Bridging Structure and Evolution

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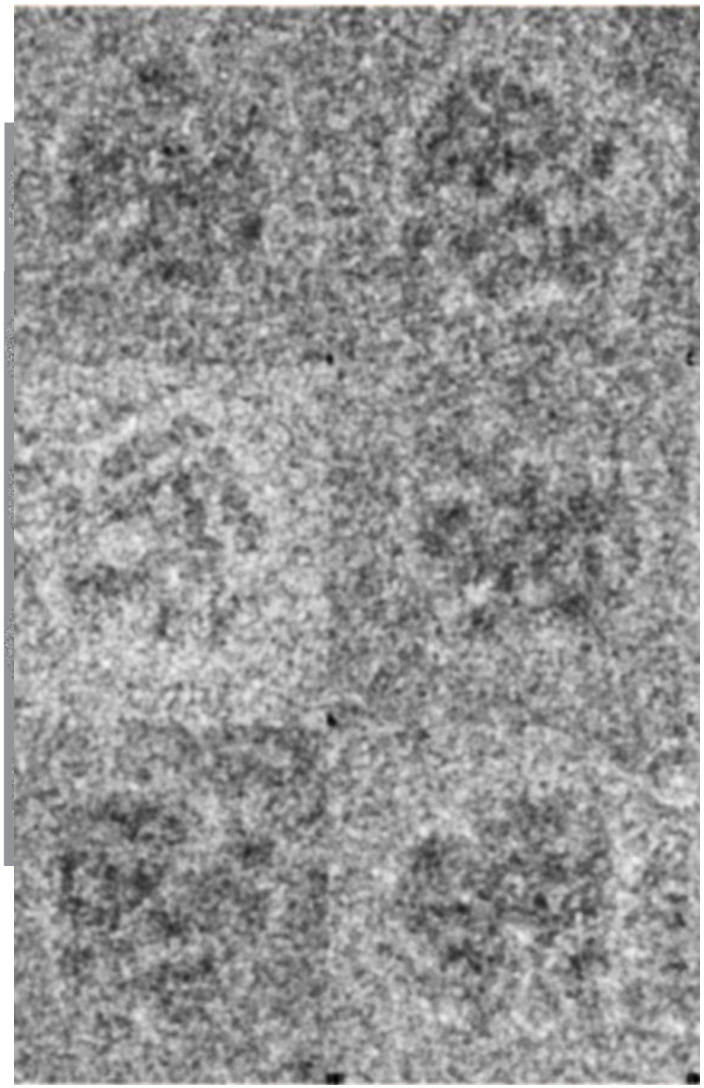
Friday June 21, 2013

The Initial Model Problem



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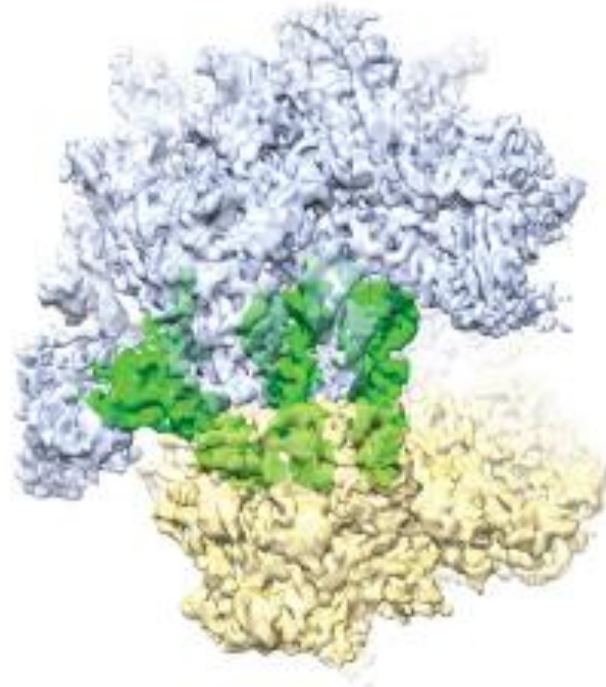
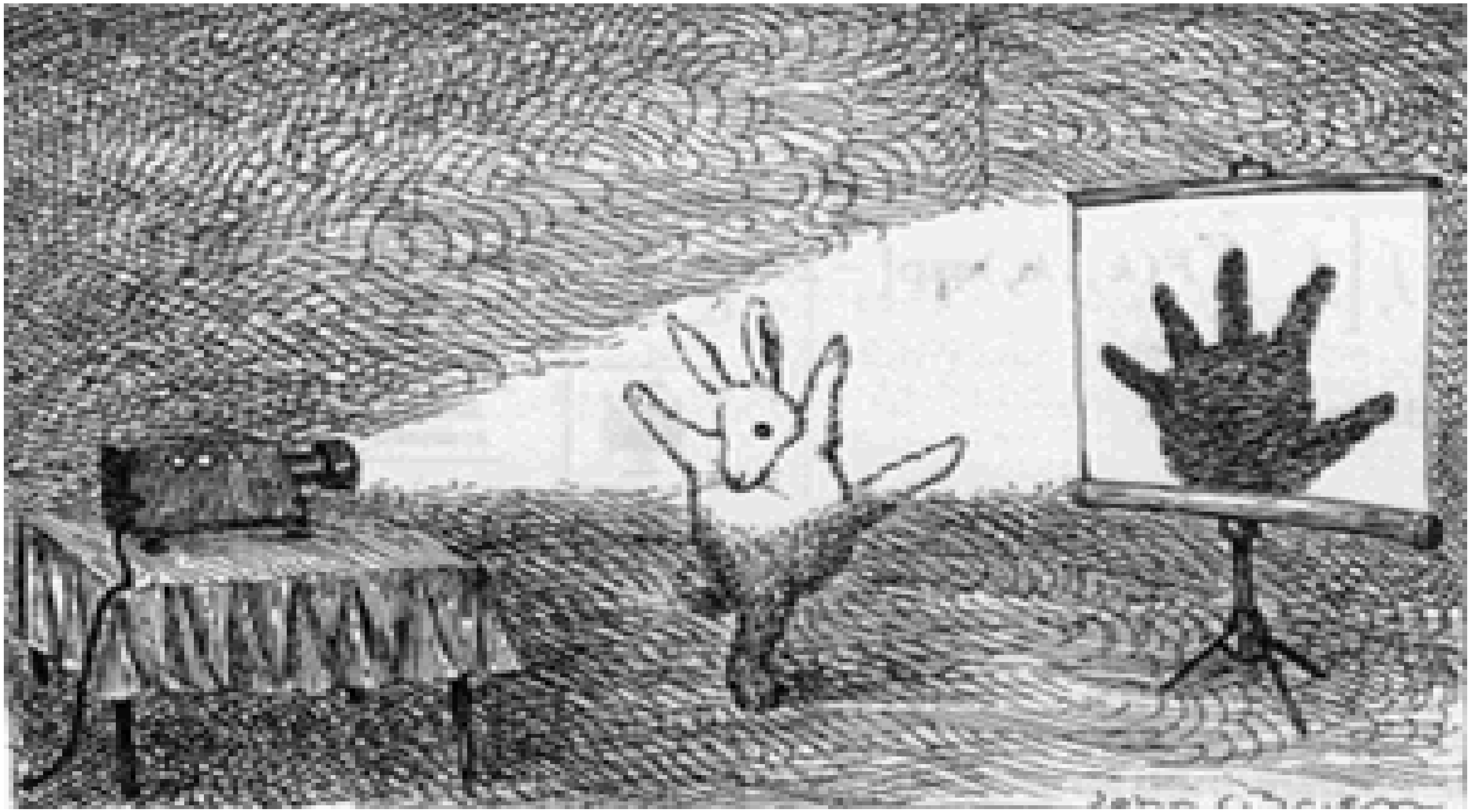


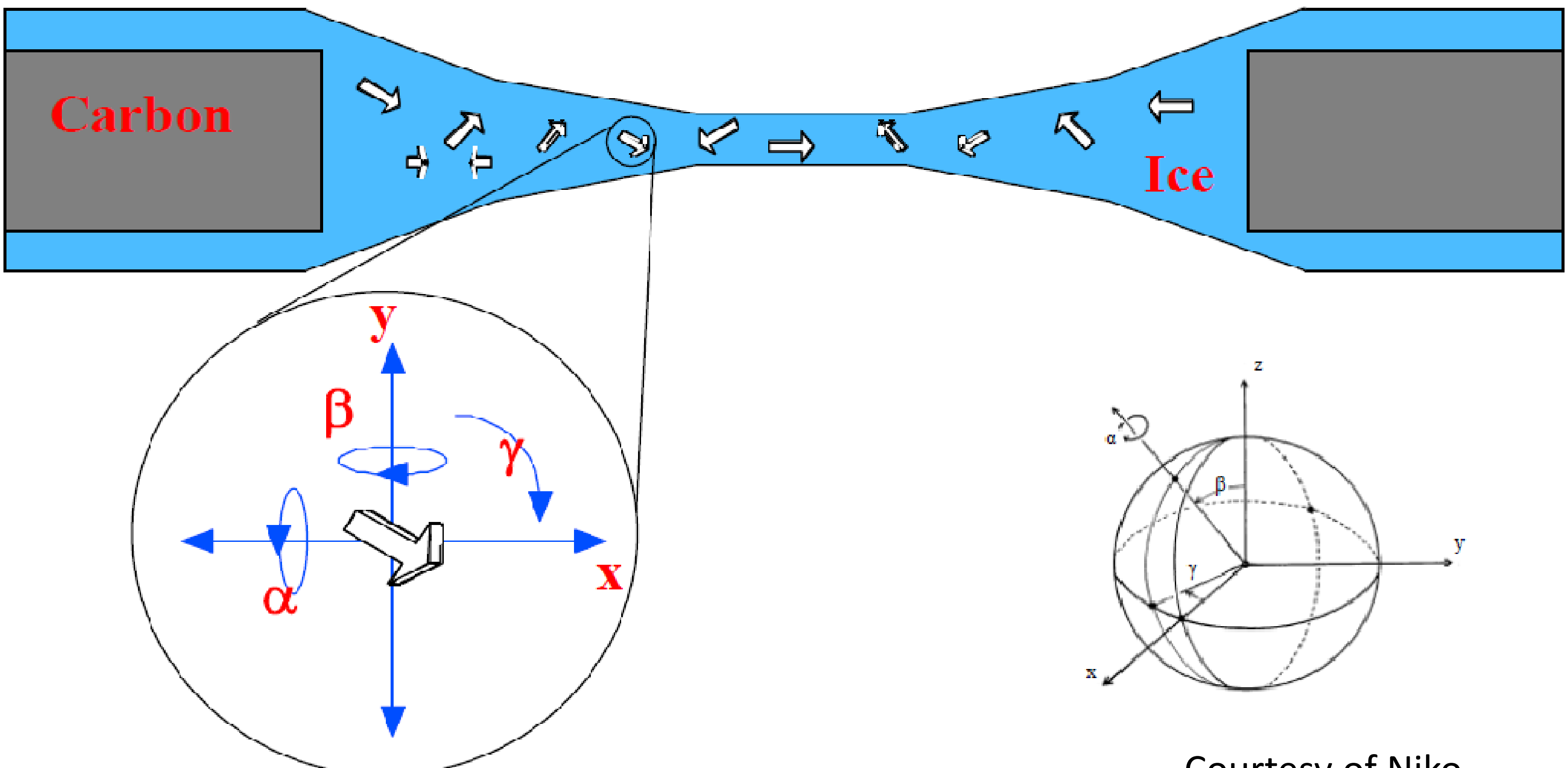
Divining the shape from the “projection”



The New Yorker

The Initial Model Problem

5 Parameters to determine



Courtesy of Niko

Methods

Direct Methods

Random Conical Tilt

Tomography

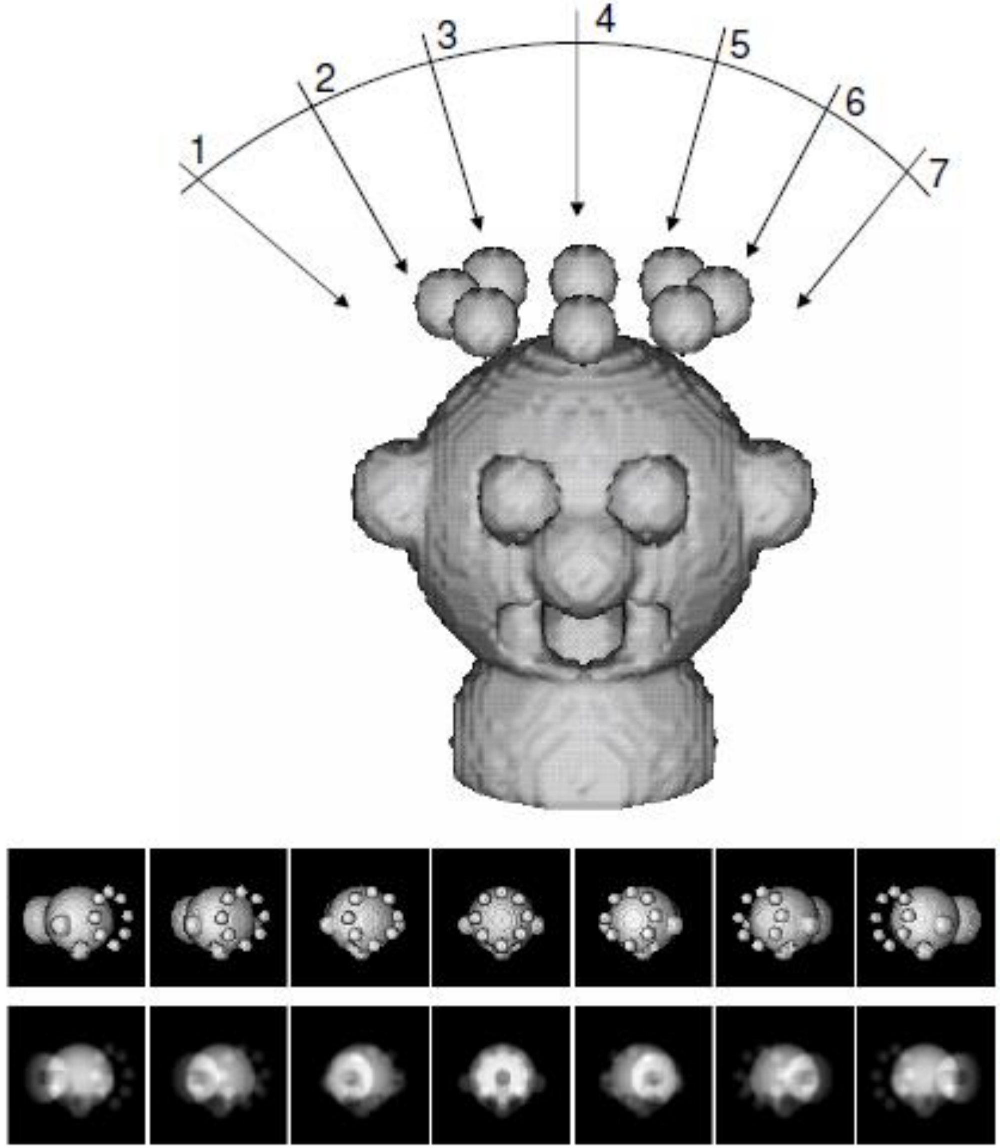
Orthogonal Tilt Reconstruction

Computational Methods

Common information based

Projection Matching based

The Central Section Theorem

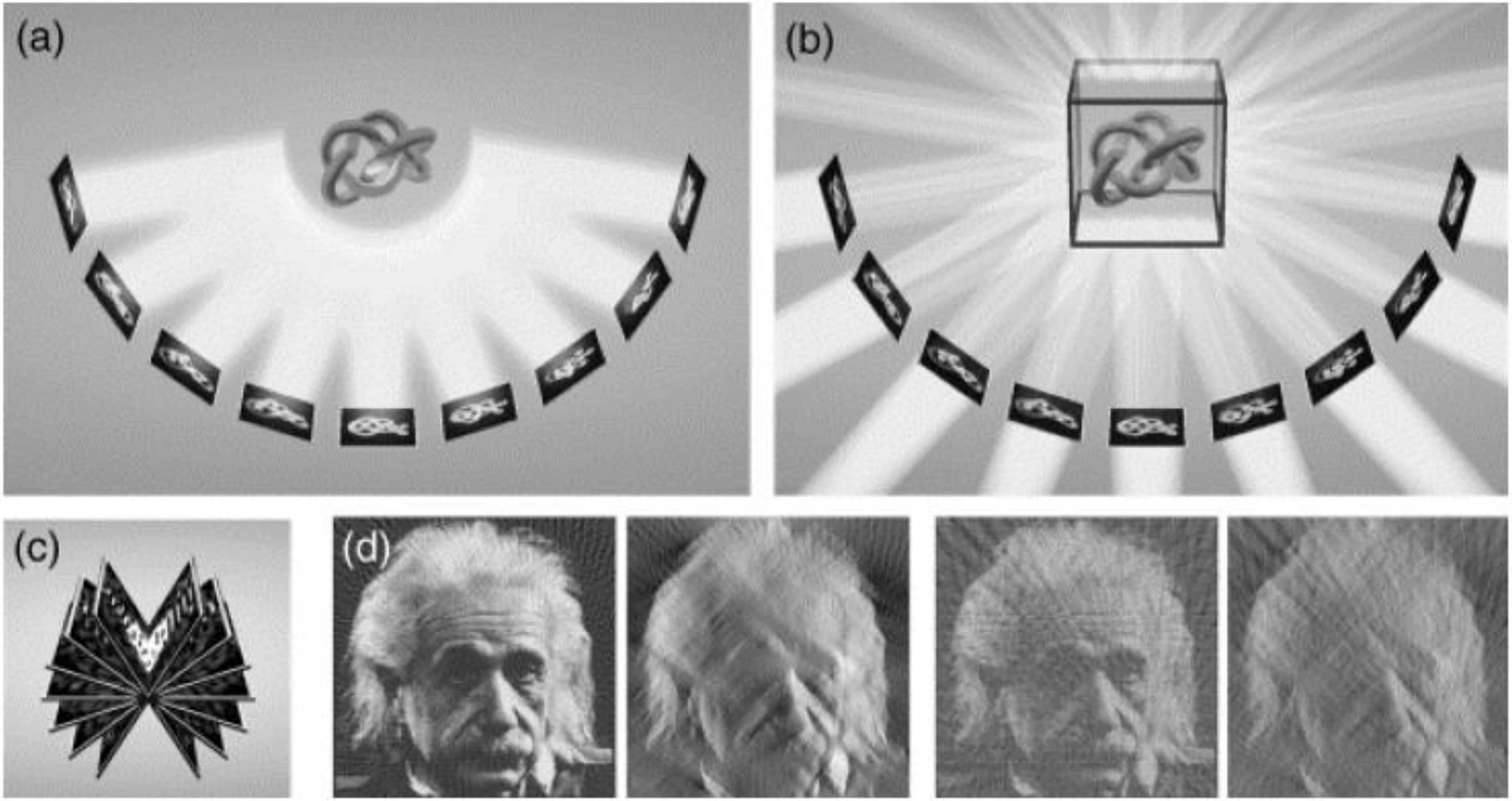


In reciprocal space, every 2D projection of a 3D object corresponds to a central section in the 3D Fourier transform of the object. Each central section is orthogonal to the direction of of projection.

Trying to get all of the representative views of a particle is analogous to filling in the 3D fourier Transform with central sections.

Stolen from N. Boisset EMBO Lecture

Tomographic reconstruction



± 90° 2° steps | ± 60° 2° steps | ± 90° 5° steps | ± 60° 5° steps

Baumeister et al., 1999 (Stolen from N. Grigorieff lecture)

Difficulties and Issues with Direct Methods

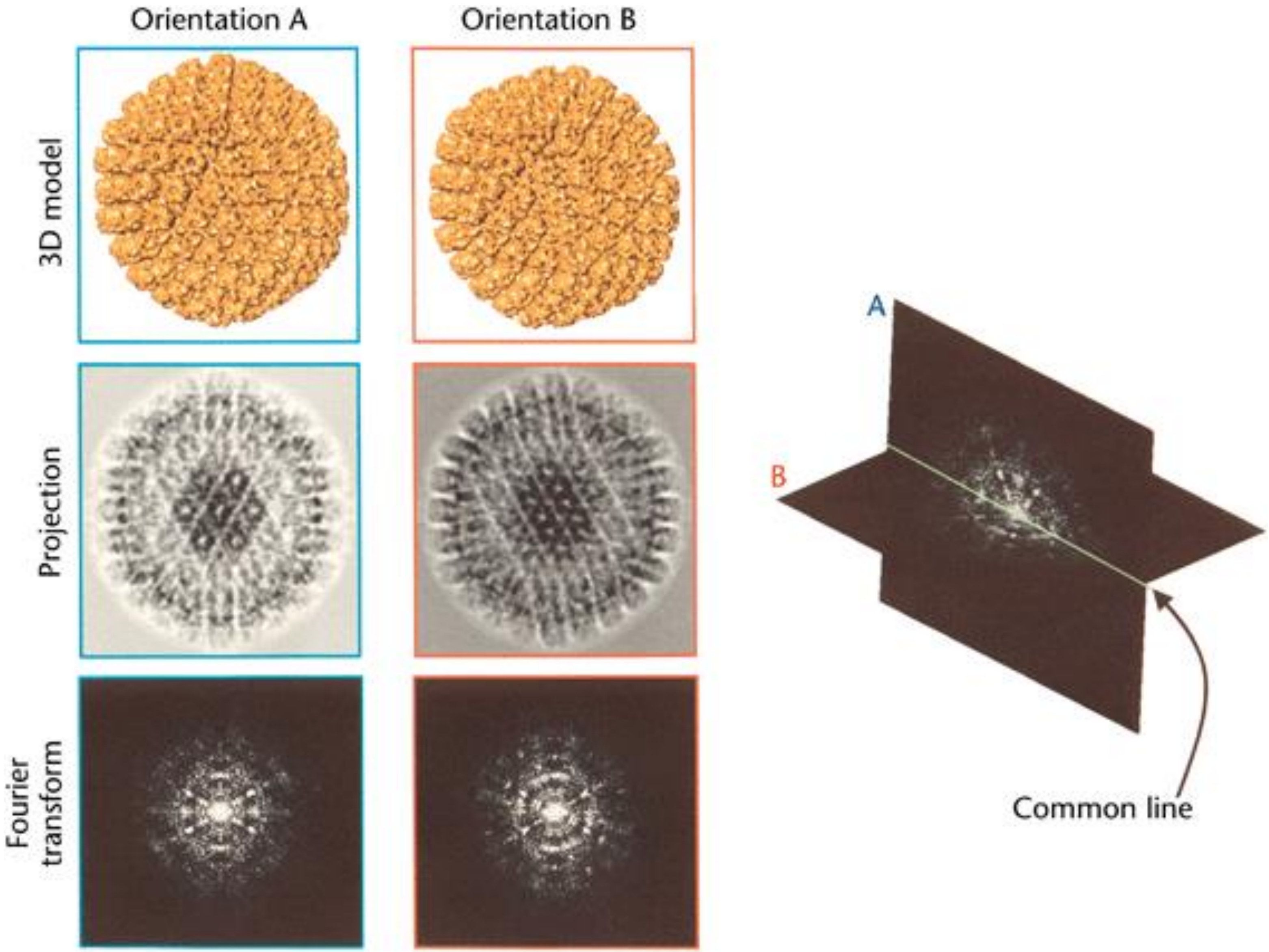
Experiments can be technically very difficult and time-consuming

Dose fractionation leads to lower SNR and resolution in reconstructions

Reconstructions have artifacts which can be difficult to correct

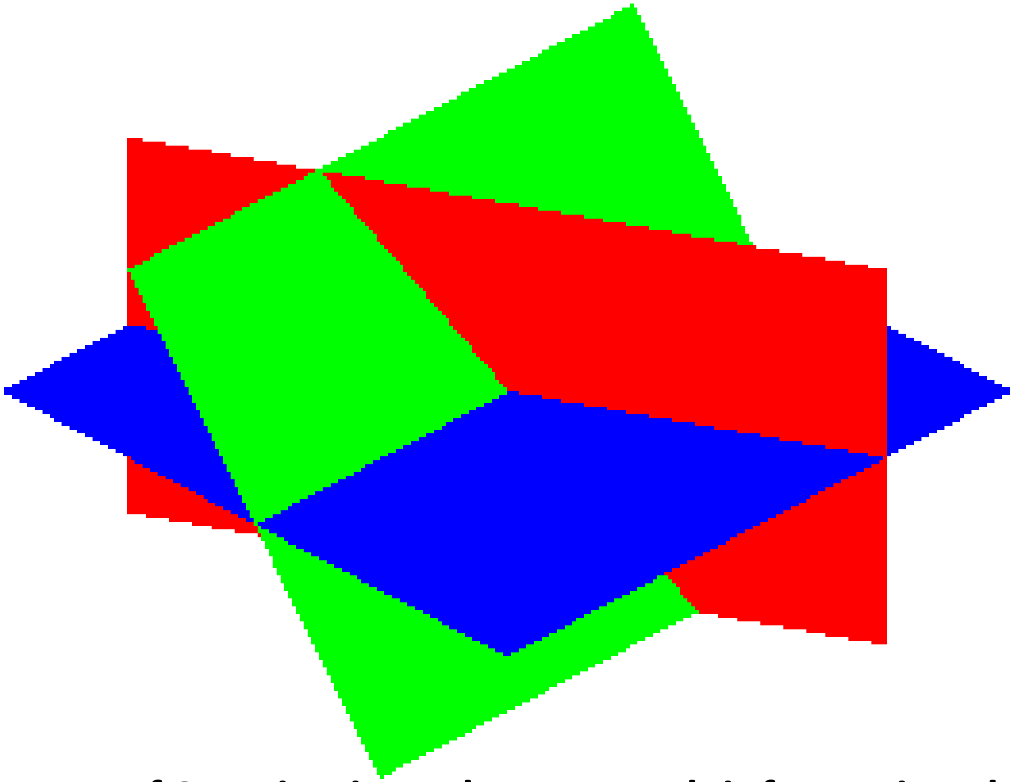
Data obtained is useless in the generation of a high resolution reconstruction

Common lines



Projections share information, which is located along a "common line" in Fourier space

Intersecting Central Sections

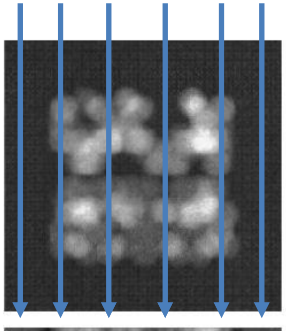


Any set of 3 projections share enough information that they can uniquely define their respective relative orientation

"The common-line-projection theorem states that two different 2D projections of a 3D object always have a one-dimensional line-projection in common."

Van Heel et al., 1997, Scanning Microscopy
(original papers: Van Heel et al. 1987, Vainshtein et al., 1986)

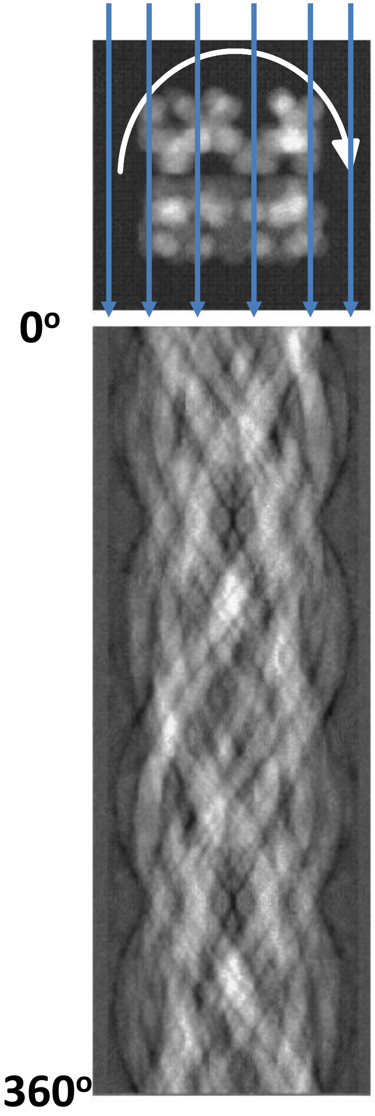
Sinograms


0º

Project through the 2D image, obtaining line projection

Van Heel et al., Scanning Microscopy

Sinograms



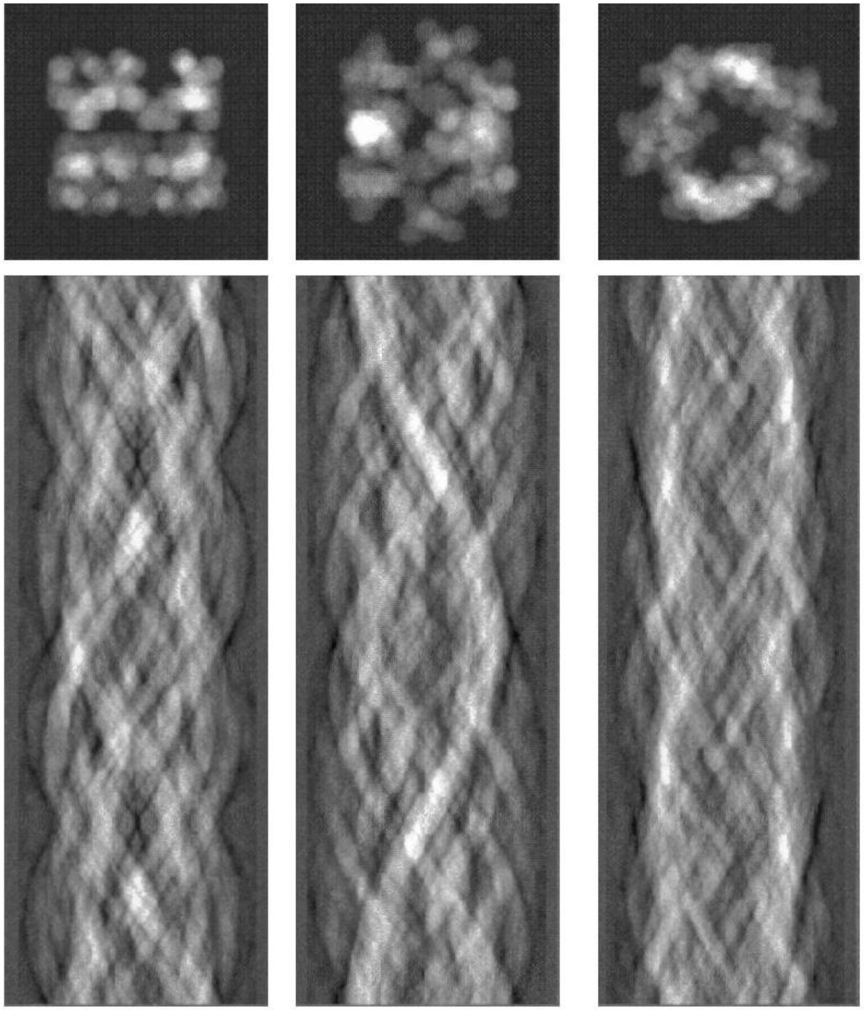
Project through the 2D image, obtaining line projection
(which is the real space version of a central section of the 2D FT)

Rotate the image, 1 degree at a time,obtaining projections,
to obtain a sinogram

Van Heel et al., Scanning Microscopy

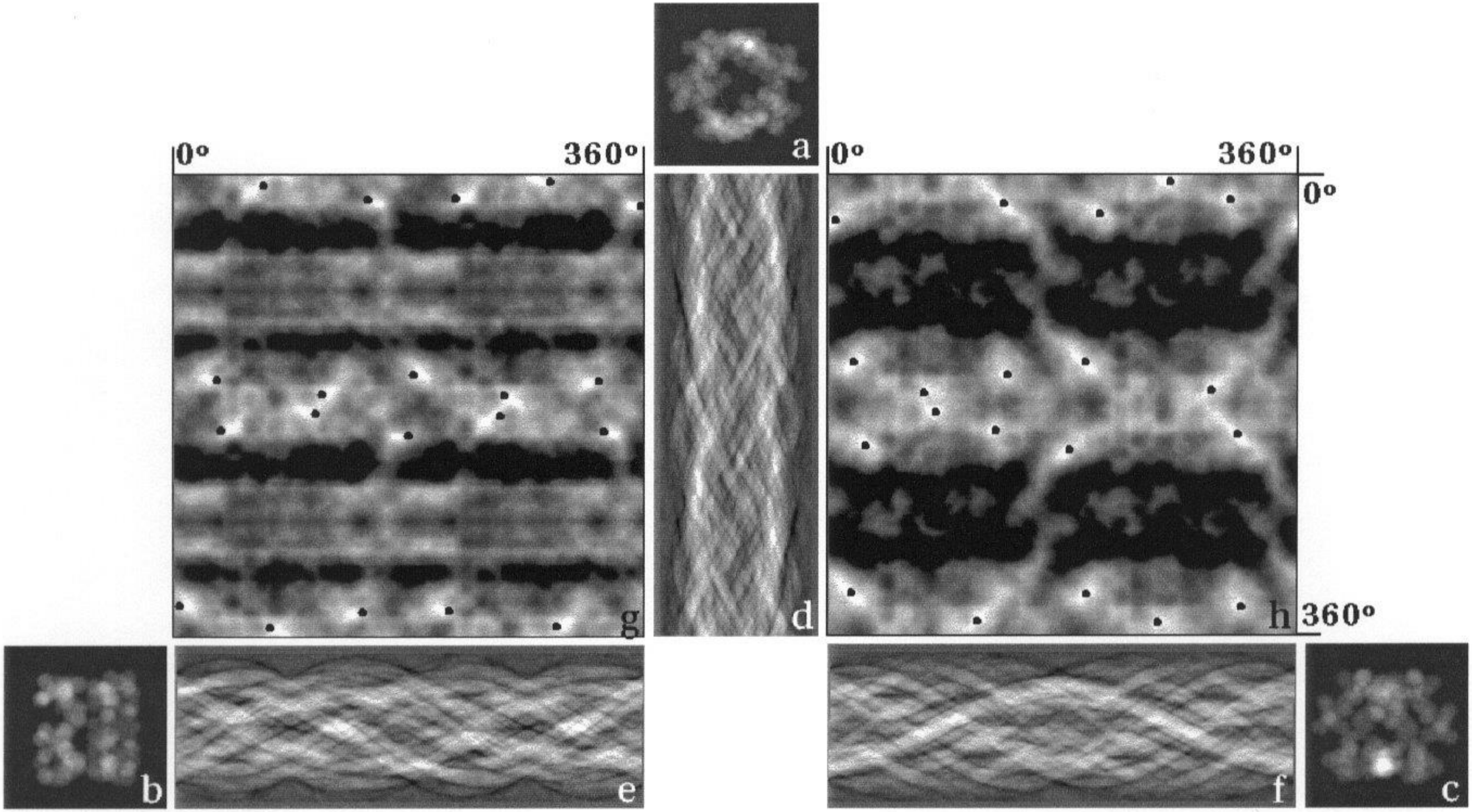
Angular Reconstitution

Repeat for a set of three images



Van Heel et al., Scanning Microscopy

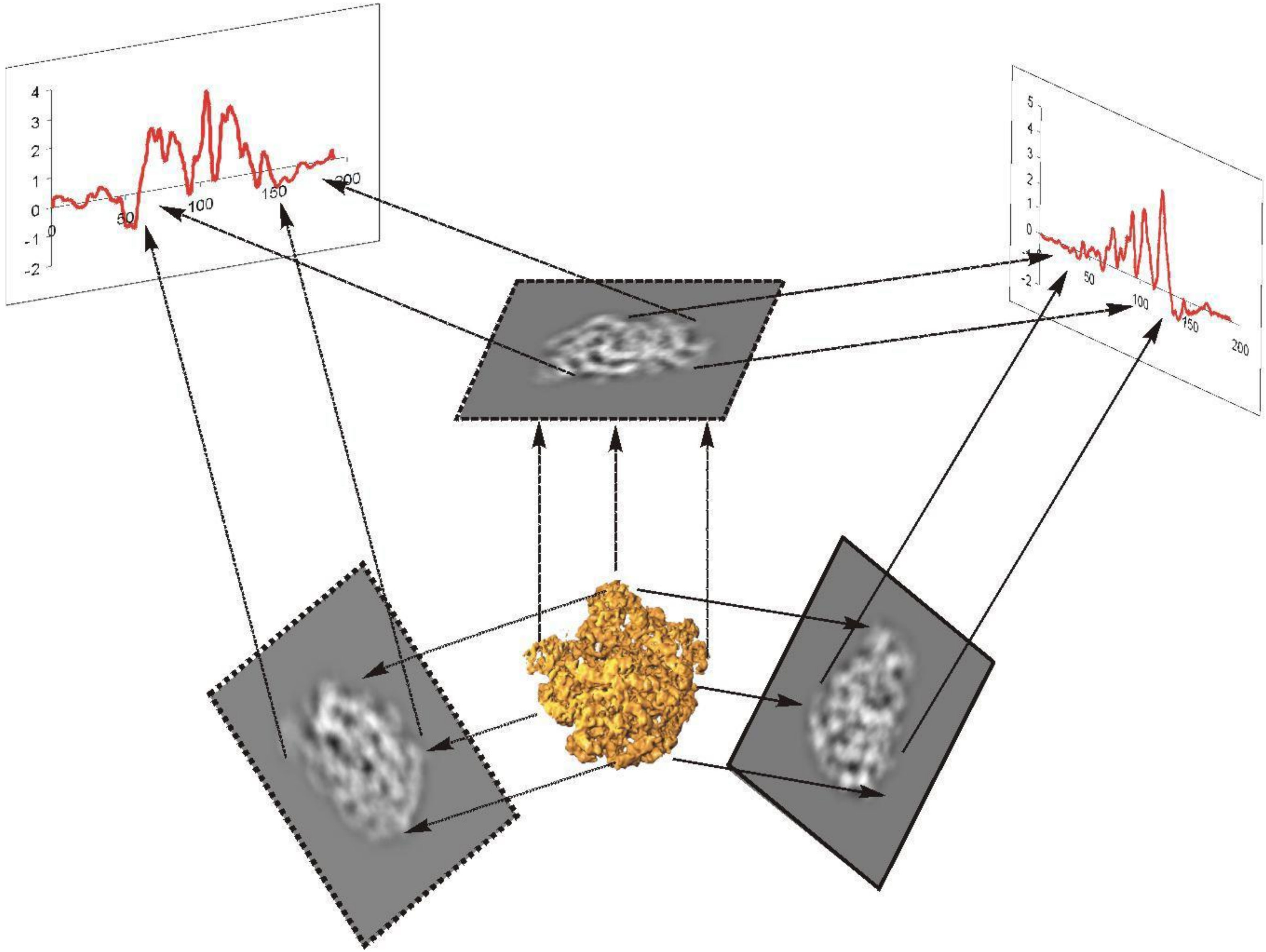
Direct Methods for Obtaining Initial Models



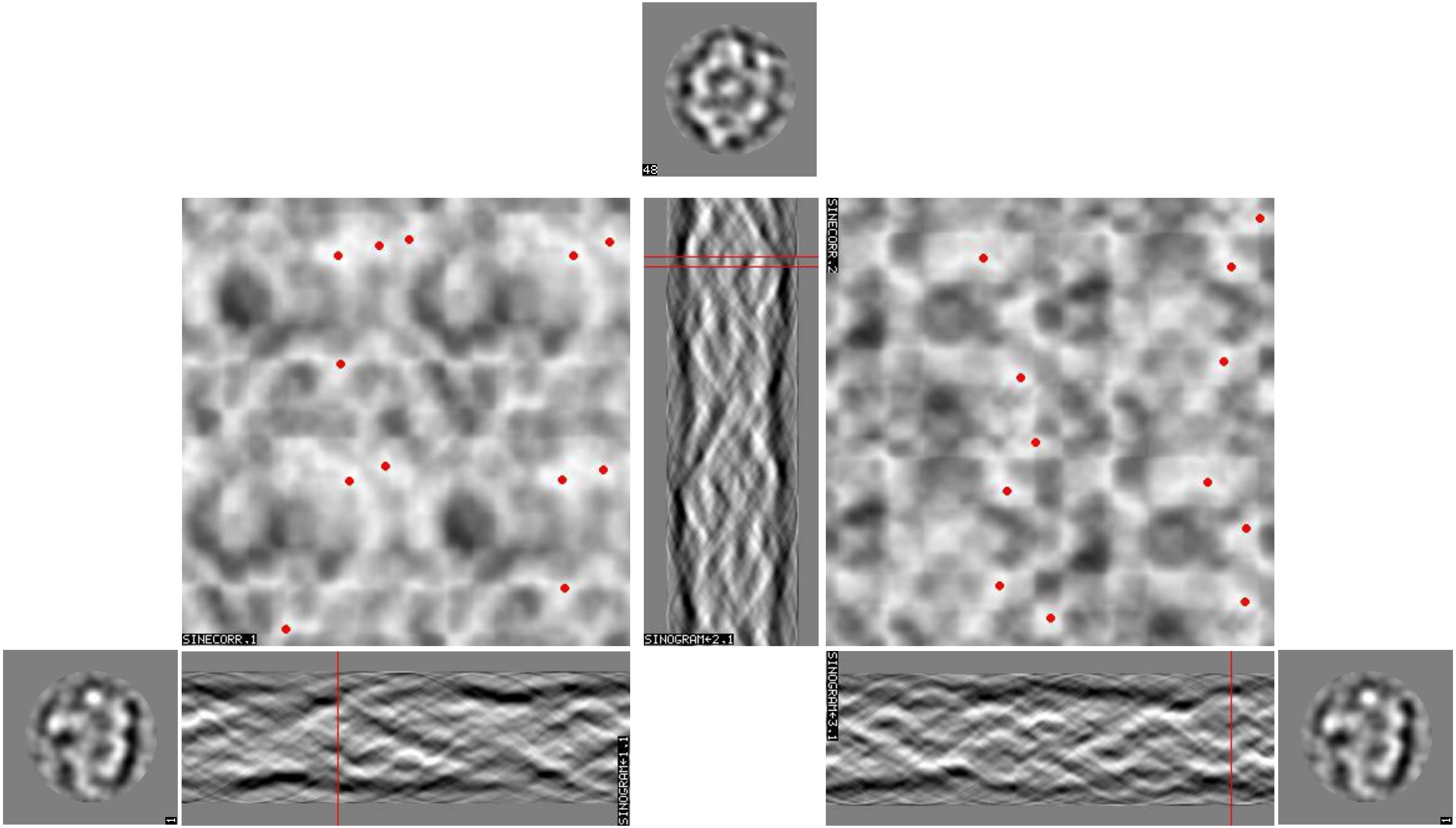
Calculate the Sinogram Correlation Function (line by line comparison of the sinograms). Find peaks.

Van Heel et al., Scanning Microscopy

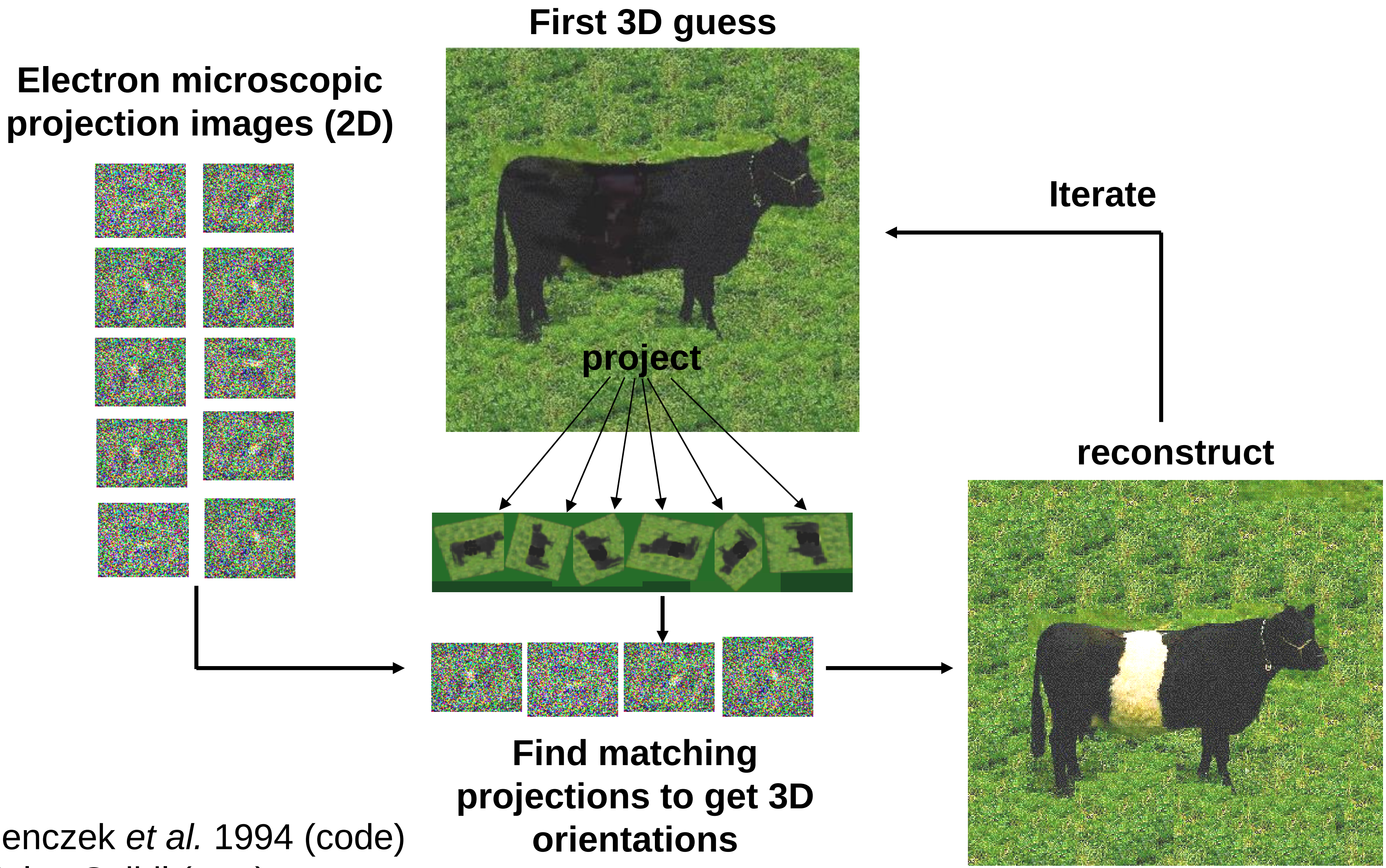
Angular Reconstitution



Direct Methods for Obtaining Initial Models

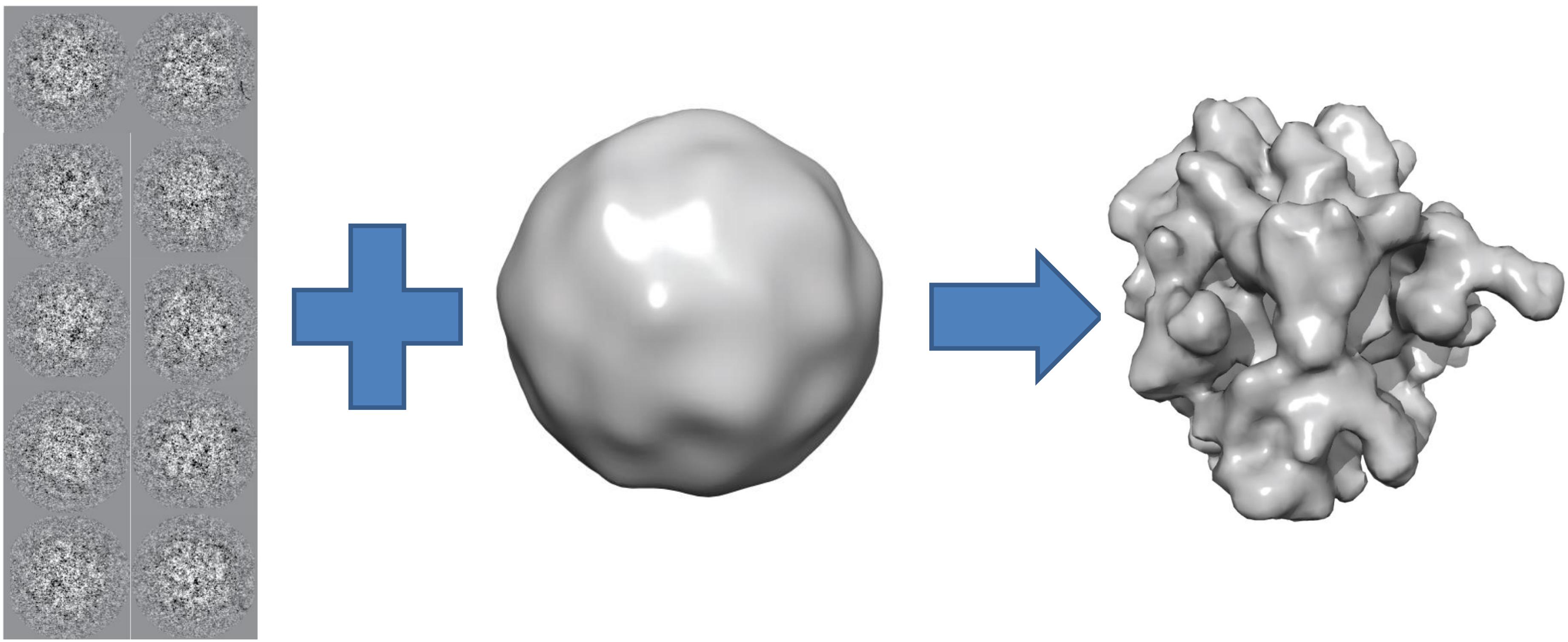


Projection Matching Illustrated

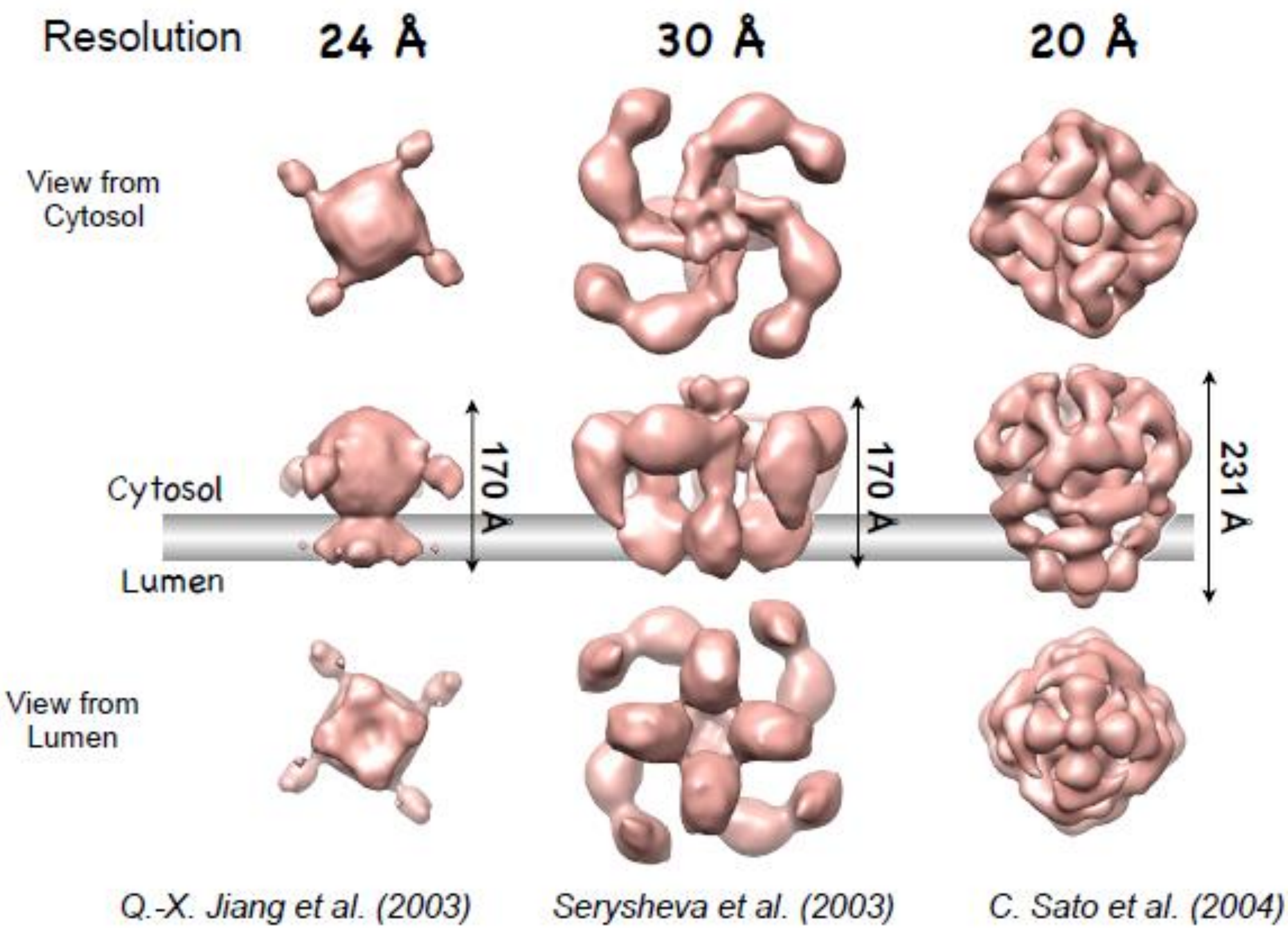


Penczek *et al.* 1994 (code)
Helen Saibil (cow)

Projection Matching Methods



Caveats Illustrated



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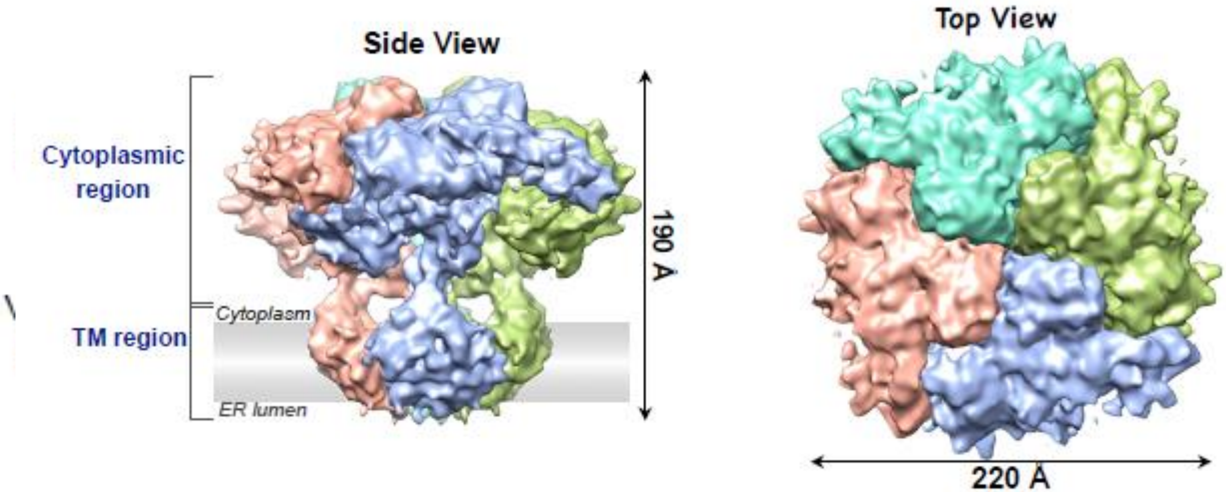

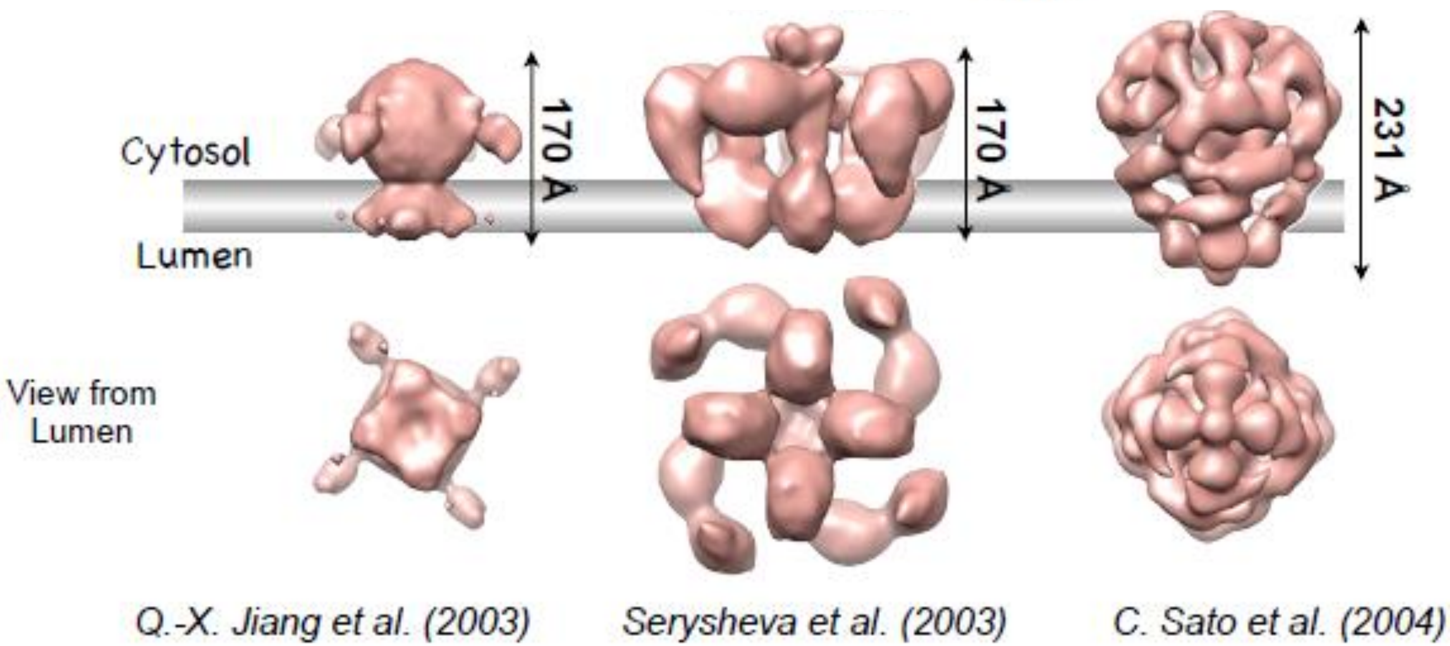

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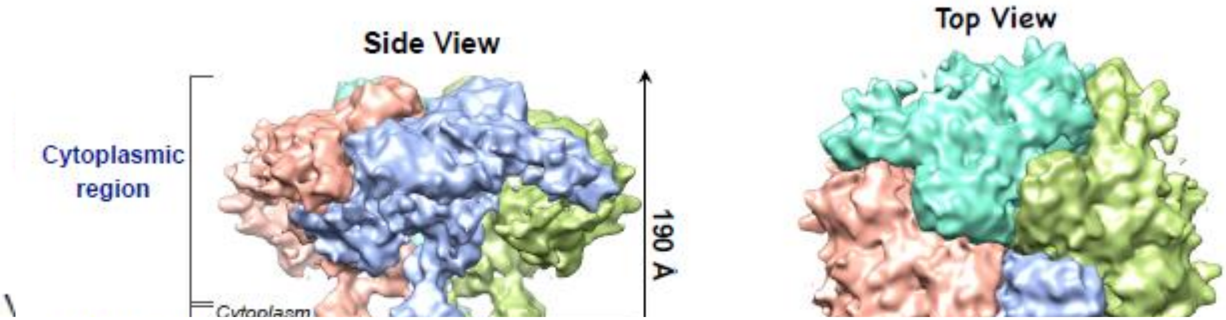

It is easy to obtain a solution where your reprojections can seem to appear consistent with your data, but are not representative of the sample.

There are many steps in processing which can go wrong, and which depend on decisions made by the user (e.g. which classes/images are “good”)

Due to the low SNR, it can be very difficult, or impossible to generate a good solution from an initial bad solution.

It is easy to be tempted to interpret noise as signal . (All of these wrong structures attempted to fit crystal structures into their density, for example).

Q.-X. Jiang et al. (2003)   *Serysheva et al. (2003)*   *C. Sato et al. (2004)*