



EMAN

Tutorial Session #2

Steve Ludtke

Quick Initial Refinement

- `cd ../stage4`
- `cat 000script`
- `./000script`
- `wait a while`
- `eman`
- `look at:`
- `classes.*.img, x.*.mrc`
- `Cp ~/public/anim.py .`
- `http://ncmi.bcm.tmc.edu/tmp/anim.py`

High Resolution Refinement

- `cd ../stage5`
- `cat 000script`
- `precomputed (looong job)`
- `eman`
- `look at:`
- `classes.*.img, x.*.mrc`
- `analysis -> convergence`
- `chimera animscript.py`
-
- `apix*box/32`

Measures of Resolution

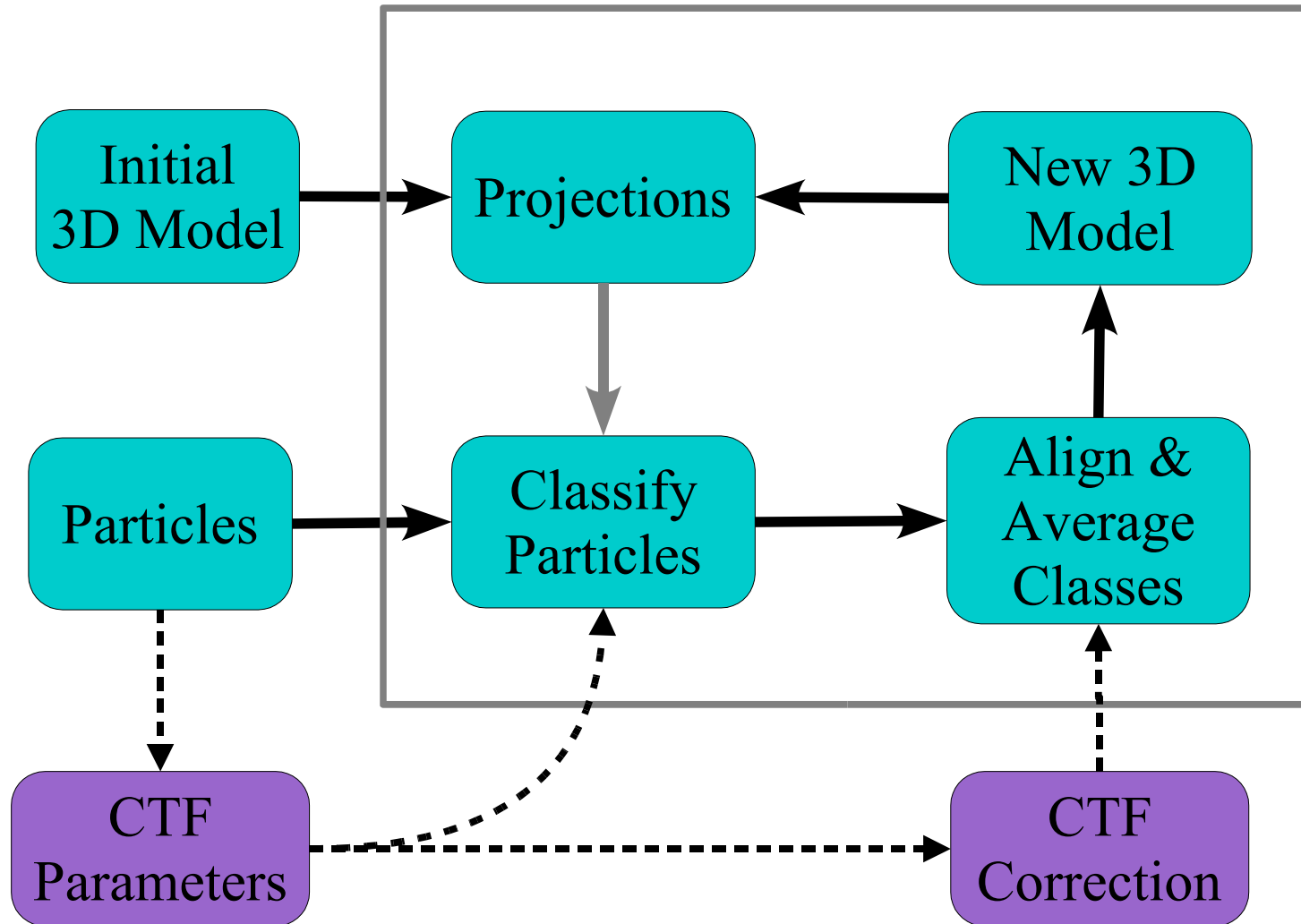
- Masking demo
- Rotational averaging
- Eotest vs split refinement

Simple Docking and Segmentation

- *cd ../stage6*
- *./000script*
- *chimera fh.0.ent shrunk.mrc ../stage5/threed.8a.mrc*
- *./000script2*
- *use qsegment*
- *use chimera*

Easier and better ways of doing this will be discussed later in the workshop.

CTF Correction - EMAN



Possible Corrections

- Phase flipping
 - Astigmatism
- Amplitude contrast correction
- Envelope function correction
 - Drift
 - Multi-parameter envelope
- Inter-micrograph weighting

CTF Parameter Determination

- *fitctf* - only if you have a real or simulated structure factor curve
- *ctfit* - check results, or fit if you don't have a structure factor, evaluate micrograph quality
- *ctfit* used with 3 micrographs can be used to produce a pseudo-structure factor for fitting

Initial Model Bias

- `cd data/model_bias/GroEL.stage4gaus`
- `eman`
- `Analysis -> Convergence`
- look at `x*.mrc`, `classes*.mrc`

Initial Model Bias

- `cd ~/data/model_bias/KIF.sim/stage1`
- `./000script`
- `cat 000script` (in a different window)
- when done, look at `iter.final.img`
- `cat 000script2`
- pick a method and make an initial model

Initial Model Bias

- make sure your model is threed.0a.mrc
- `cd ../stage2`
- `edit 000script`
- remove `proc=52`
- `./000script`
- This will run overnight, those with laptops might start it before bed and let it run until morning