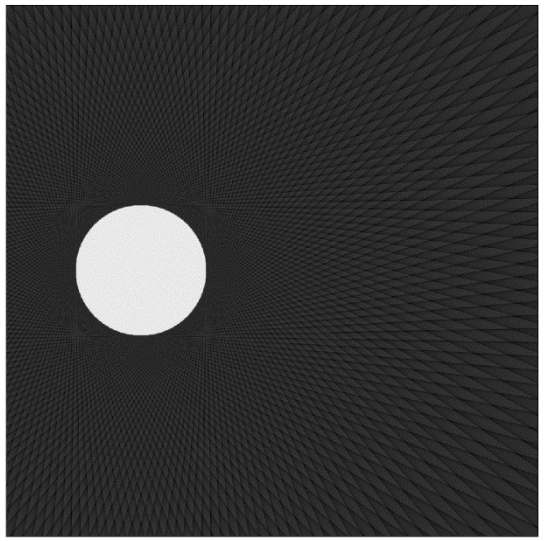
Inverse Radon Transform
Filtered Backprojection



Original Object



Backprojection

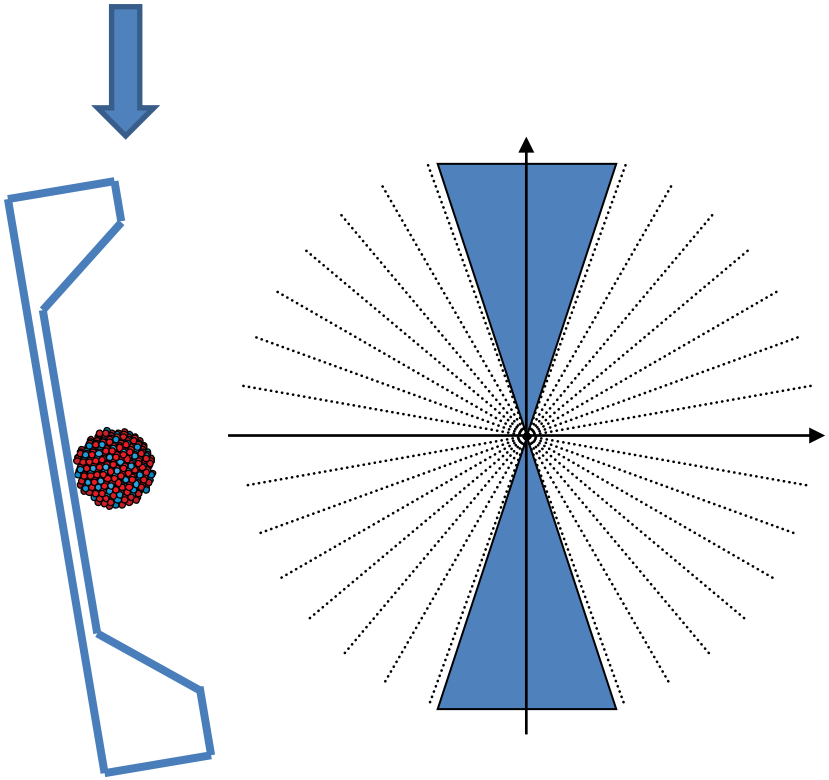


Filtered Backprojection

More details about tomography reconstruction principle:

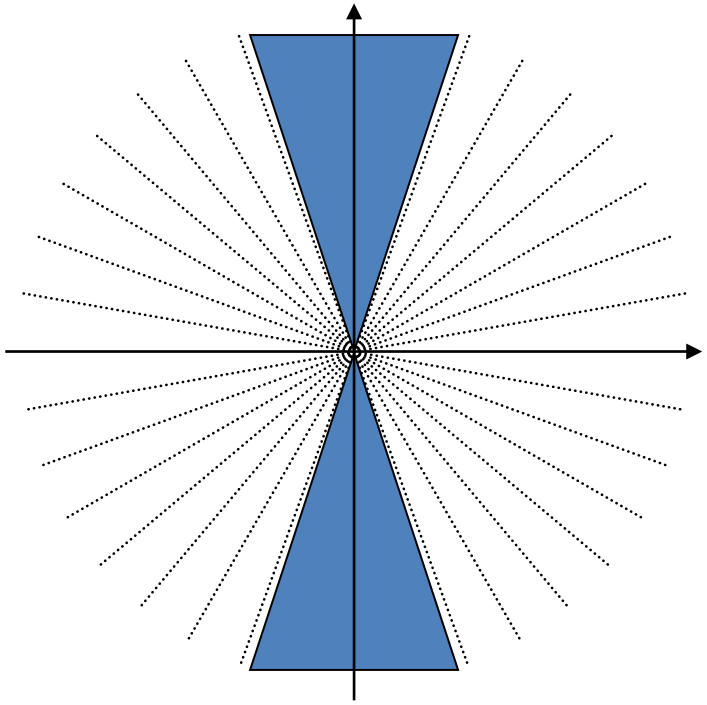
https://www.youtube.com/watch?v=2sk0xe8k_uI

Missing Wedge Problem



- Hardware geometry
  - Sample holder, goniometer limits, grid shadowing

Electron Dose Limit

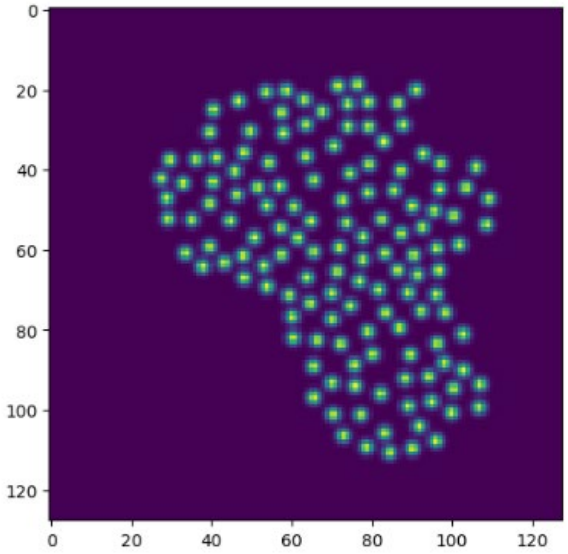


- Some samples can be easily damaged (biological sample) -> CryoEM
- Material science samples are relatively sturdier, but still there is knock-on damage, carbon contamination, etc.
- Minimize electron dose -> Minimize # of projections measured

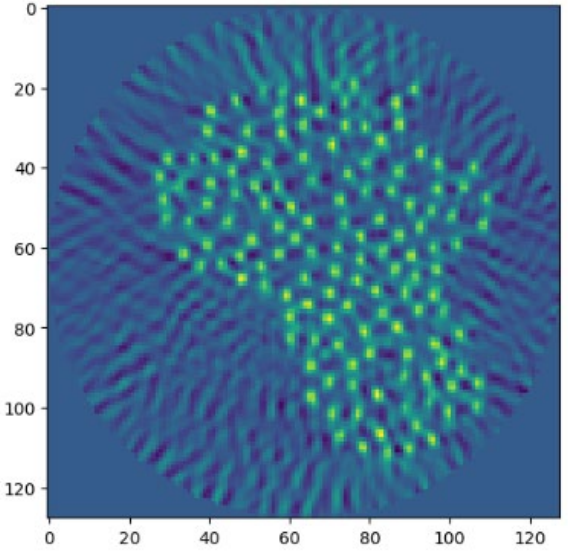
2. Neural-Network based Data Augmentation

Missing Data Problem

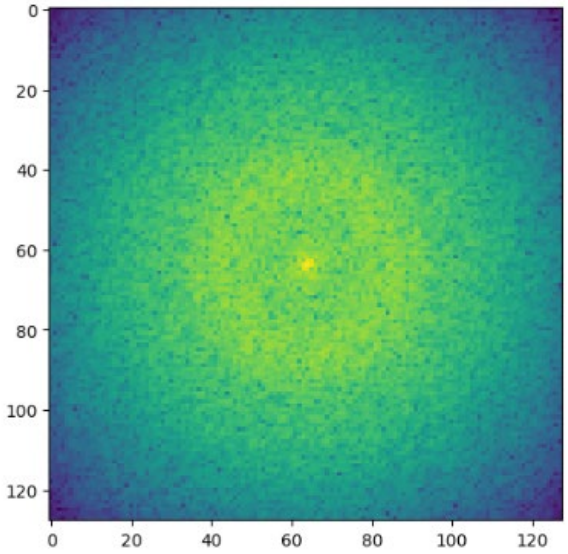
Ground Truth



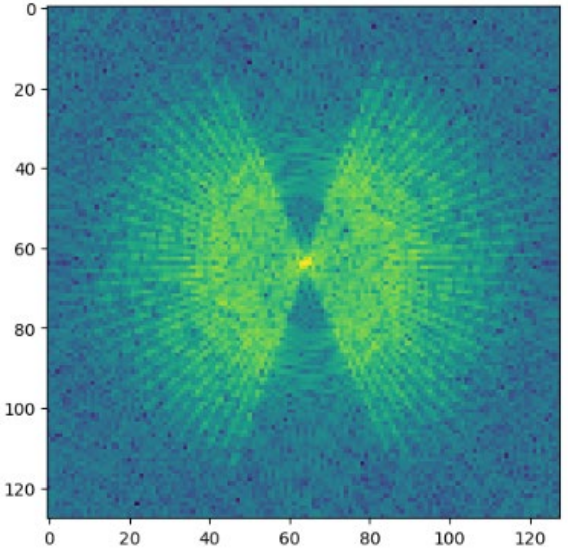
FBP Reconstruction
+/- 70 deg, 4 deg step



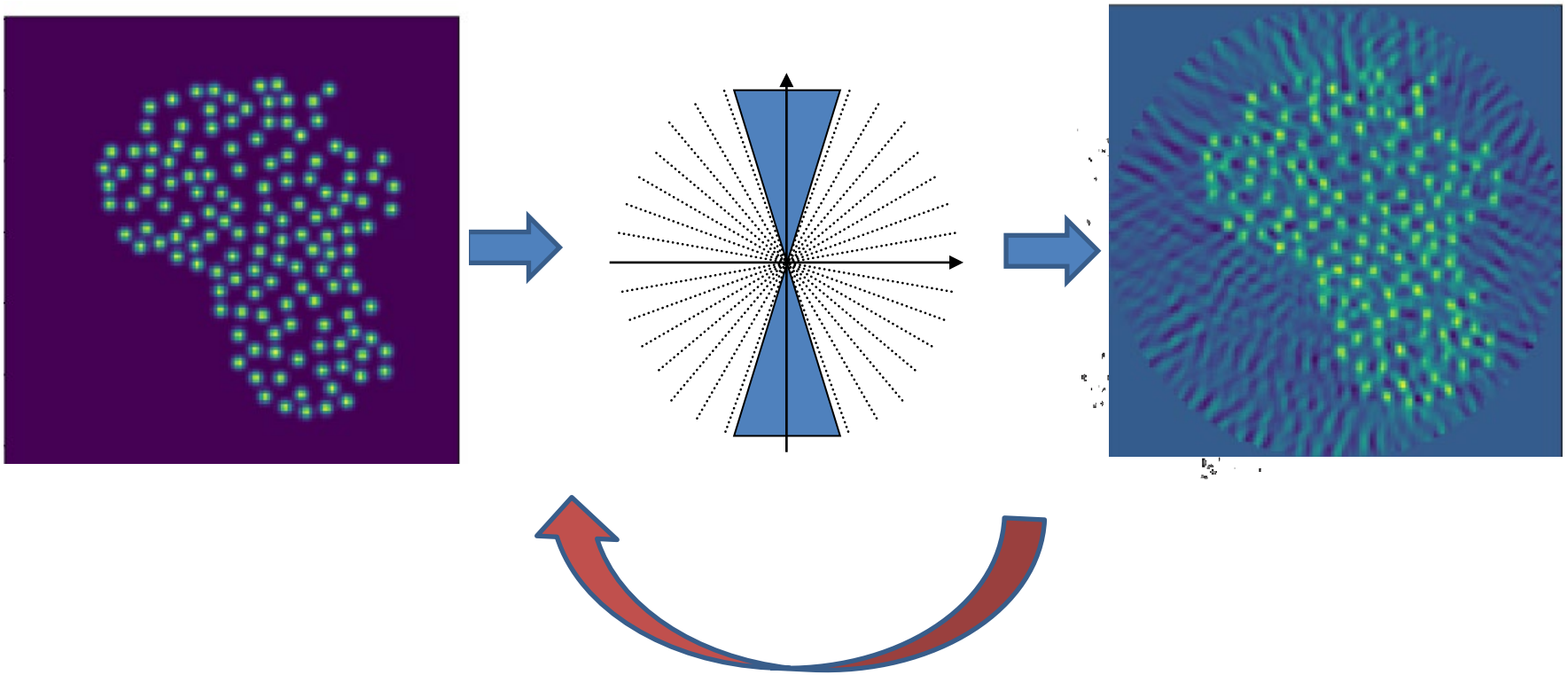
Real Space



Fourier Space

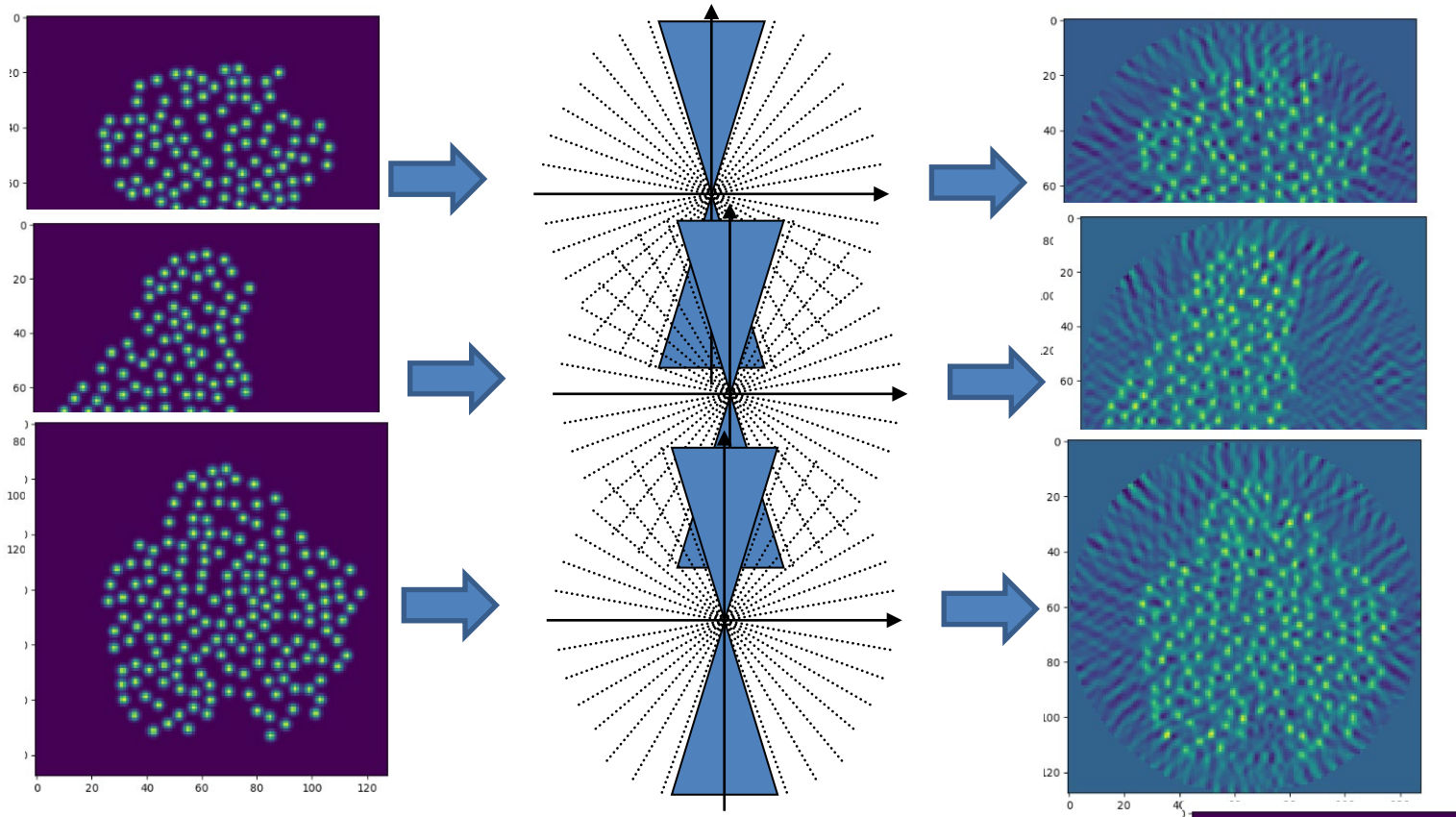


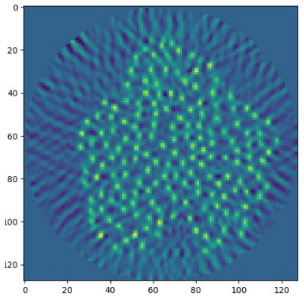
Missing Data Problem

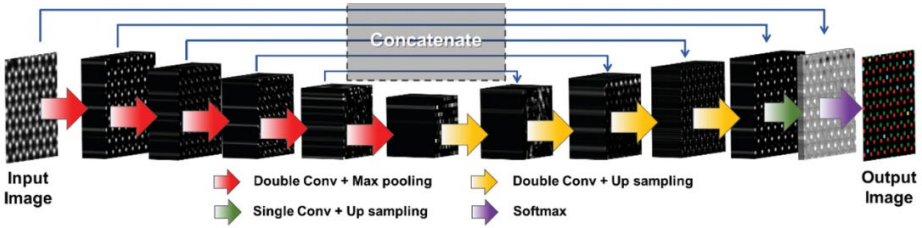


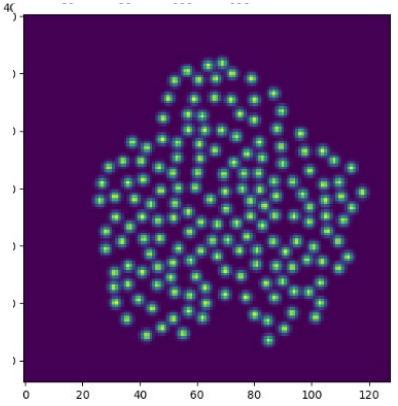
Inverse?

Deep Learning-based Augmentation (Simulation)

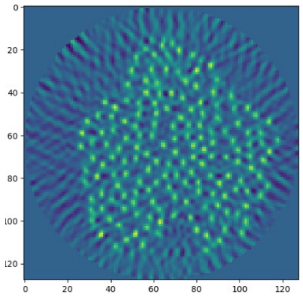


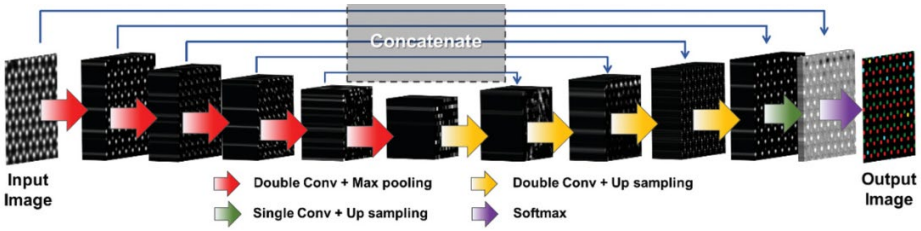


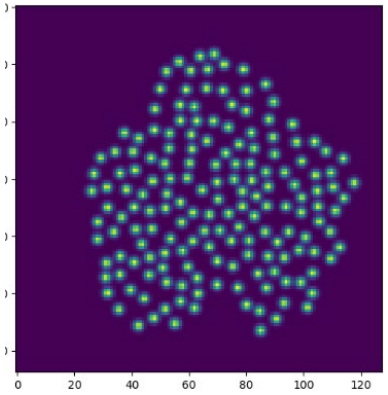


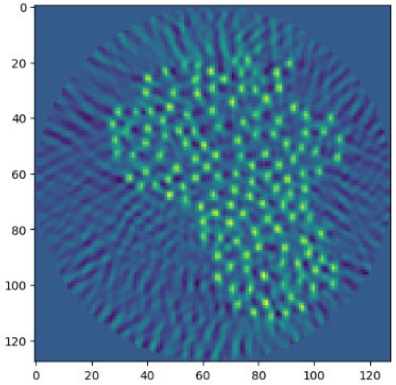


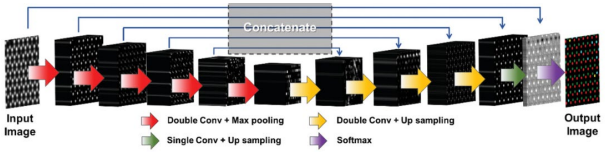
Deep Learning-based Augmentation (Simulation)

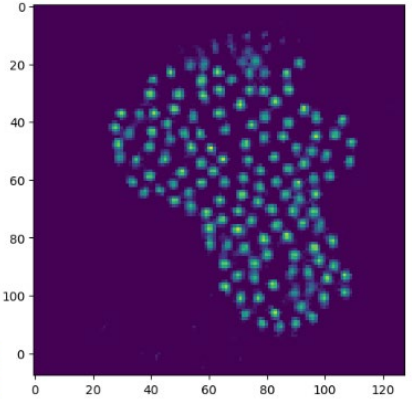


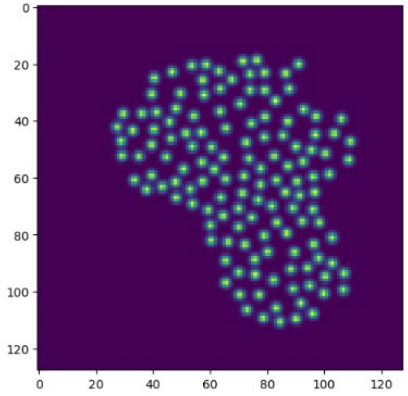


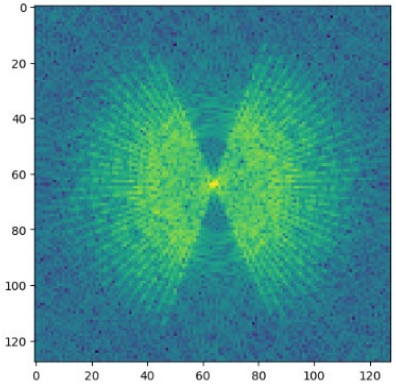


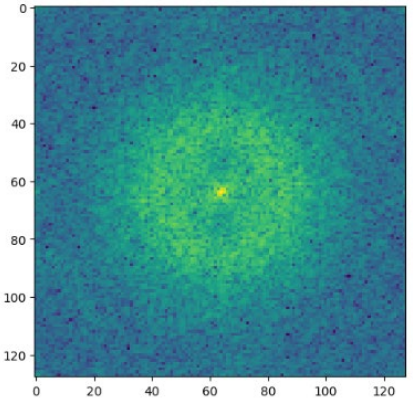


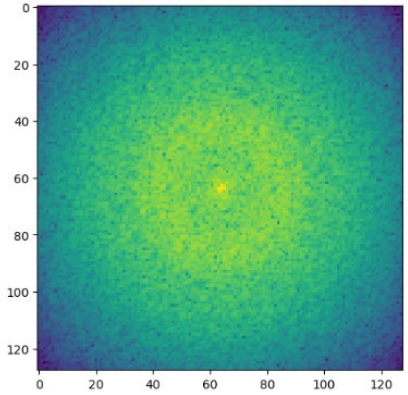




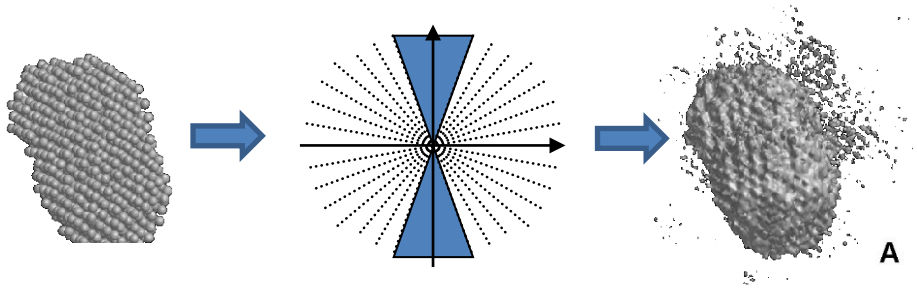




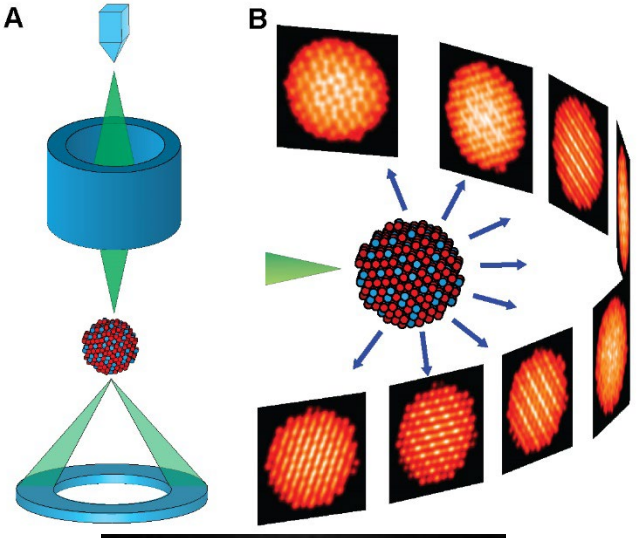




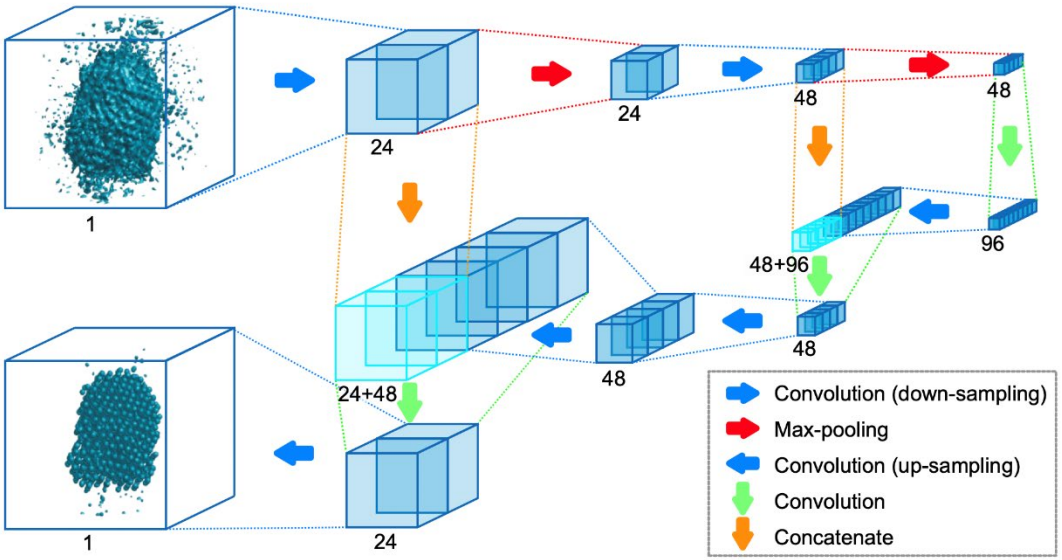
Deep Learning-based Augmentation (Simulation)



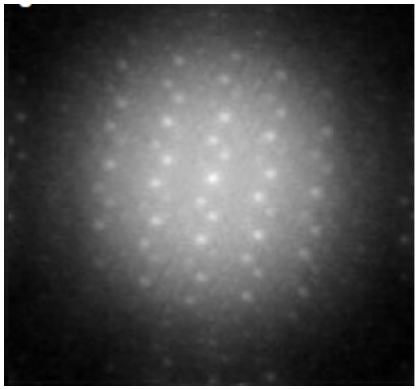
FCC Pt nanoparticle, random shape, 22pm RMSD, ~0.5% defect



Reconstruction (Missing Wedge)



J. Lee et al., *Nat. Commun.* **12**, 1962 (2021).



After DL Augmentation

Questions?