Retrieval of missing information in 2D-Electron Crystallography

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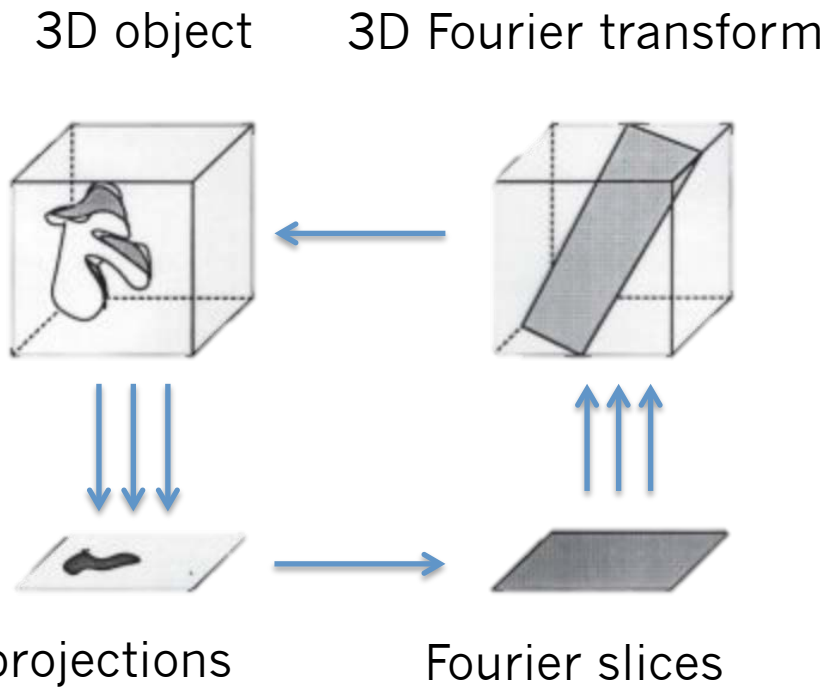
C-CINA

2DX
2D Electron Crystallography
Image Processing Suite

MISSING CONE

2D to 3D

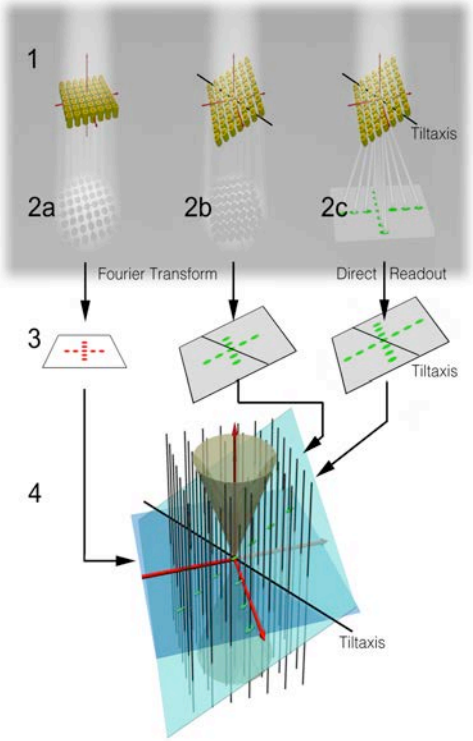
- Central projection theorem



2D to 3D

Merge non-titled and tilted datasets

Fill 3D Fourier space



Missing cone

A void of data in the Fourier transform which is of the shape of cone

Images can be recorded only up to a certain tilt angle (typically 60°)

- Sample thickness increases
- Sample movements
- Lack of flatness
- Correcting for defocus

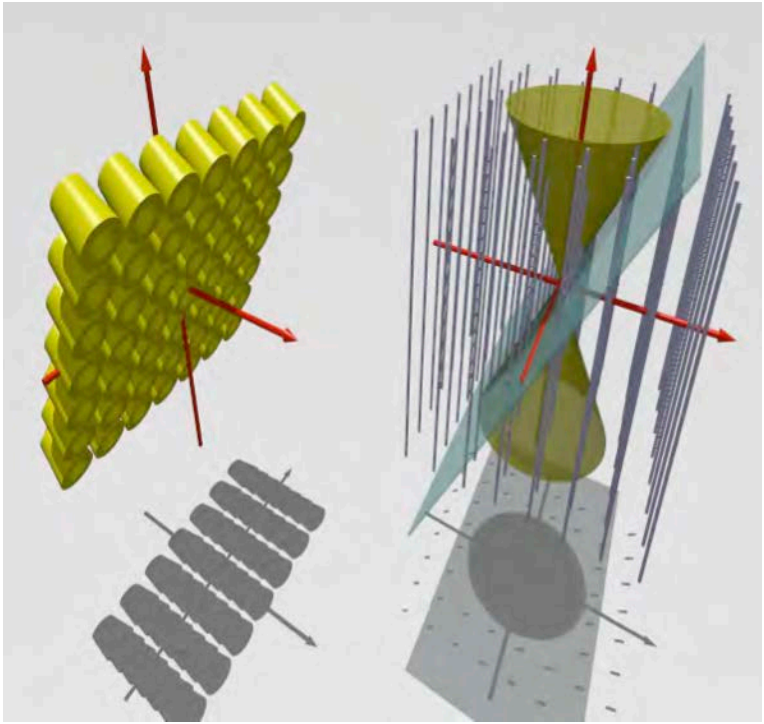
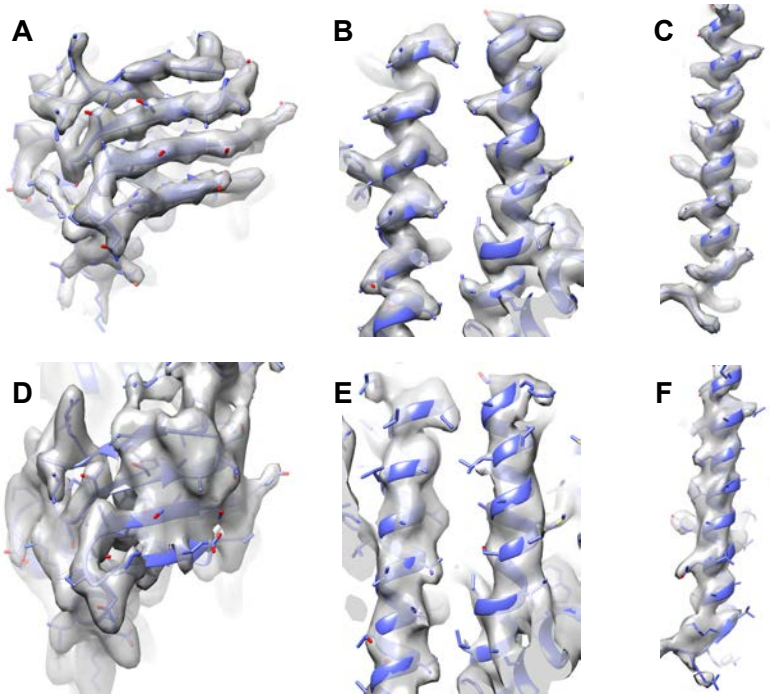


Illustration of missing cone

5Å atomic model map

with missing cone



Problem statement and Algorithm

THEORY

Problem statement

Signal reconstruction problem

Given a part of of signal

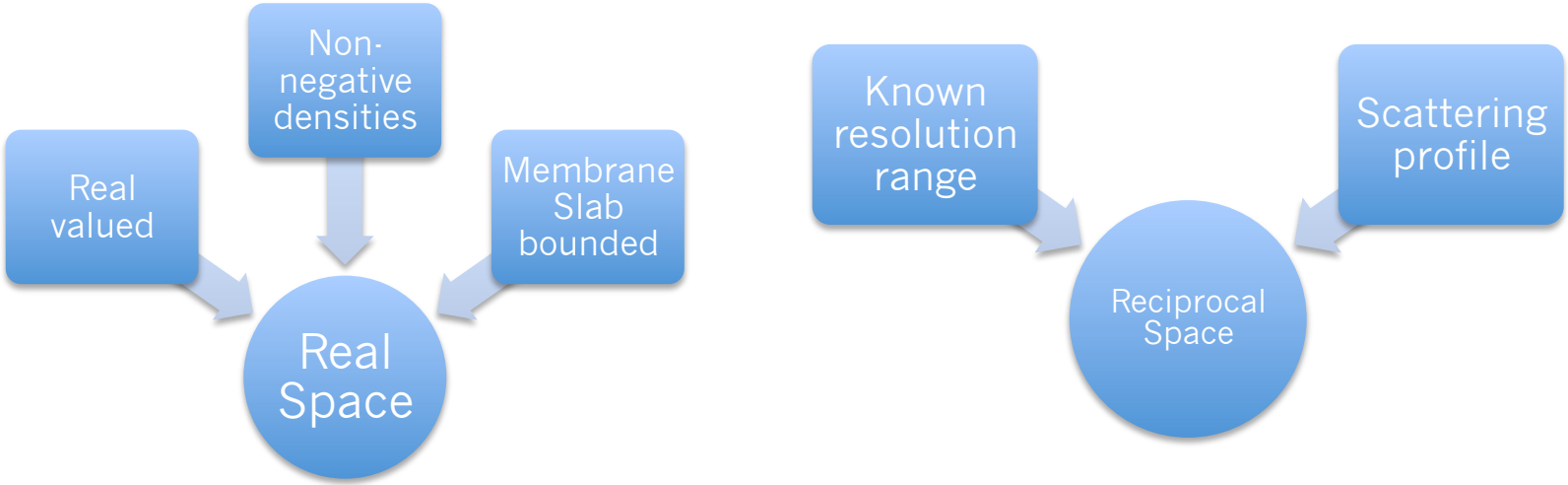
(Fourier transform of the object)

Calculate remaining signal

Using additional information about the target object

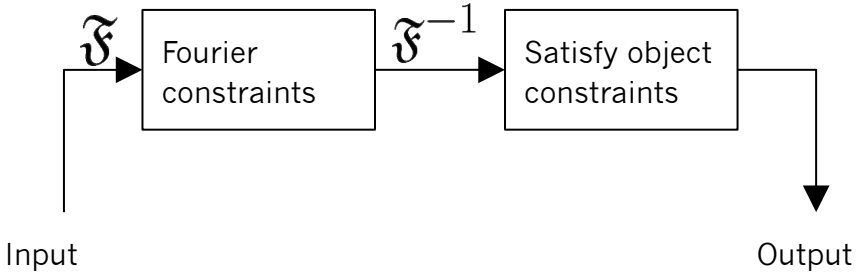
Key Idea

Apply the knowledge/constraints available:



Iteration schema

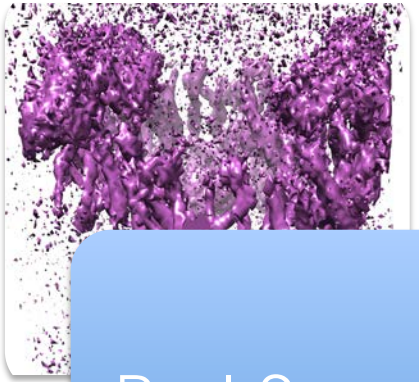
$$Given : s_n$$
$$s'_n = P_F(\mathfrak{F}(s_n))$$
$$s_{n+1} = P_O(\mathfrak{F}^{-1}(s'_n))$$



Gets an estimate of the object!

SHRINKWRAP OPTIMIZATION

Shrinkwrap algorithm

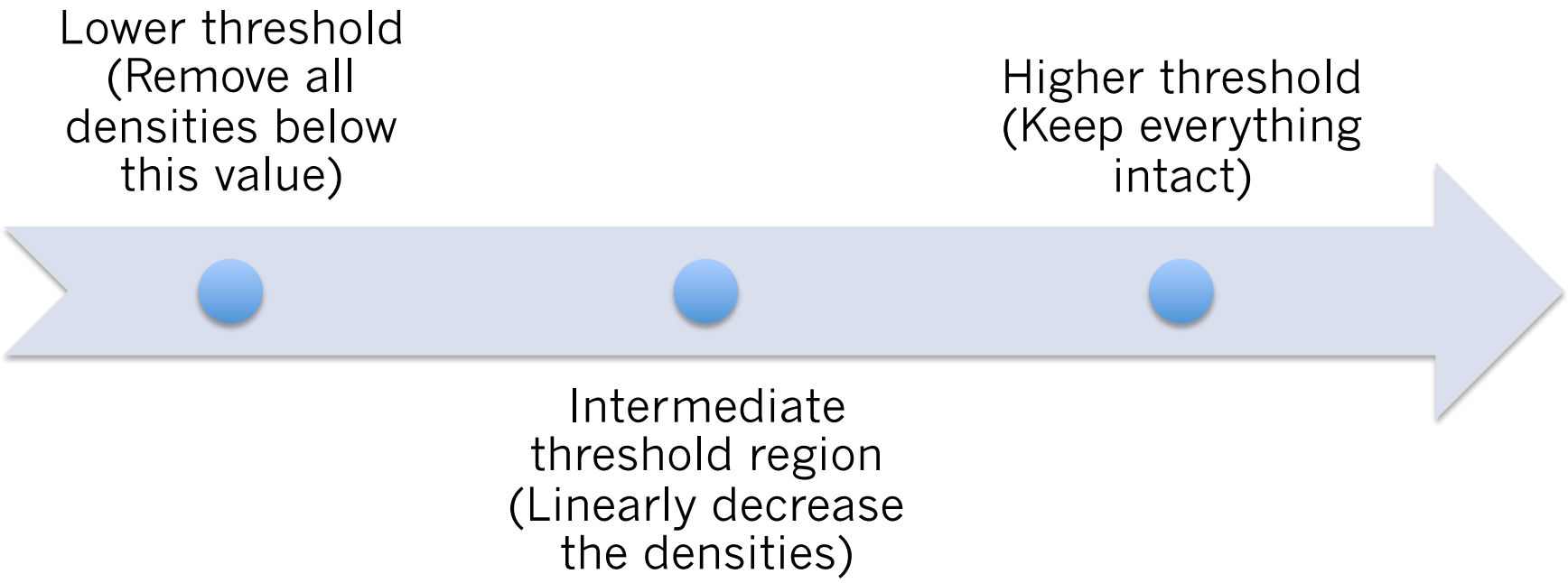


Real Space Volume

Low passed envelope

Density thresholded mask/ support

Modified shrinkwrap algorithm



Modified shrinkwrap algorithm

Advantages:

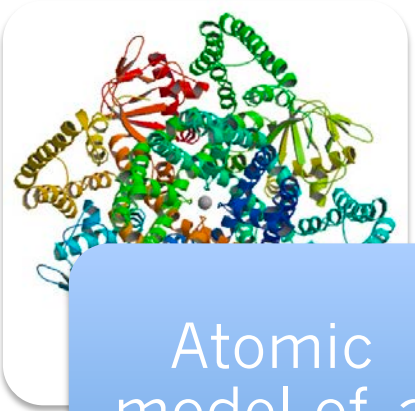
Controls sudden increase in the energy

Reduces the risks of assumption that the densities can be labeled either noise or signal!

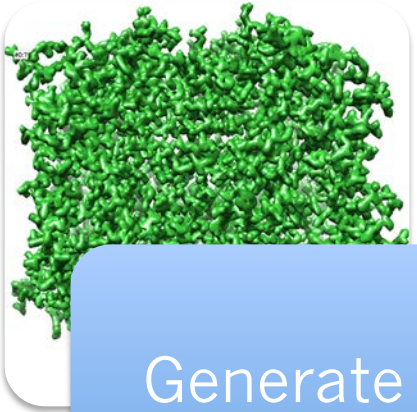
Algorithm applied on a simulated dataset

SIMULATIONS

Setup



Atomic model of a protein complex

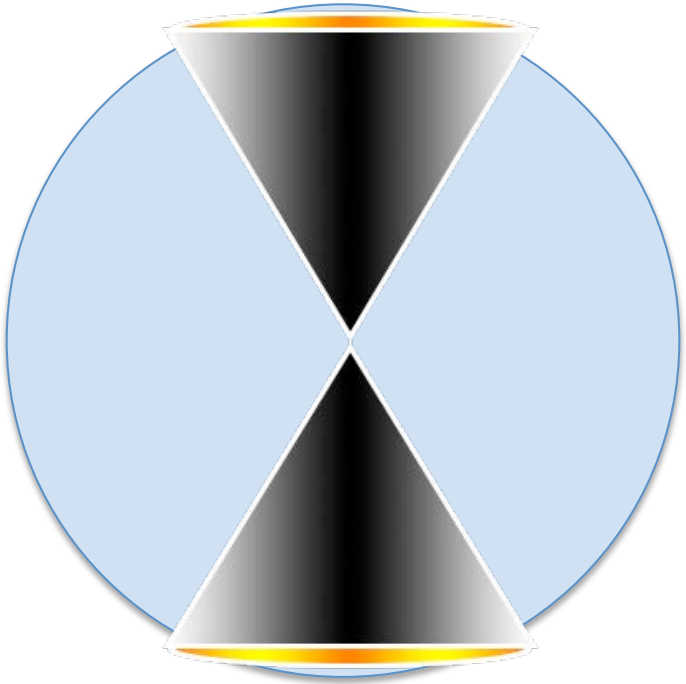


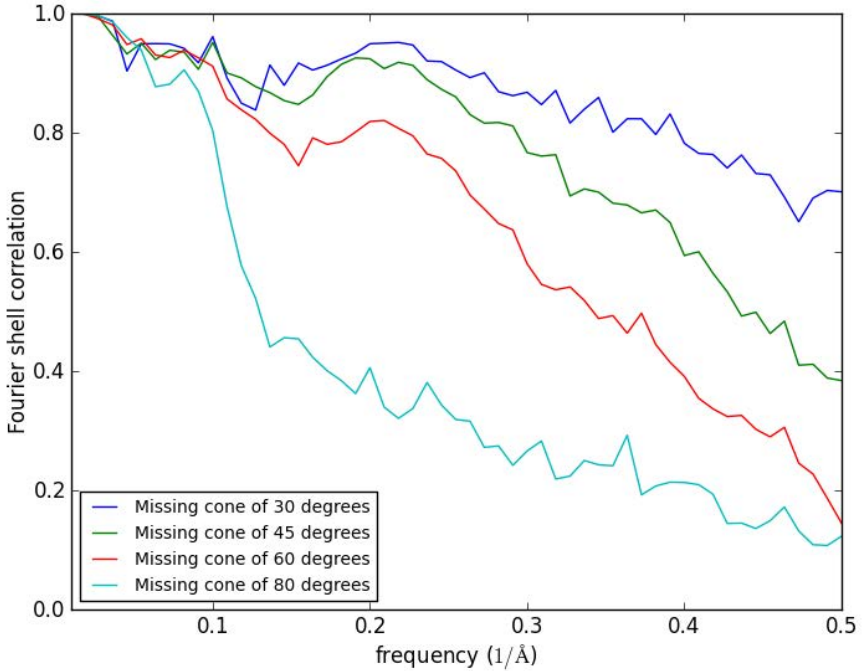
Generate density map

Fourier transform to get the initial 3D data

Retrieving missing cone

- A cone was cut from Fourier space
- The degree of cut was varied from 30^{o} to 80^{o}



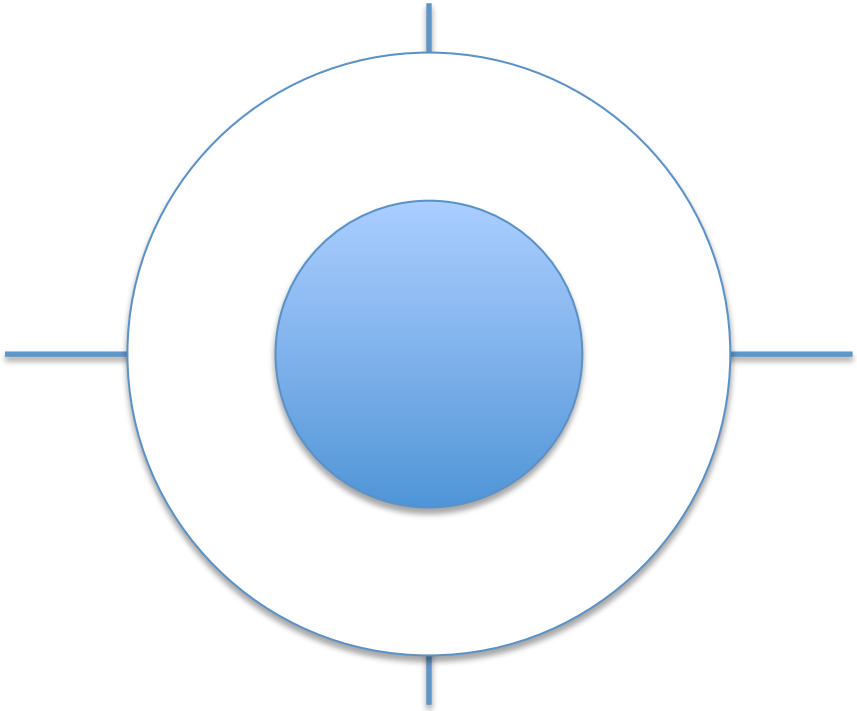


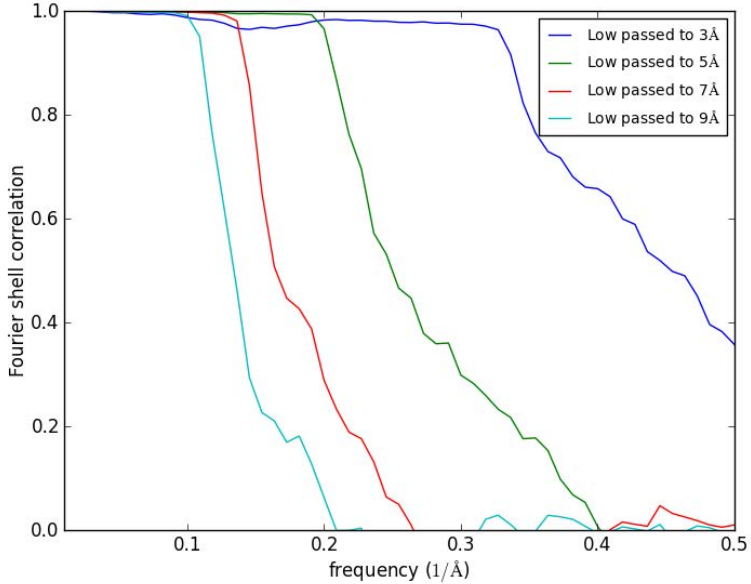
Retrieving missing cone

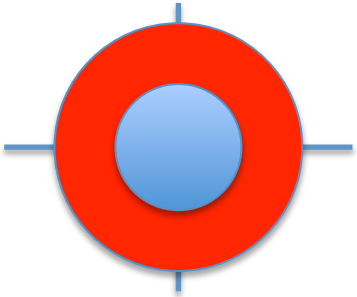
Plot of FSC between the original cones and the recovered cones of various angles. In general the low resolution data is preserved even for high cuts.

Performance at high resolution

- Delete the high resolution data by low pass filtering
- Compare the produced results with the original data







Performance at high resolution

The plot shows FSC curves between the original and the recovered Fourier volumes.

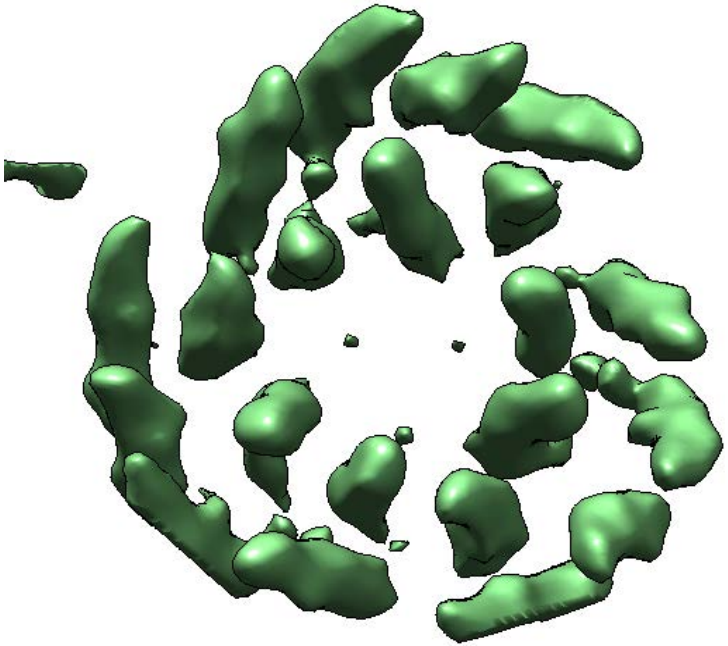
Algorithm applied to experimental 2D crystallogarphic datasets

EXPERIMENTAL DATASET

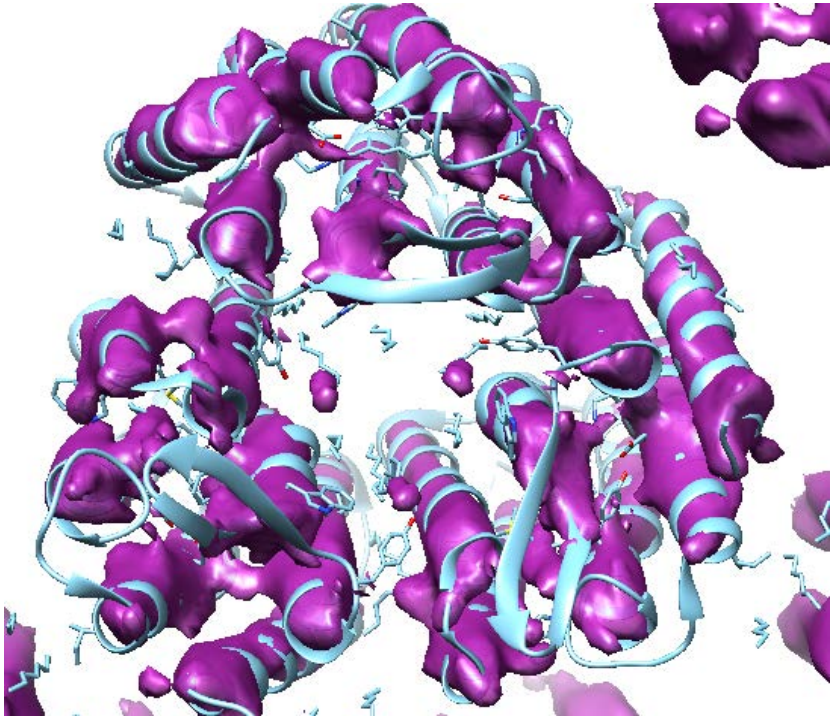
Bacteriorhodopsin dataset

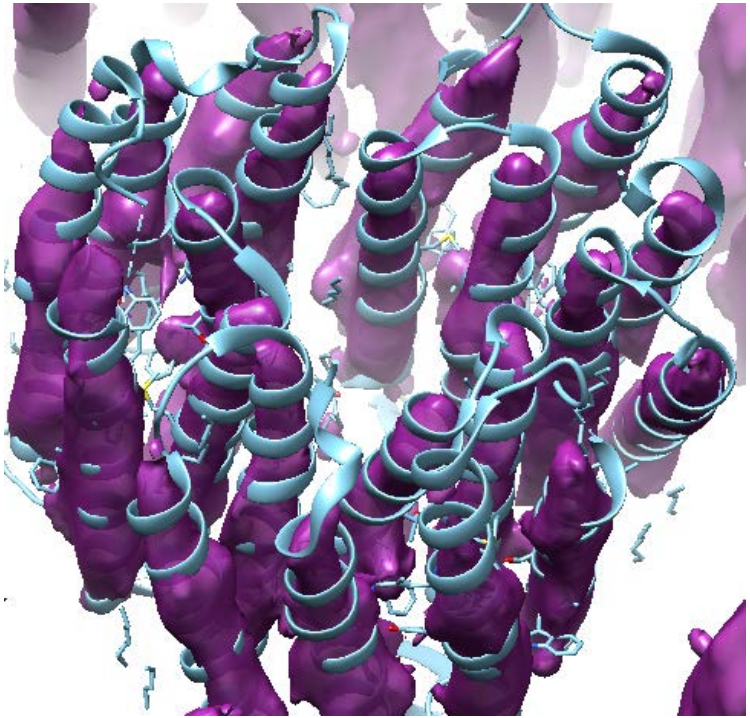
- A tilt-limited reconstruction using nominal amount of images (33) was made
- Algorithm applied and compared correlation with atomic model 3NS0

Raw 3D reconstruction

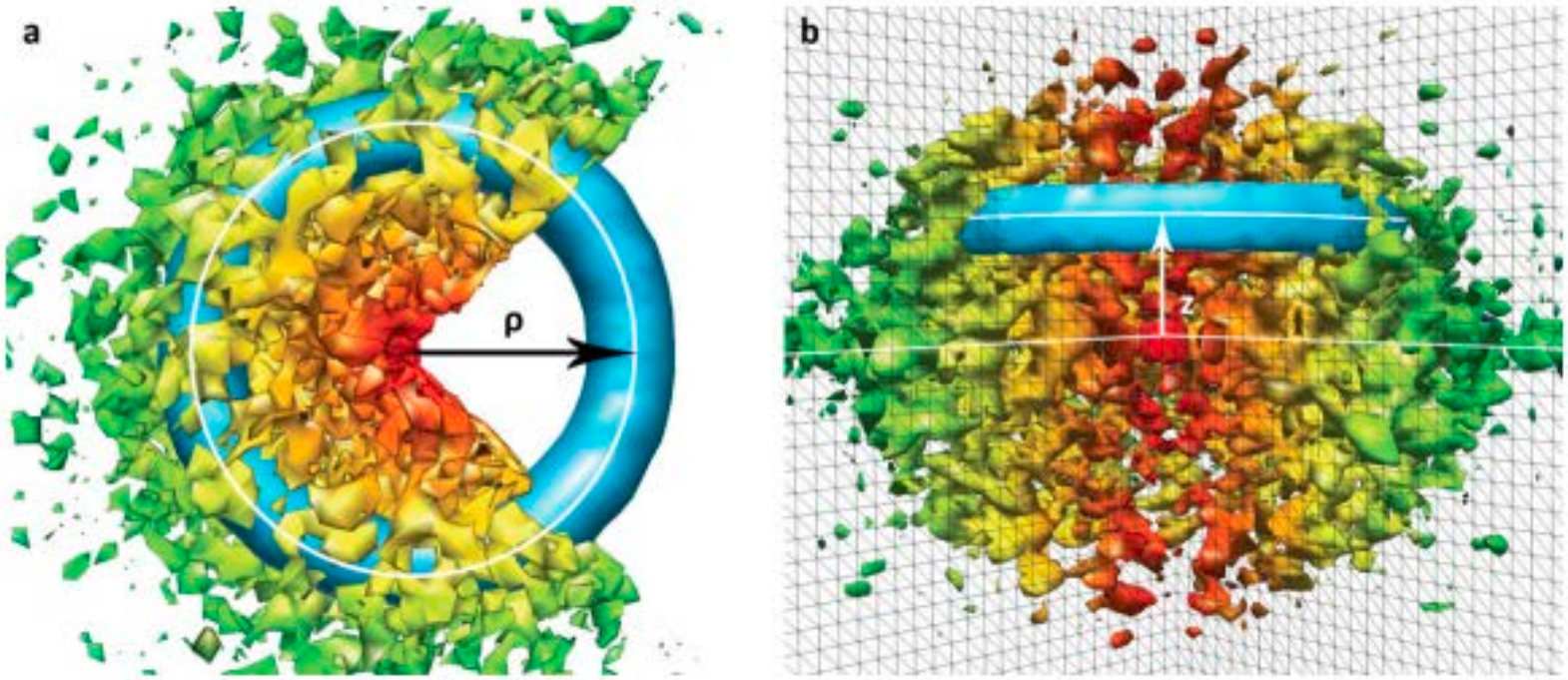


Refined map

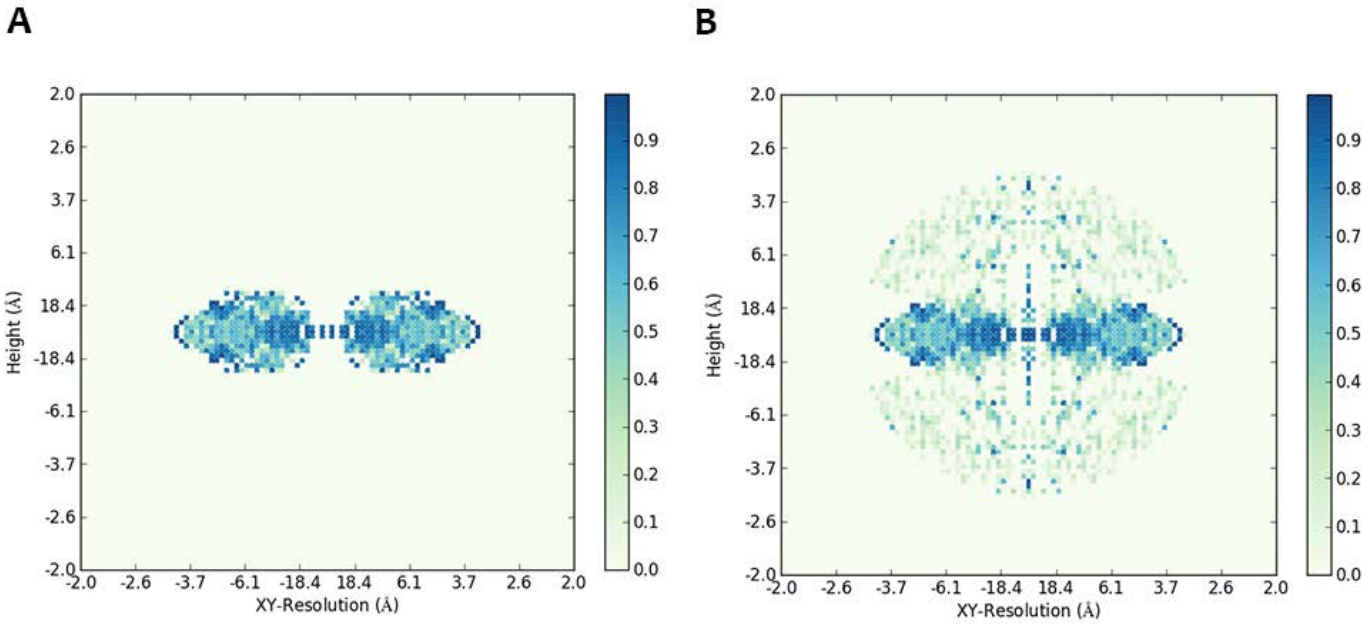




Cylindrical ring correlation (CRC)



bR raw and refined CRC



Summary

Electron density maps generated by 2D electron microscopy are deficit of data in reciprocal space

We present an easy to implement iterative algorithm to generate the missing data in Fourier space

The algorithm relies on applying constraints in orthogonal object and reciprocal space

We apply the algorithm to a simulated dataset and an experimental dataset where we observe the reproducibility of missing data