

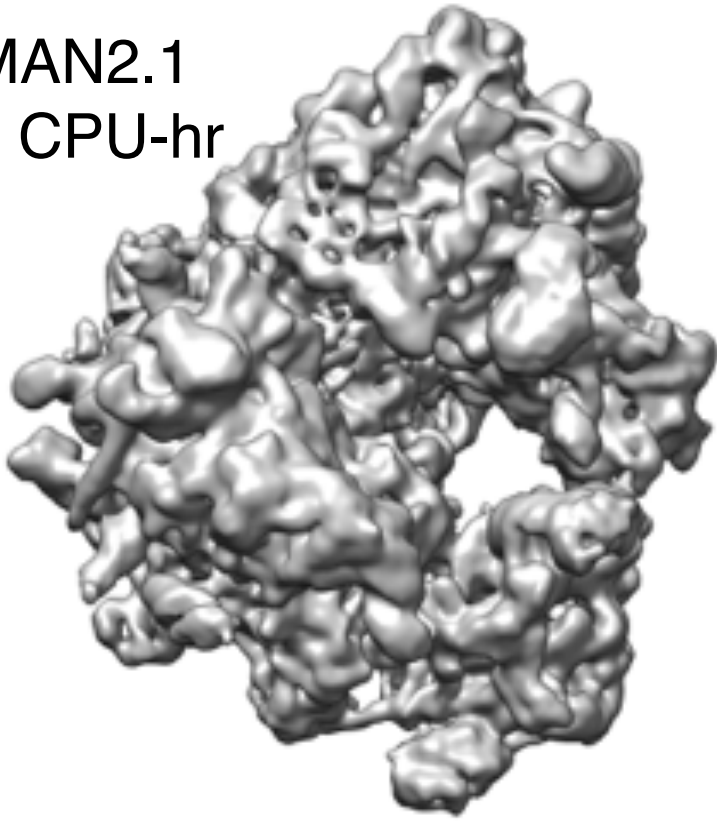
Welcome to the
7th Biennial

NCMI Workshop on Single
Particle Reconstruction, Structural
Variability and Modeling

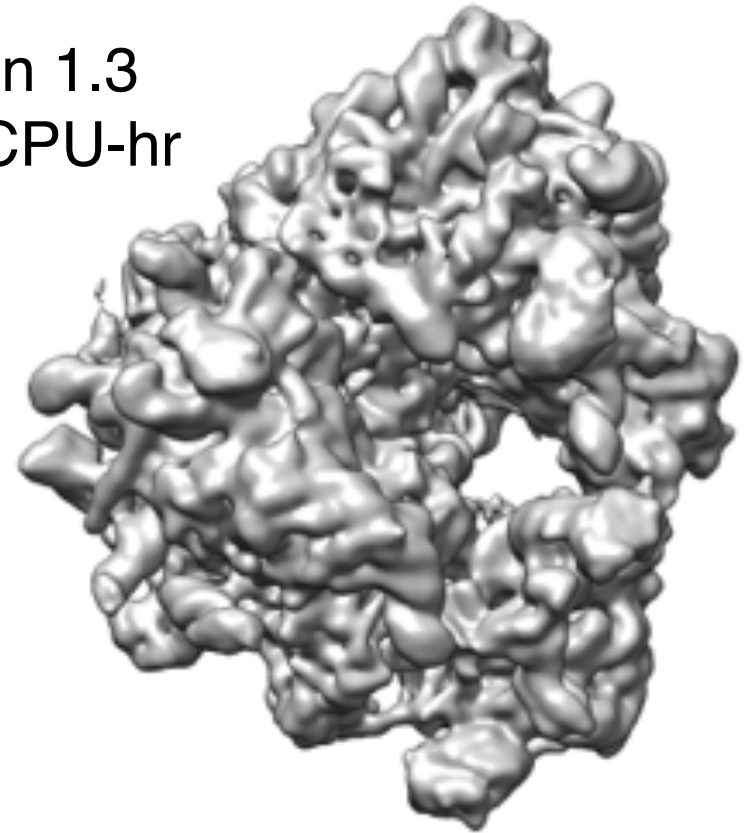
CryoEM

- Movie mode alignment/averaging
- Particle Picking
- CTF
- 2-D Class-averaging
- 3-D Reconstruction
- Conformational and Compositional Variability
- Tomography & Subtomogram Averaging
- Helical Reconstruction
- 2-D Crystals
- Phase Plates

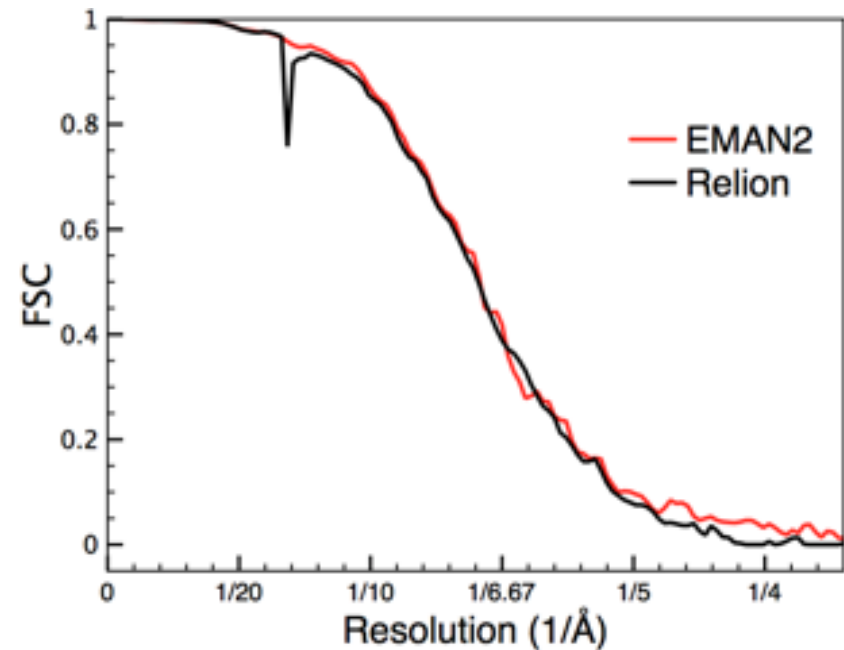
EMAN2.1
320 CPU-hr

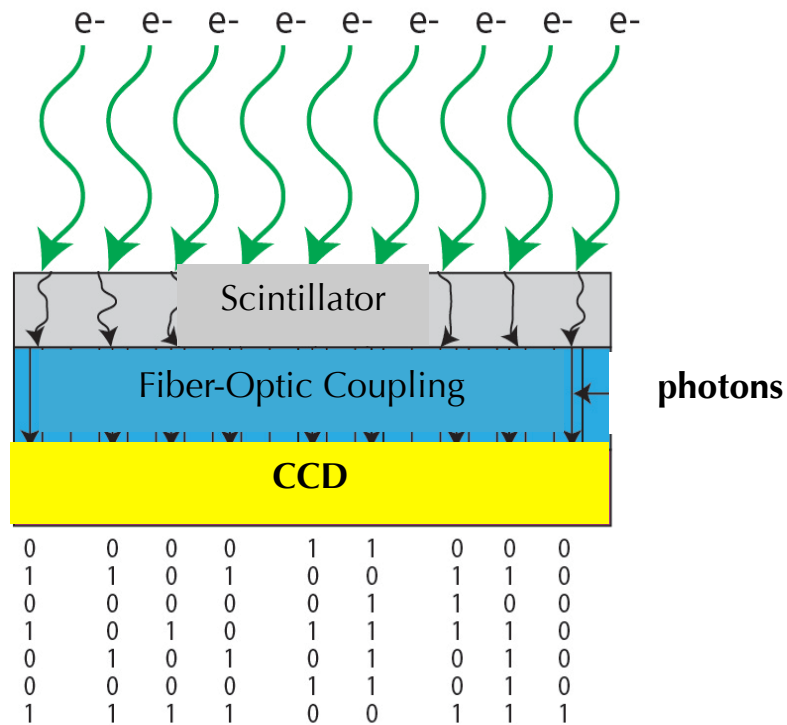


Relion 1.3
2200 CPU-hr



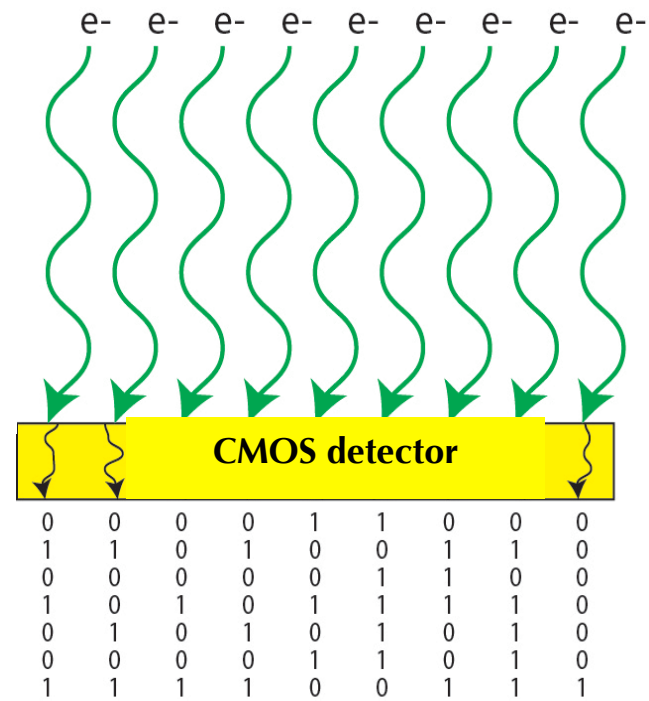
S. Cerevisiae 80S Ribosome (EMD-2275)
Data taken from PDBe 3DEM test data
no movie alignment performed
Dataset 10002 (Bai XC, Fernandez IS,
McMullen G, Scheres SH)





CCD Camera

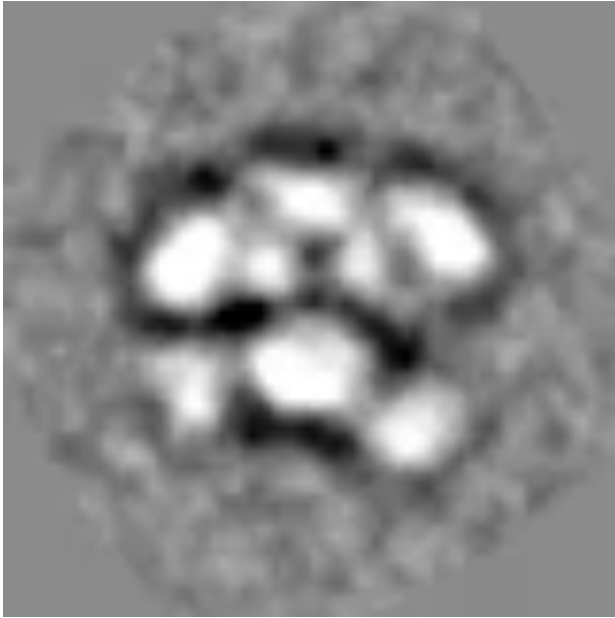
- Single Frames
- Poor DQE past 1/2 Nyquist



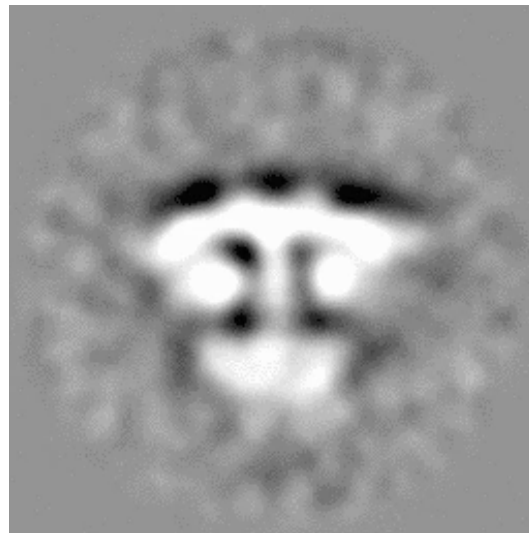
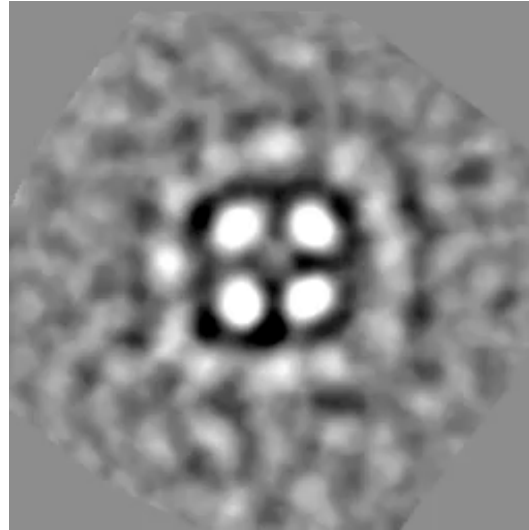
Direct Detection Camera

- Movies
- Good DQE to Nyquist
- Counting Mode
- Supersampling
- (4 TB/day!)

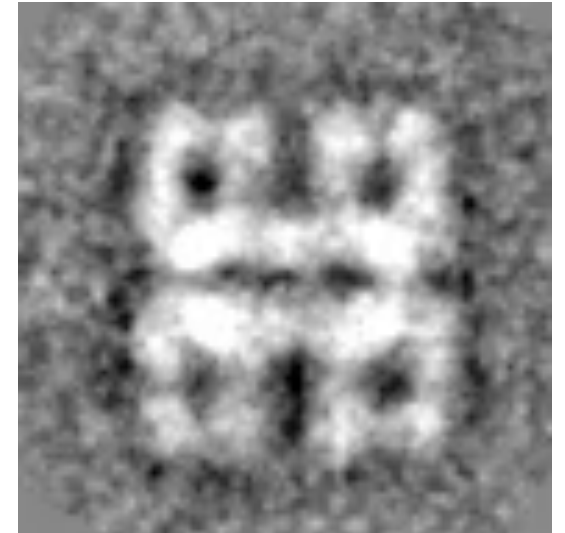
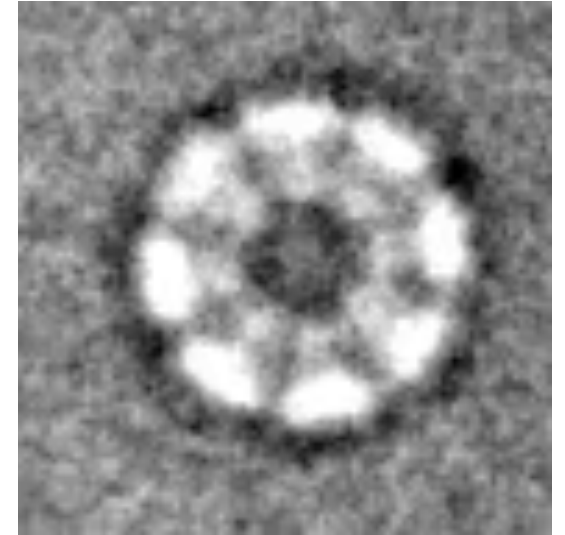
Fatty Acid Synthase
~30 Å motion



IP3 Receptor
~15 Å motion



TriC (open)
~12 Å motion

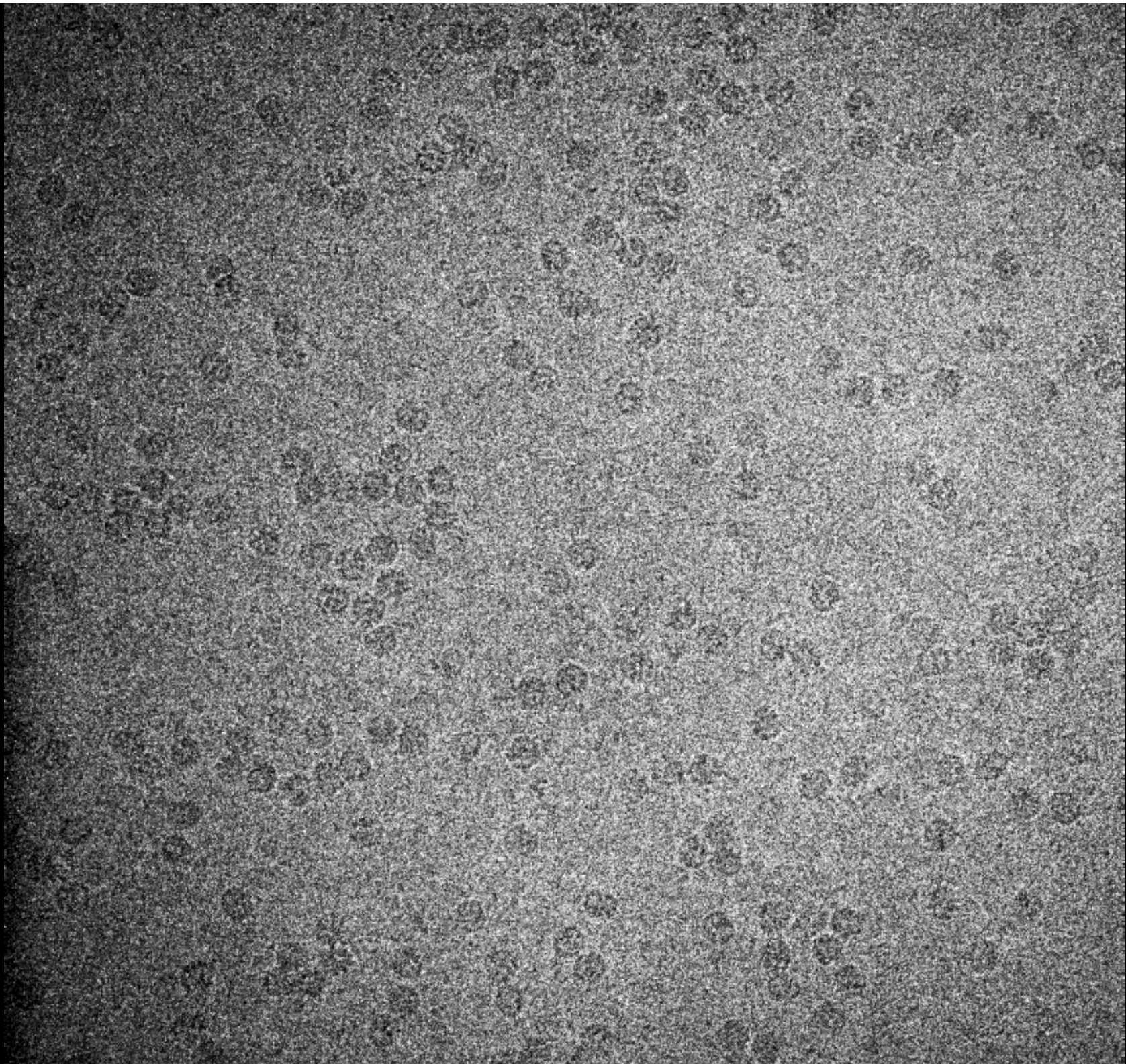


CryoEM

- ~~Movie mode alignment/averaging~~
- ~~Particle Picking~~
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- ~~2-D Crystals~~
- ~~Phase Plates~~

The Plan

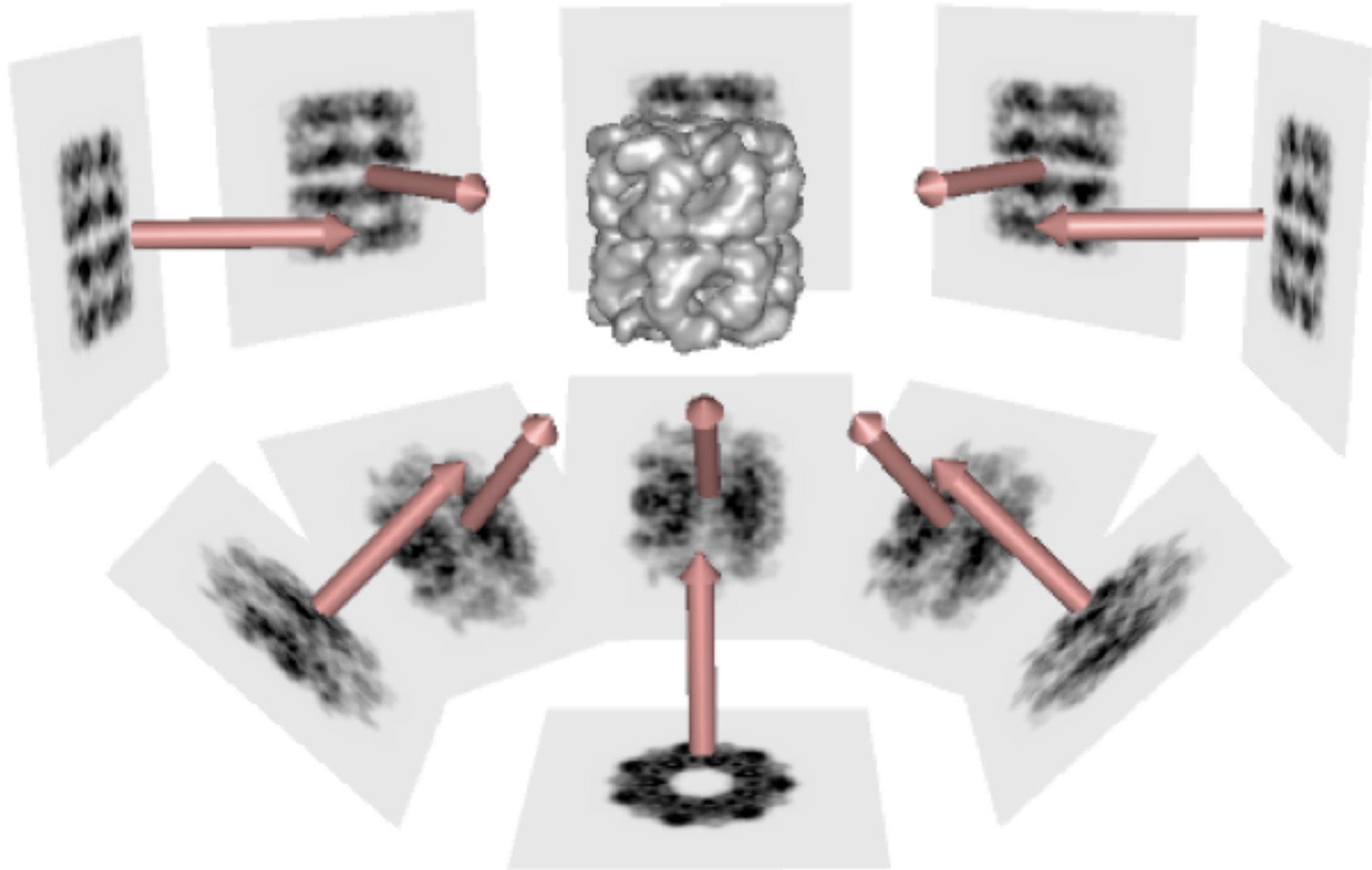
- Day 1 - Intro Lectures & EMAN2.12 tutorial
 - Dinner @ BCM-> Vendor Talks
- Day 2 - Structural Variability, Relion Demo
 - Early Release for Halloween
- Day 3 - Structural Variability, SPARX, EMAN Tutorials
 - Dinner @ BCM -> Participant Short talks
- Day 4 - Map Assessment & Model Building
 - Banquet at Trevisio

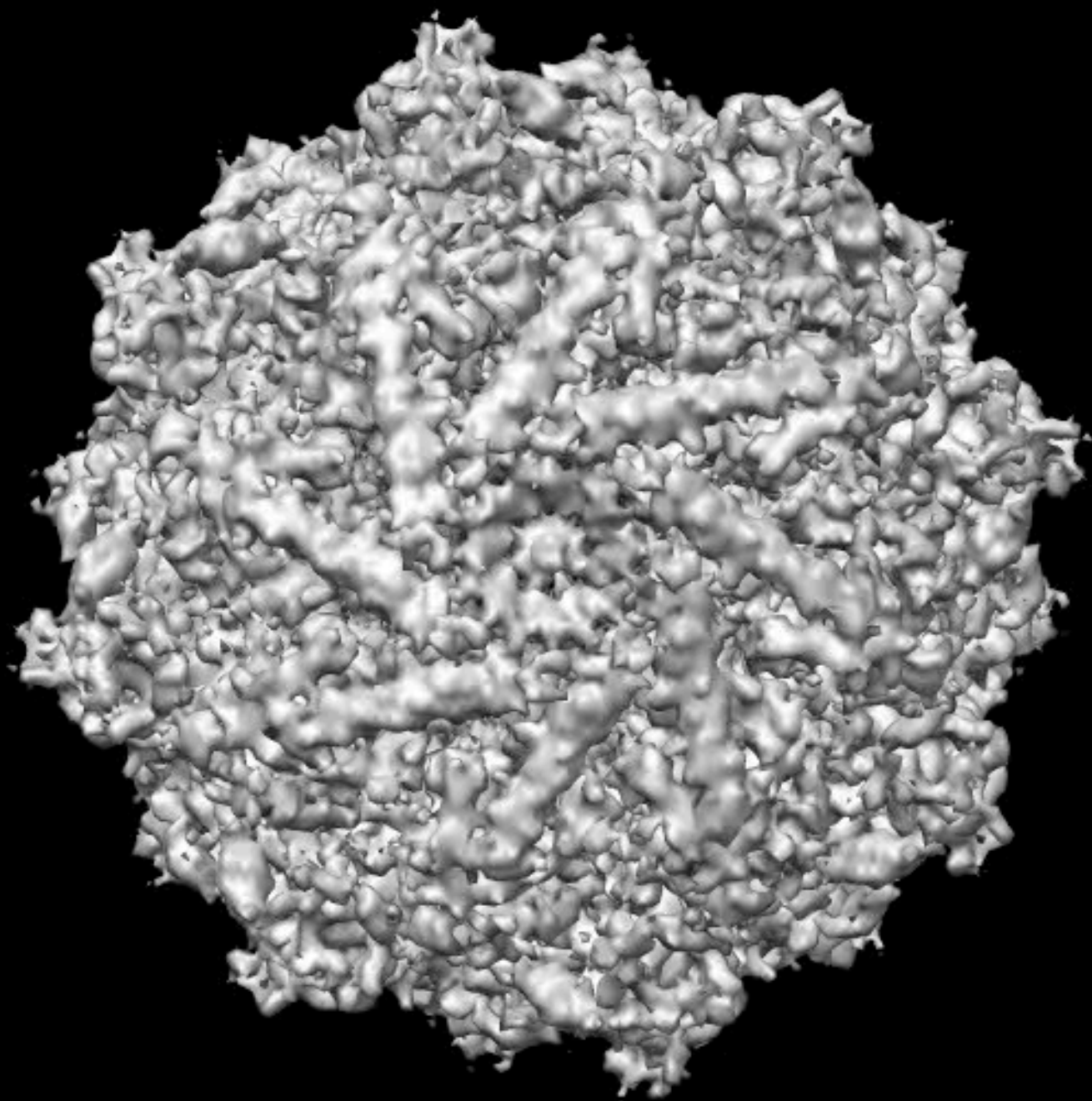




432/30,000 particles

TEM Produces Projections





High Resolution SPA

Stage	Data	Typ Processing
Data Collection	~4 TB/day Typ ~2 days	
Preprocessing	6 TB -> ~150 GB	~30 hr data I/O
Particle Selection	150 GB -> ~20 GB	varies
CTF Correction, etc	20 GB -> 50 GB	minimal, ~1 CPU-hr
2-D Class-Averages	~500 MB	~10 CPU-hr
Initial Model	~100 MB	~10 CPU-hr
Refinement	~10 GB tmp ~100 MB final	10-10,000 CPU-hr

EMAN2

- EMAN2 Wiki:

- <http://blake.bcm.edu/emanwiki/EMAN2>

- Software Download page:

- http://ncmi.bcm.tmc.edu/ncmi/software/software_details?selected_software=counter_222

- Discussion Mailing List/Google Group:

- <https://groups.google.com/forum/?fromgroups#!forum/eman2>

EMAN2 Architecture

Ease of Use



Flexibility

Project Manager
Interface

High-Level Programs

Command-Line Programs

Python Core

C++ Core

Programs

- Command-Line Programs (EMAN2)

syntax:

`e2<name>.py --help`

`e2<name>.py <file> [--option=value] [--option] [-O]`

`<>` - required parameter

`[]` - optional parameter

- `e2help.py <category>`

File Formats

MRC	R/W	IMAGIC	R/W
SPIDER	R/W	HDF5	R/W
PIF	R/W	ICOS	R/W
VTK	R/W	PGM	R/W
Amira	R/W	Xplor	W
Gatan DM2	R	Gatan DM3	R
Gatan DM4	R	FEI SER	R
TIFF	R/W	Scans-a-lot	R
LST	R/W	PNG	R/W
Video-4-Linux	R	JPEG	W

Extensible Core

Type	Description	#
Processor	Generic image processing algorithms, filters, masks, thresholds, etc.	180
Aligner	Algorithms used to align 2 images or volumes to each other	22
Projector	Routines to generate 2-D projections of 3-D objects	6
Reconstructor	Routines to reconstruct 3-D objects from 2-D projections	11
Cmp	Similarity metrics used to compare two images or volumes	10
Averager	Average together stacks of images in various ways	7
Analyzer	Perform various operations on sets of images, such as classification or PCA	6
Orientgen	Routines describing how projections cover the asymmetric triangle	6

Utility Programs

- `e2version.py` - Display version info
- `e2speedtest.py` - Test machine performance
- `e2help.py` - Documentation for modular functions
- `e2display.py` - GUI for general visualization
- `e2proc2d.py` - 2d image processing of stacks and single images
- `e2proc3d.py` - 3d image processing of 3-D stacks and single volumes
- `e2iminfo.py` - general image information tool
- `e2.py` - Python command-line for EMAN2

GUI

- e2projectmanager.py - Project management and workflow
- e2display.py - General image/volume display
- e2filtertool.py - Interactive 2/3D image processing
- e2evalimage.py - Whole micrograph quality/CTF evaluation
- e2boxer.py - Interactive particle picker
- e2helixboxer.py - Filament picker
- e2tomoboxer.py - Interactive tomogram picker
- e2ctf.py - Particle-based CTF analysis
- e2evalparticles.py - Class-based particle separation/evaluation
- e2eulerxplor.py - Evaluate particle orientation distributions
- e2simmxxplor.py - Evaluate how well orientations can be determined

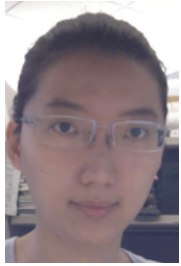
High Level Programs

- `e2refine2d.py` - reference free class-averages
- `e2initialmodel.py` - Make initial models from a few class-averages
- `e2refine_easy.py` - Standard single particle 3-D refinement
- `e2eotest.py` - even/odd test for resolution assesement
- `e2refinemulti.py` - multiple map simultaneous refinement
- `e2classifyligand.py` - Split data into 2 groups based on 2 models

Interoperability

- `e2refinetoelion2d.py` - Seed a 2D Relion refinement
- `e2refinetoelion3d.py` - Convert project for 3D Relion refinement
- `e2refinetoelalign.py` - Convert project for Frealign refinement
- `e2runelalign.py` - Execute Frealign
- `e2refinefromelalign.py` - Process the results of a Frealign run
- `e2runresmap.py` - Run ResMap on an EMAN2 refinement

Ask These People For Help!



Boxue Ma



Vernon Williams



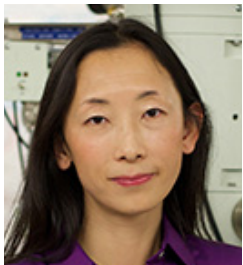
Zhaoming Su



Jason Kaelber



Muyuan Chen



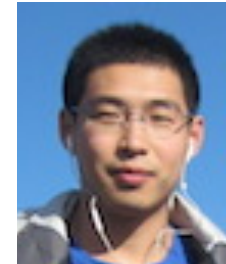
Wei Dai, Ph.D.



Jesus Galaz, Ph.D.



Brandon Smith



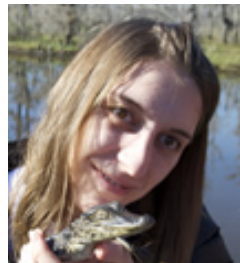
Kaiming Zhang



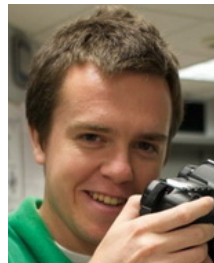
Bo Chen



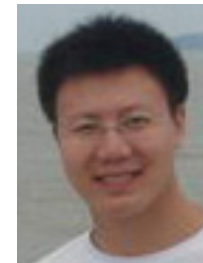
Hun Roh, Ph.D.



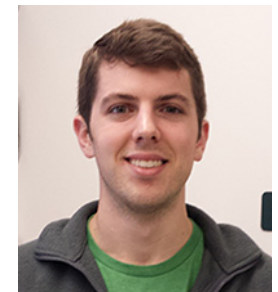
Rossi Irobalieva



Corey Hryc



Zhao Wang



Michael Bell