

Participate in the Practical Session

IF YOU DID NOT REGISTER, PLEASE GO TO:

http://ncmi.bcm.tmc.edu/ncmi/events/workshops/workshops_7/participant_really

- 48 PC's in the computer lab
- your laptop with Linux (or OSX)/EMAN (4 gigs of free disk space)
- your laptop with one of our external drives and a boot CD (EMAN & data preinstalled, limited quantity, USB2 suggested)

Laptop should be at least 1 ghz, 512 megs RAM,
USB2, 1024x768 display (larger is better)

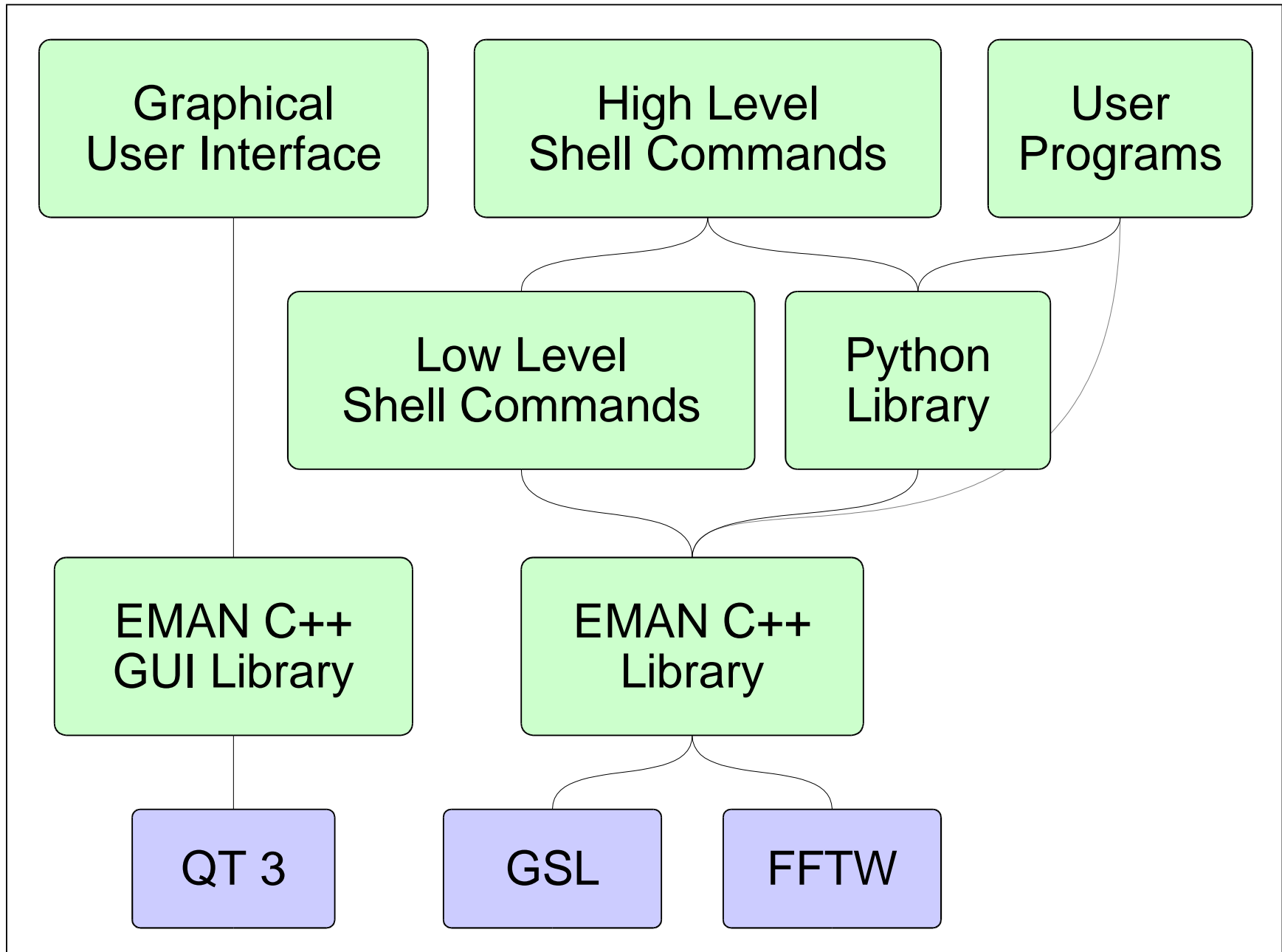


Introduction to EMAN

Steven Ludtke

EMAN Philosophy

- Automate what can be automated
- Make the rest user-friendly (GUI tools)
- Interoperability
- Python scripting for flexibility
- Open Source
- Free



Supported Image Formats (auto byte-order)

- MRC (RW)
- IMAGIC (RW)
- SPIDER (RW)
- PIF (RW)
- ICOS (RW)
- VTK (RW)
- PGM (RW)
- Amira (RW)
- Xplor (W)
- Gatan DM2 (R)
- Gatan DM3 (R)
- TIFF (8/16 bit R)
- Scans-a-lot (R)
- LST (RW)

Supported Euler Conventions

- EMAN (az,alt,phi)
- MRC (theta,phi,omega)
- IMAGIC (alpha,beta,gamma)
- Quaternions (e0,e1,e2,e3)
- Spin-Axis (ang,x,y,z)
- SGI (Q,n1,n2,n3)
- Rotation Matrix (3x3 matrix)

EMAN Conventions

- Euler Angles:

$z, x, z' \rightarrow az, alt, phi$ usually specified as alt, az, phi

- Symmetry:

C_n, D_n - n -fold on z -axis

D_n - 2-fold on x -axis

Oct - 4-fold on z -axis

Icos - 5-fold on z -axis (may be changing?)

Suggested Computer Configuration (March 2005)

- Cost: ~\$1200 + monitor
- Athlon64 3400
 - Outperforms a 3.6 Ghz Xeon/P4 by more than 50%
 - G5's have very poor performance, better compilers ?
- 2+ Gigs of ram
- 250 gig ATA hard drive
- Nvidia GeForce FX or ATI Radeon
- Use 2.6 linux kernel

EMAN Documentation

- $\langle \rangle$ denotes a parameter to fill in, ie $\langle \text{input file} \rangle$
- $[\]$ denotes an optional parameter, ie $[\text{mask}=\langle \text{radius} \rangle]$
- *italics* denote something to be typed into the computer

example:

```
proc2d  $\langle \text{input file} \rangle$   $\langle \text{output file} \rangle$   $[\text{mask}=\langle \text{r} \rangle]$   $[\text{mrc}]$   $[\text{spider}]$   $[\text{pgm}]$ 
```

```
proc2d file.hed file.spi spider mask=22
```

- $\langle \text{program} \rangle$ *help* (won't work with python scripts yet)
- $\langle \text{program} \rangle$ (shows usage information)

GUI

- eman
- boxer
- helixboxer
- ctf^{fit}
- qsegment(/chimera)
- qindex
- glmatrix

- v4
- v2

Non-EMAN Programs

- vis5d+
- chimera

Basic Image Processing

- *iminfo* <file> [all] [stat]
(image information)
- *proc2d* <infile> <outfile> [options]
(generic 2d image processing)
- *proc3d* <infile>
- *proc3d* <infile> <outfile> [options]
(generic 3d image processing)
- *procpdb.py* <infile> <outfile> [options]
(simple PDB file processing)

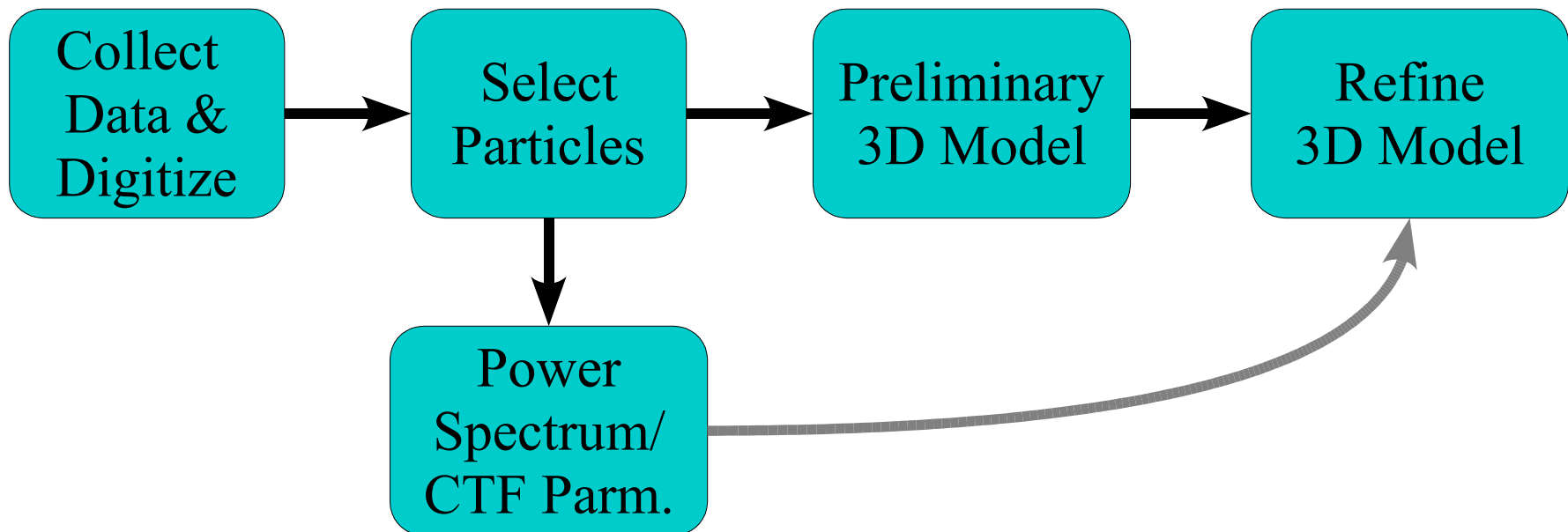
Commands Used in a Reconstruction

- `boxer/batchboxer` - particle selection
- `ctfit/fitctf` - CTF parameter determination
- `applyctf` - CTF phase flipping and parameter assignment
- `proc2d` - Generic 2D image processing
- `lstcat.py` - Generate 'LST' image files to save disk space
- `cenalignint` - Iteratively center particles before using `startcsym`
- `startcsym` - Automatic initial model generation for symmetric particles
- `volume` - Adjust electron density levels
- `proc3d` - Generic 3D image processing
- `refine` - The main command, calls many other commands
- `eotest` - Even/odd data split for resolution assessment (not completely independent)

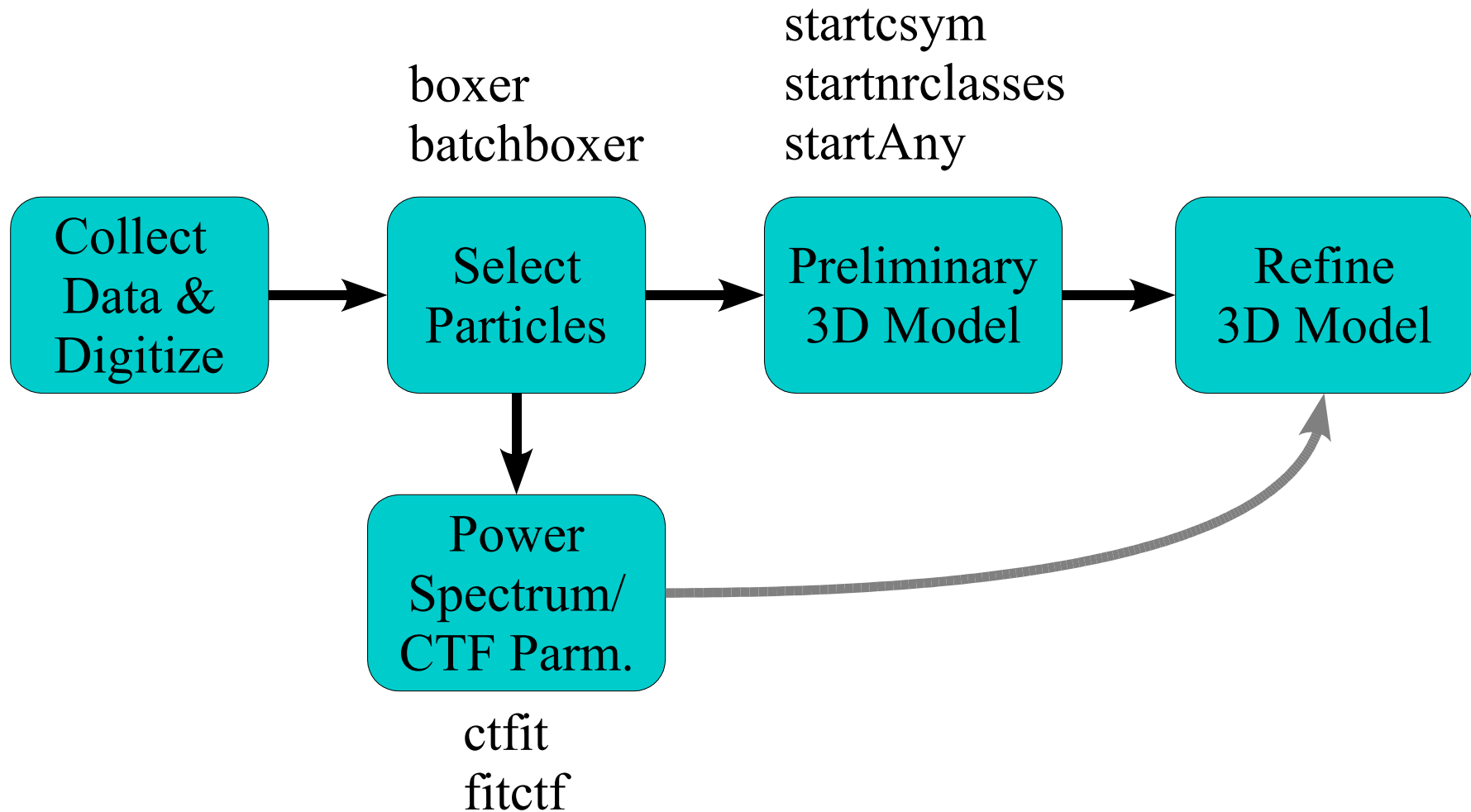
Major Commands Called by *refine*

- `proc2d/proc3d` - generic image processing
- `project3d` - Make projections of a 3D model
- `classesbymra` - Reference-based particle classification
- `classalign1` - Wrapper for `classalign2`
- `classalign2` - Iterative alignment of a set of misaligned 2D particles with CTF correction
- `make3d` - Build a 3D model from 2D particles/averages
- `volume` - Adjust densities for proper isosurface visualization

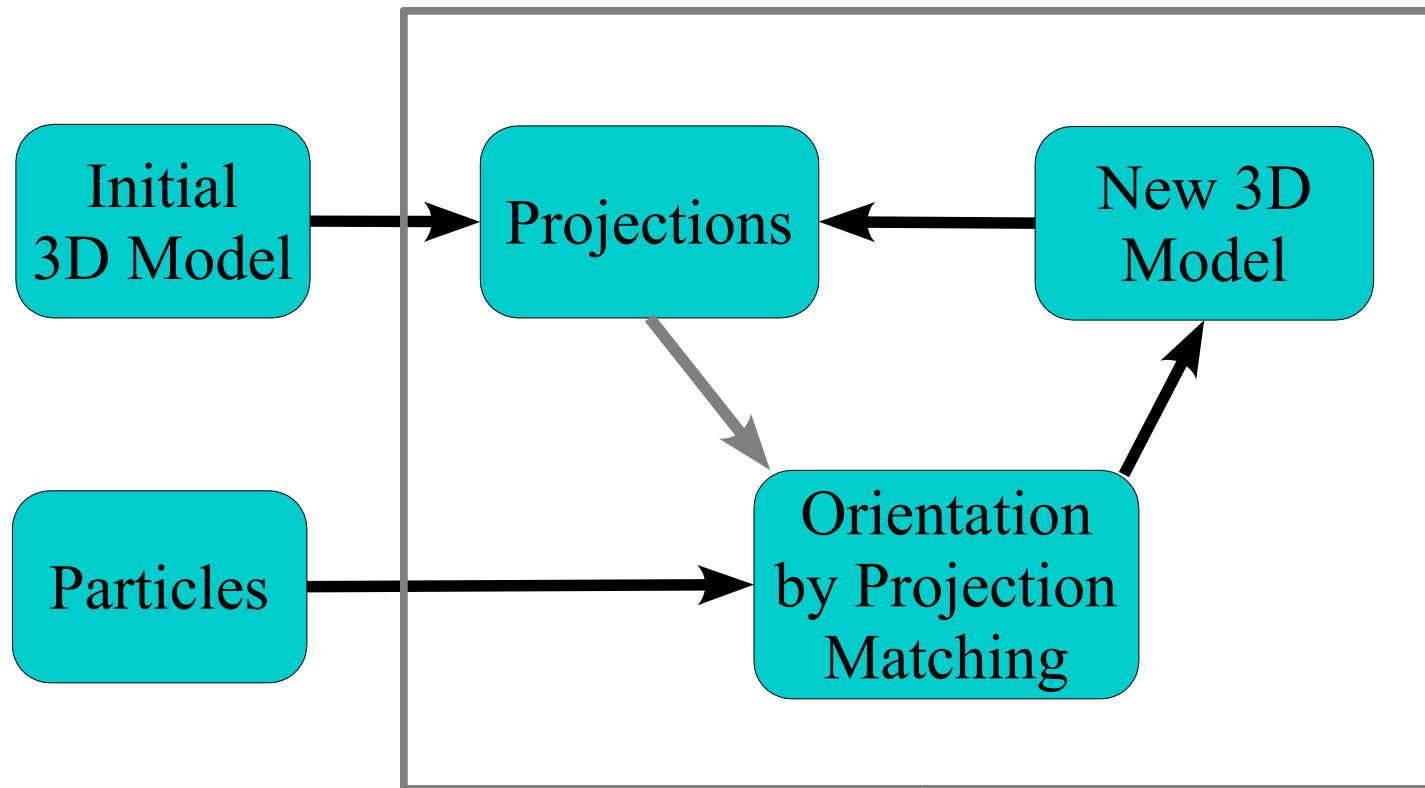
The Reconstruction Process



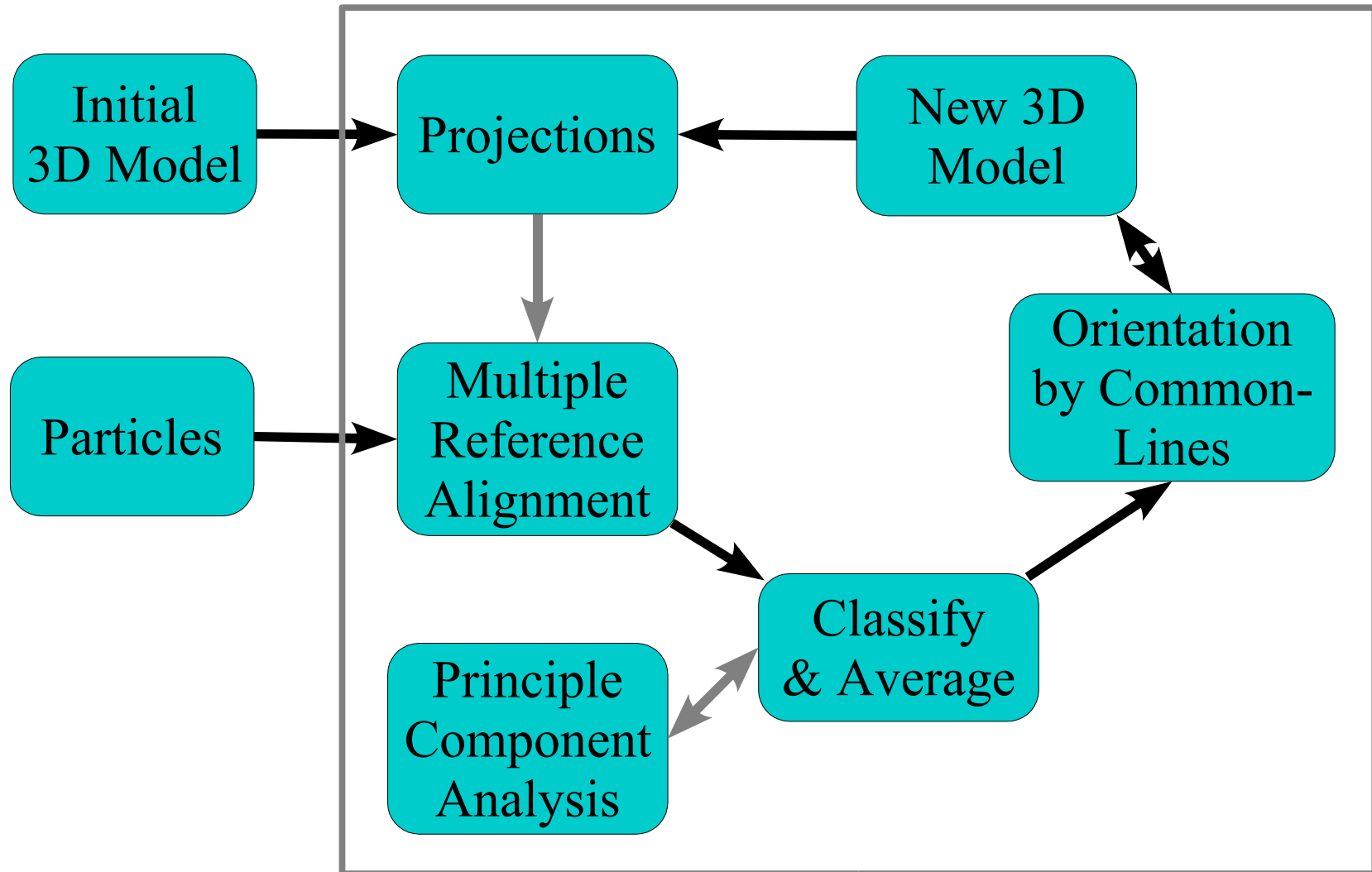
The Reconstruction Process



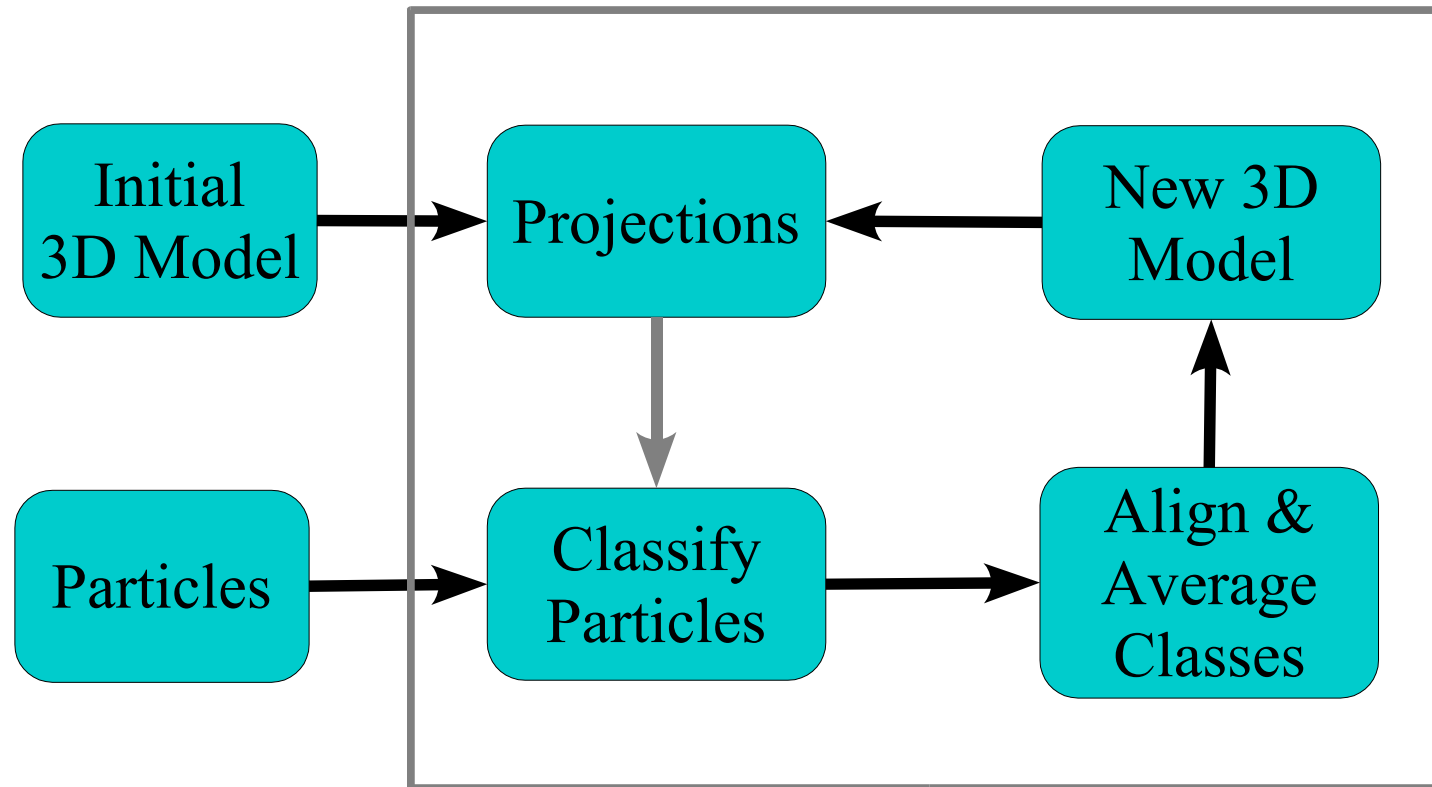
Typical Refinement - Spider



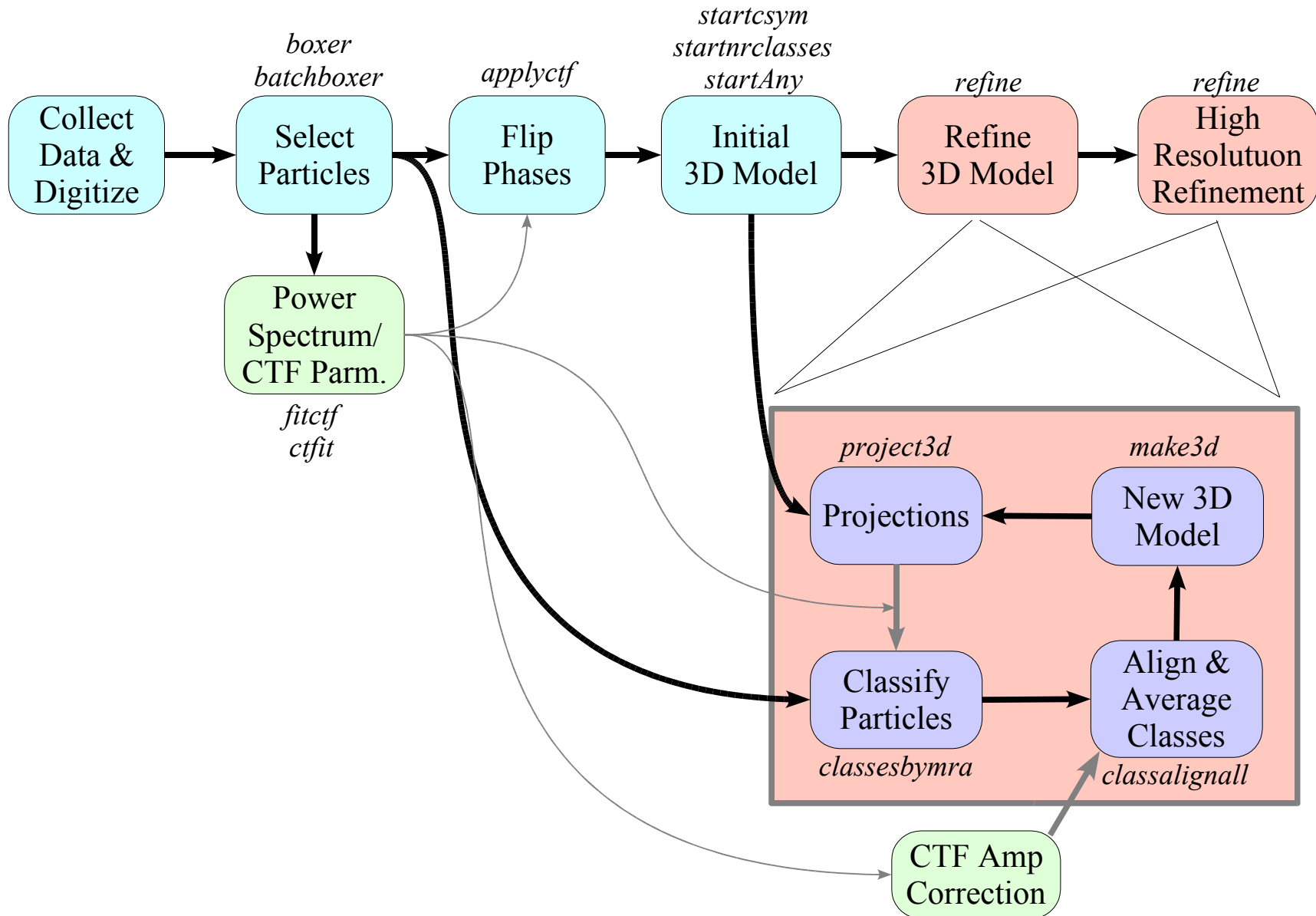
Typical Refinement - Imagic

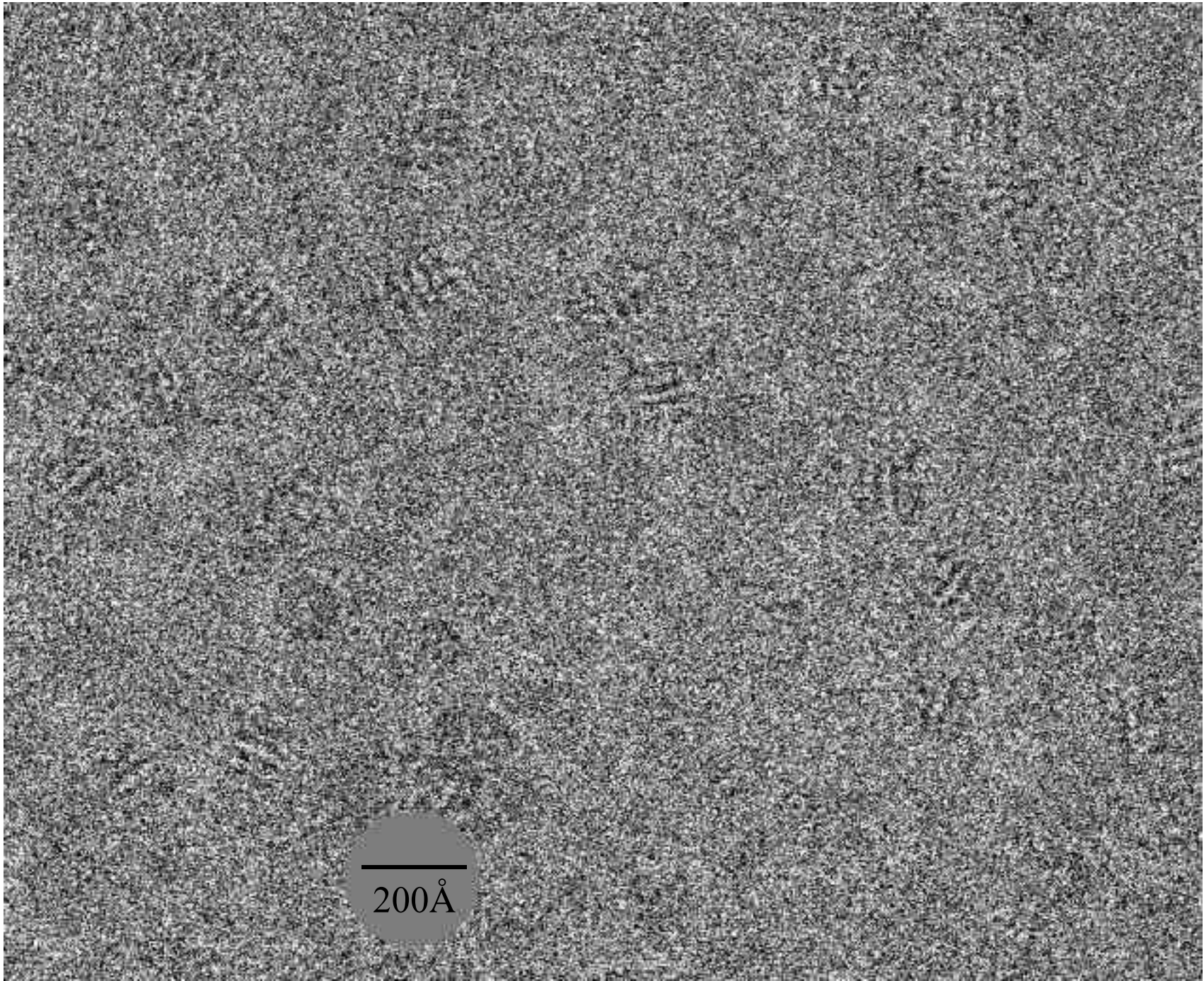


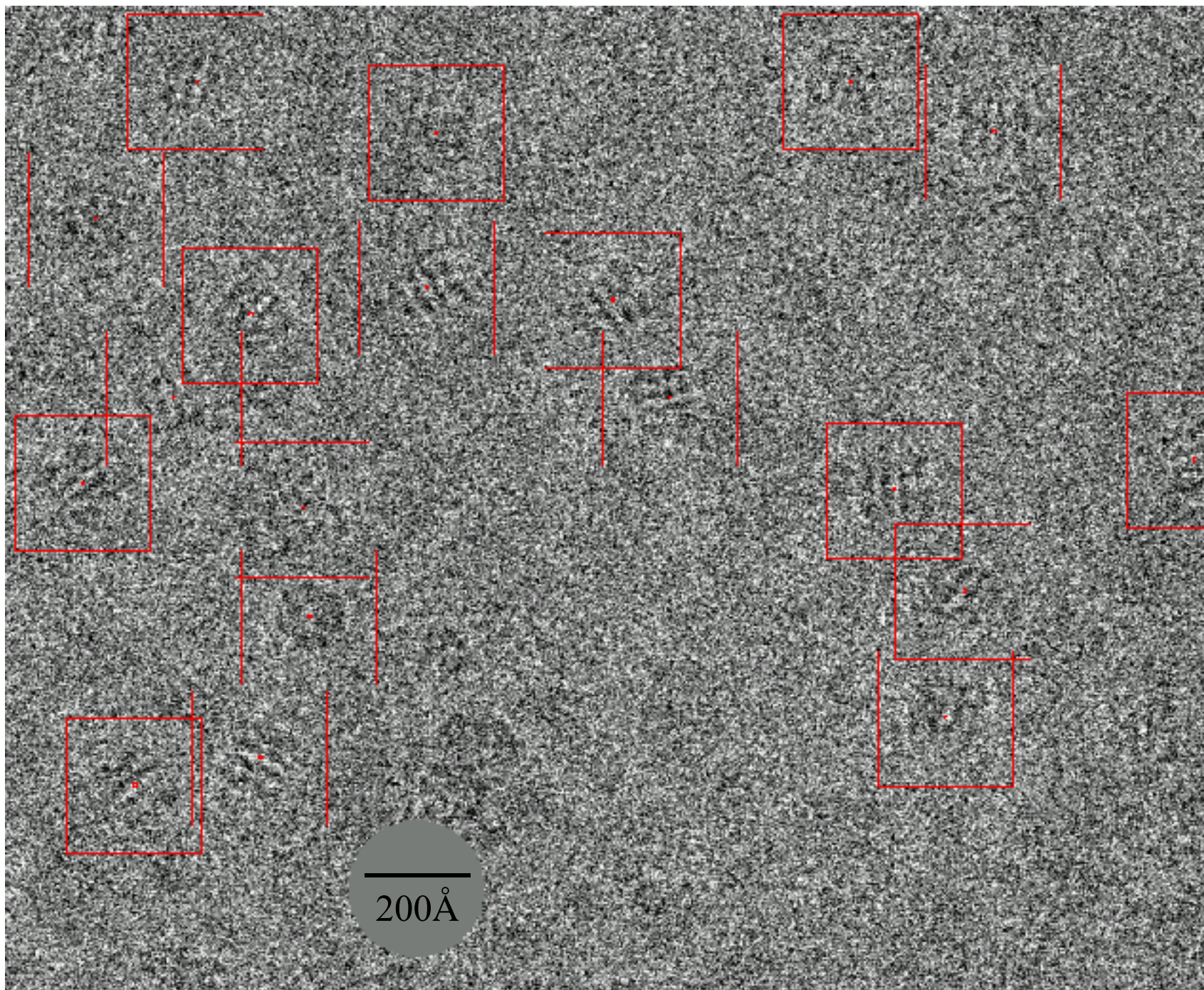
Typical Refinement - EMAN



Typical EMAN Reconstruction Strategy





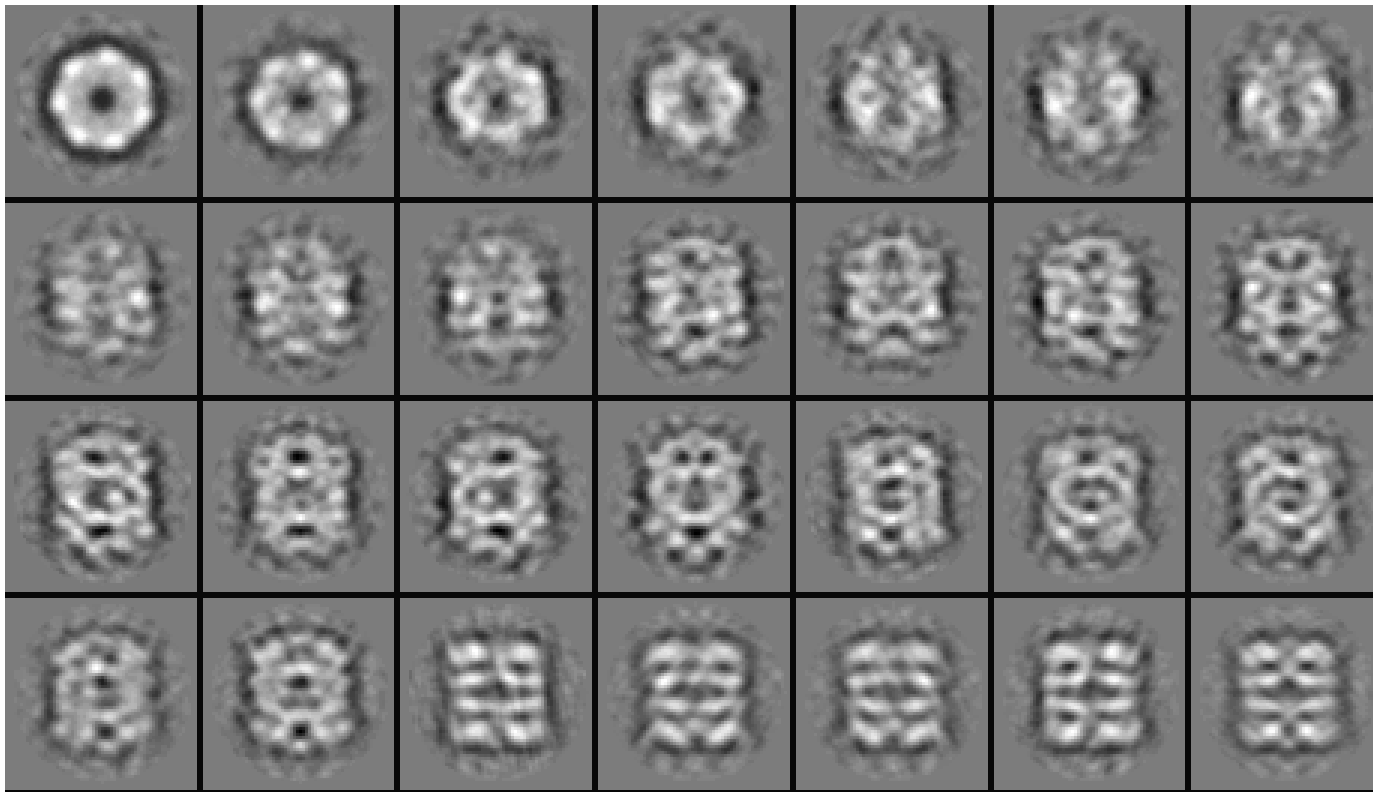


200Å

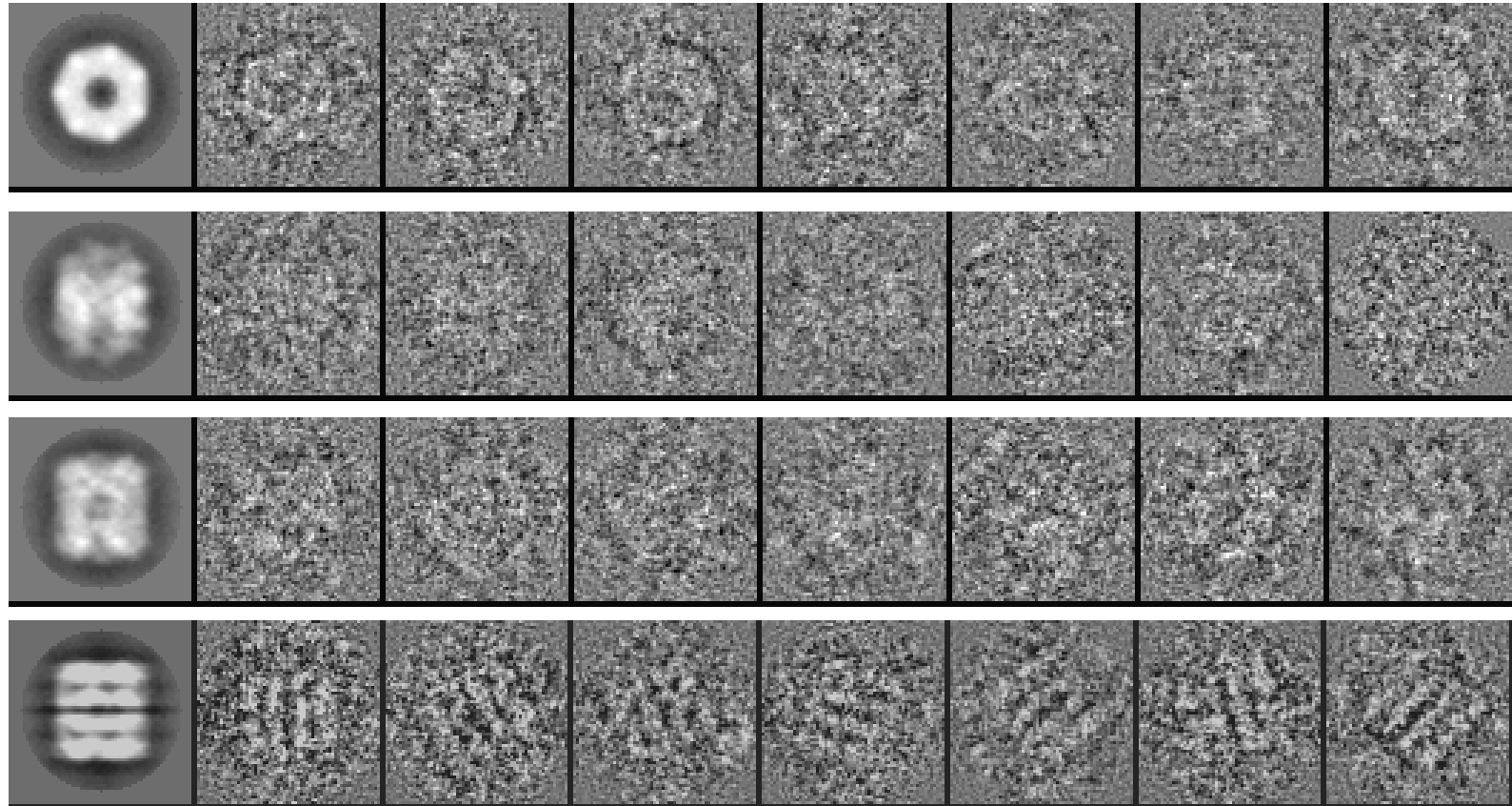
Refine from Gaussian Ellipsoid



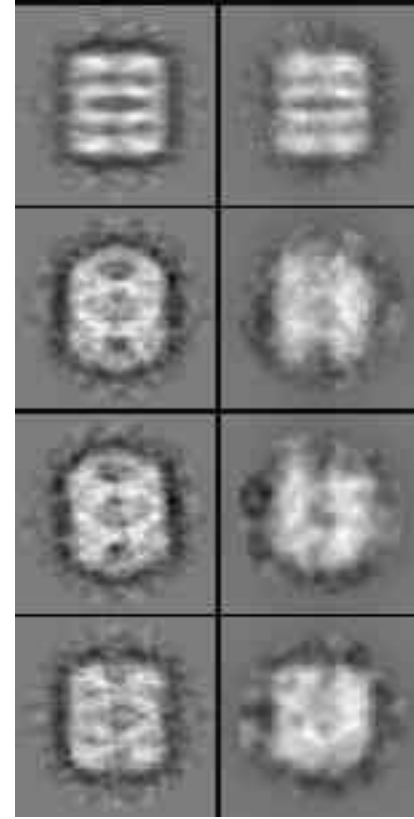
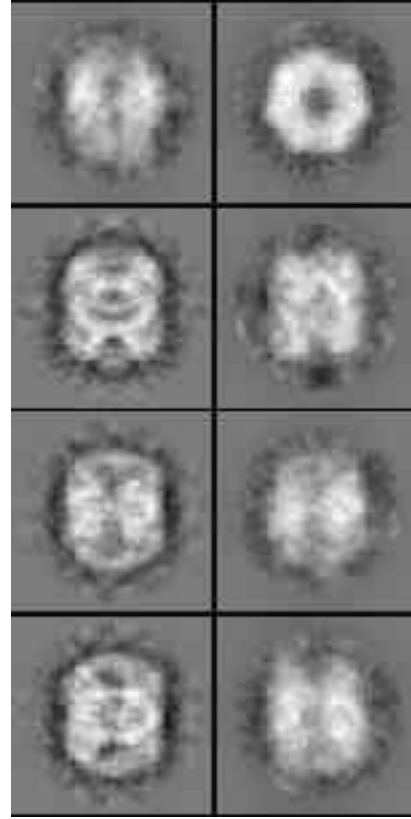
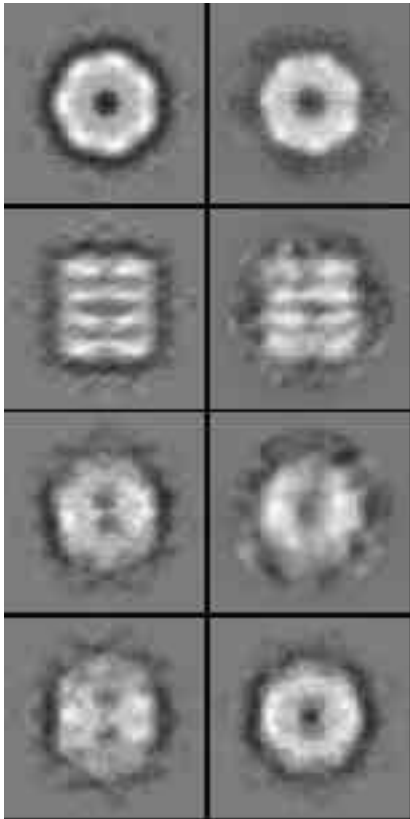
Projections



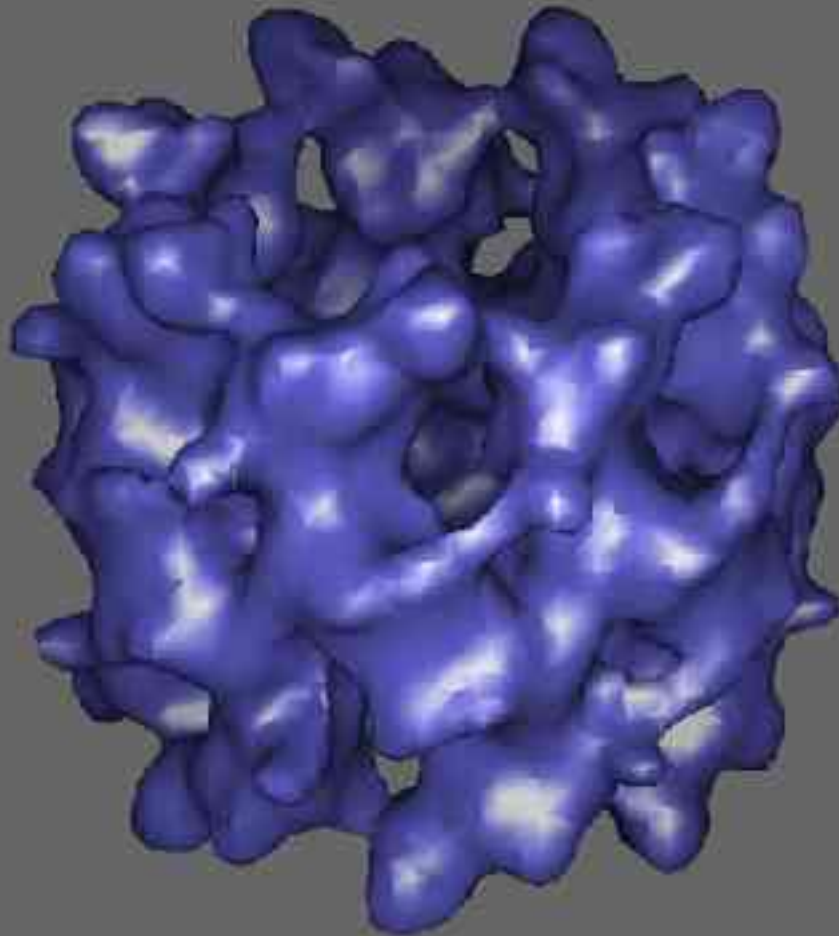
Classification



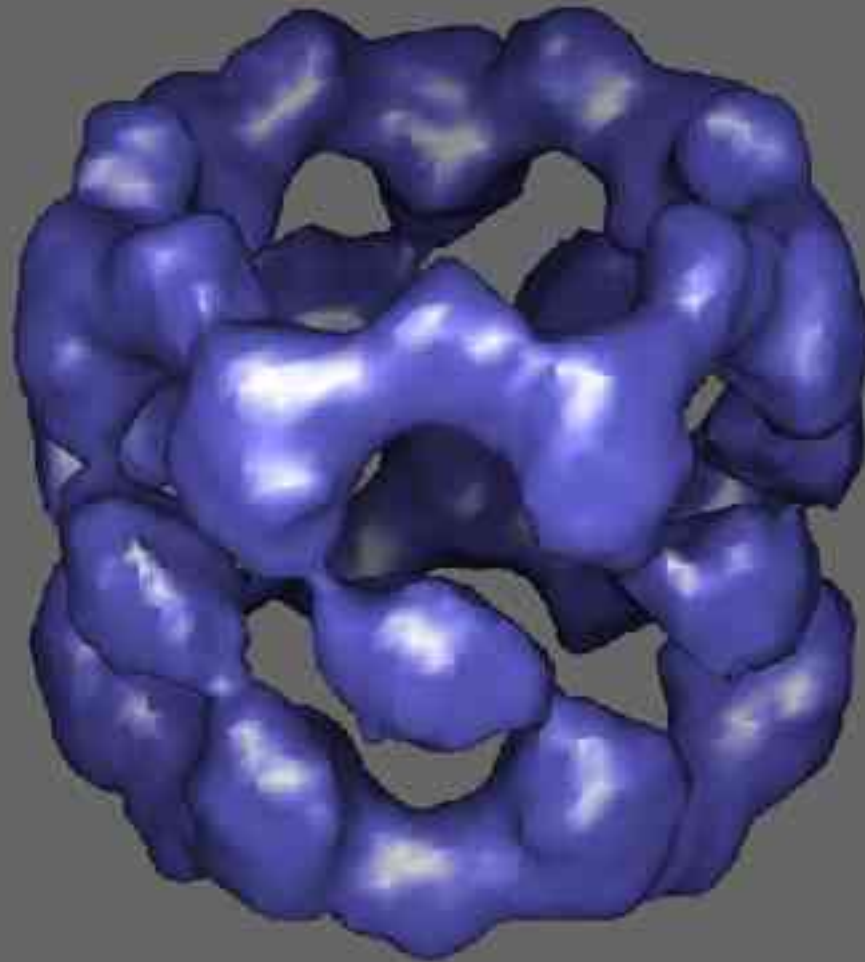
Class Averages



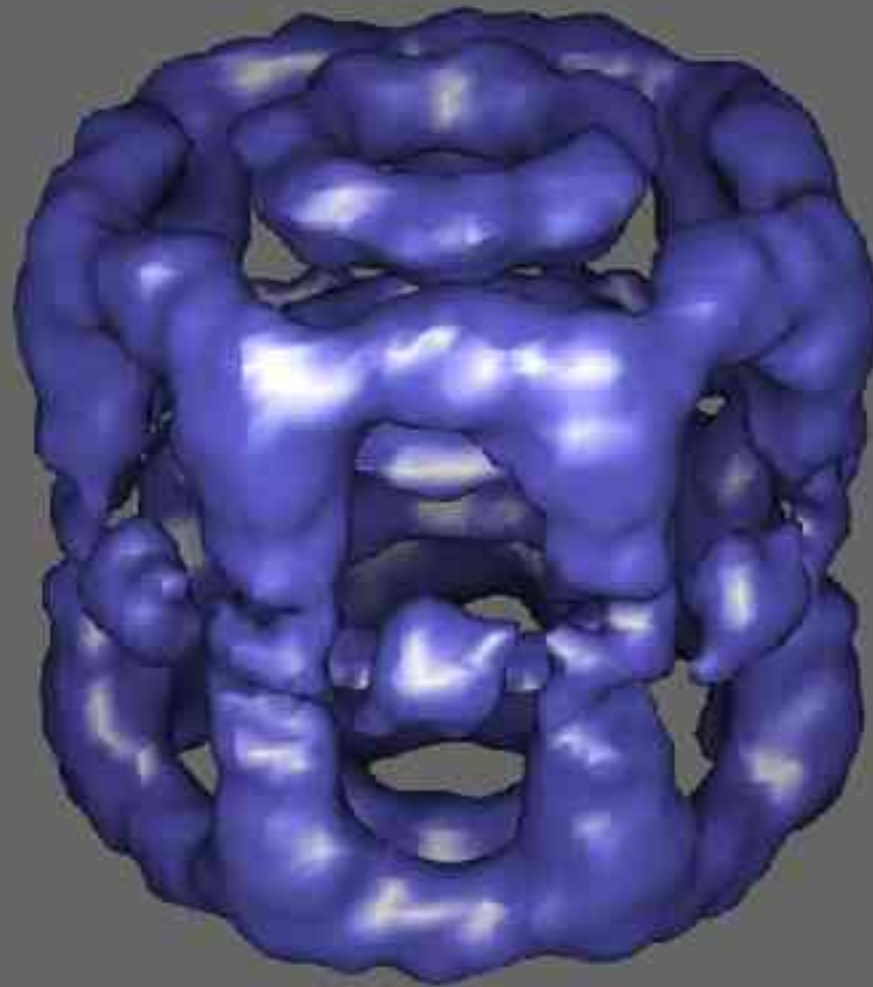
Refine from Gaussian Ellipsoid



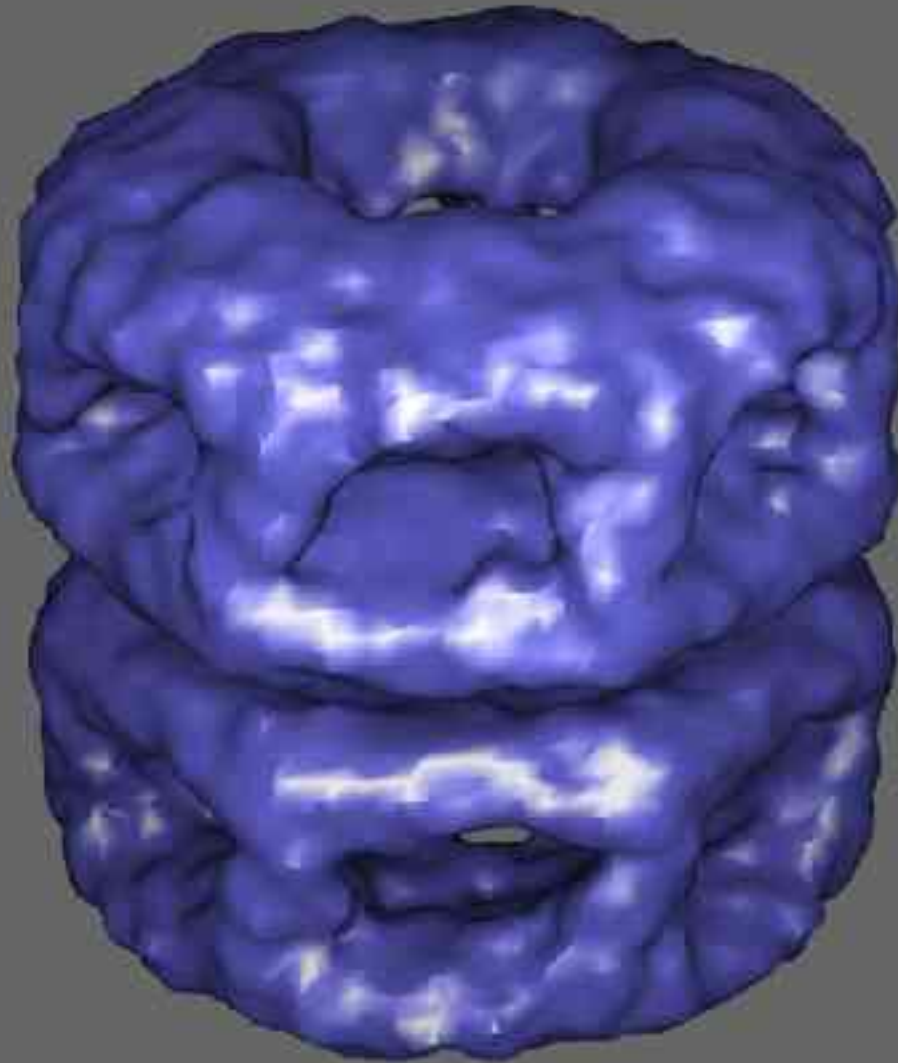
Refine from Gaussian Ellipsoid



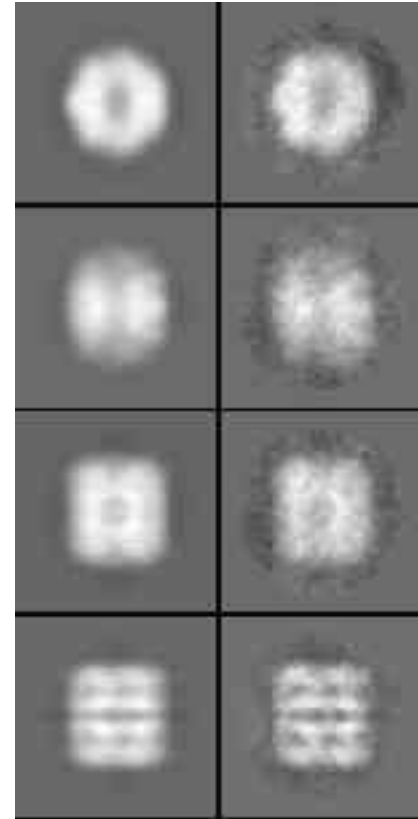
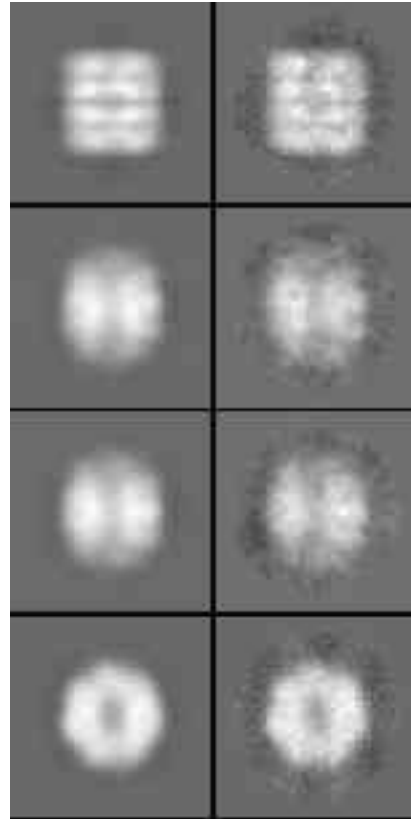
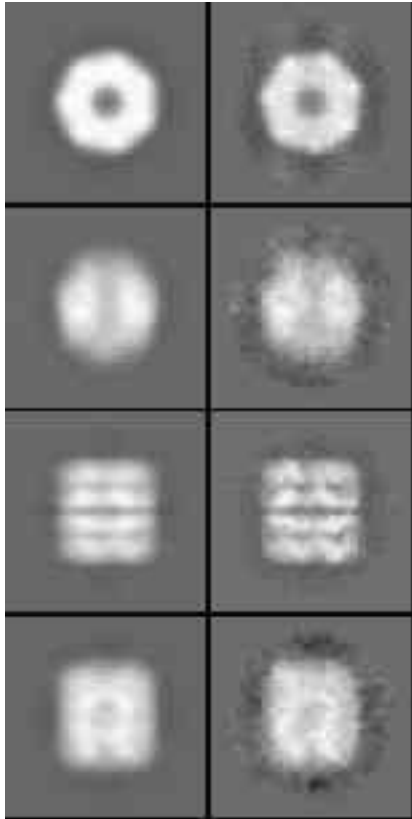
Refine from Gaussian Ellipsoid



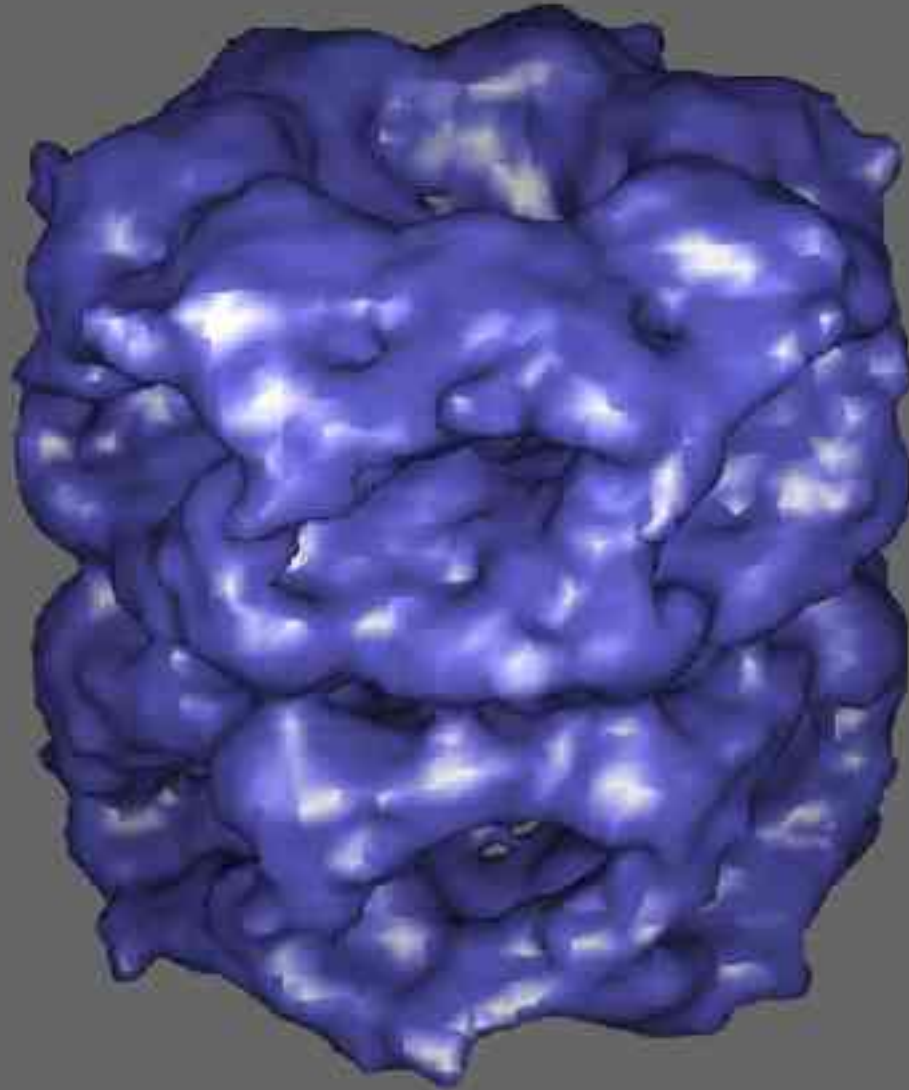
Refine from Gaussian Ellipsoid



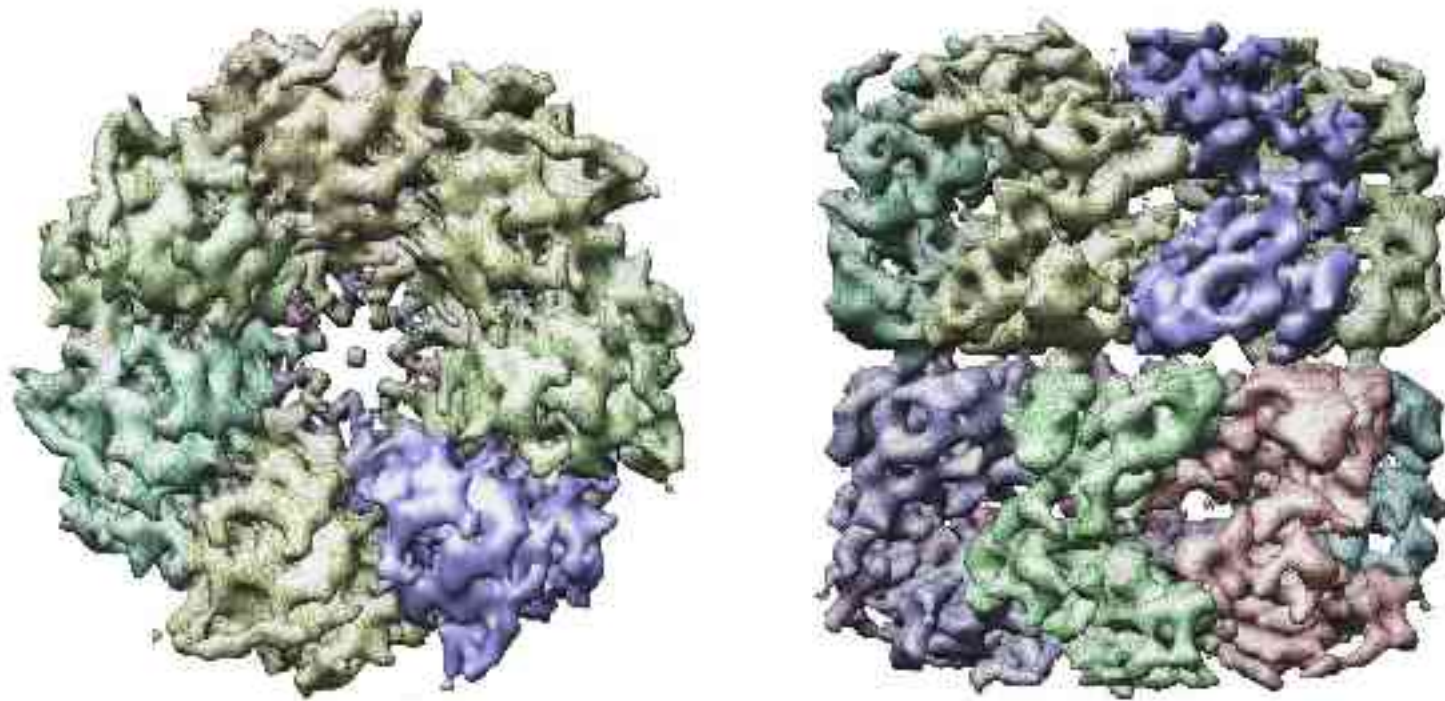
Class Averages



Refine from Gaussian Ellipsoid



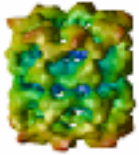
GroEL at 6 Å Resolution



Acknowledgments

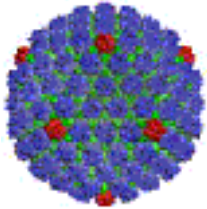
Baylor College of Medicine

- Wah Chiu
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- Dong-Hua Chen



UT SW Medical Center

- David Chuang
- Jiu-Li Song



Thanks to:



National Center for Research Resources
Agouron Institute

Prepare for Demo Session

- Computer lab PC:
log in user 'baylor' password 'EMAN2005'
get accustomed to the account
 - Your preinstalled laptop:
copy the contents of the DVD to your hard drive
chmod -R u+w * (in the directory with the copy)
 - Your laptop, our hard drive
Attach and power up the USB hard drive
Boot from the provided CD
As soon as the boot prompt appears, enter:
knoppix home=/dev/sda1
(if that fails, try)
knoppix26 home=/dev/uba1 (but don't click Faster)
- booting from the CD takes a while, but eventually you should see the workshop web page. Double-click 'Faster'. May have to reboot if it fails.