ARGONNE TRAINING PROGRAM ON EXTREME-SCALE COMPUTING

ATPESC 2018

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Volumetric Snapshot 3D Imaging (ANL-UC "SmallWorlds" project)
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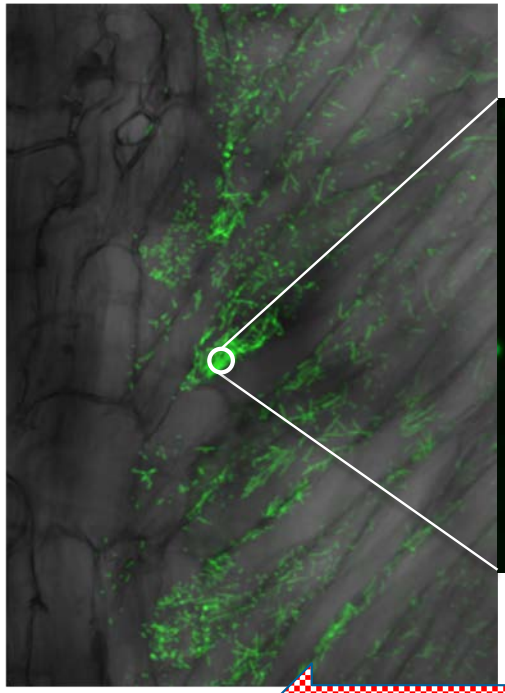
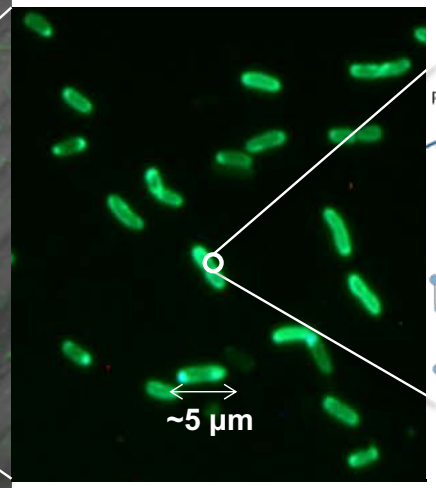
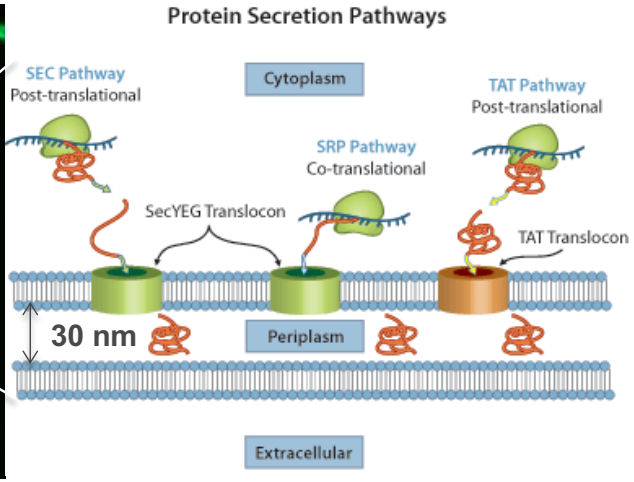
Q Center, St. Charles, IL (USA)
July 29 – August 10, 2018

MULTI-SCALE NATURE OF THE IMAGING CHALLENGE





Micrometer Scale



sub-micrometer Scale

sub-Millimeter Scale

3D-MFM

Confocal Microscopy

Functional Fluorescent Tags

optical

Correlative Imaging

STEM

Millimeters

Micrometers

Nanometers

VOLUMETRIC SNAPSHOT 3D IMAGING

Goal:

Develop an Imager to get 3D data of living (moving) cells

Volumetric: capture a 3D volume

Snapshot: acquire entire volume at the same time

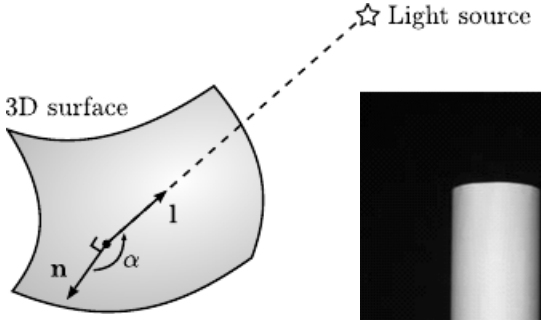
- 3D methods from Computer Vision
  - Shading
  - Focus/defocus
  - Texture
  - Multiview/Stereo
  - Structured light
- Multi-focal microscopy
  - Optical system
    - Multiple focal planes
  - Computation/reconstruction
  - Results
- Future
  - Interferometry + MFM
  - Structured light + MFM

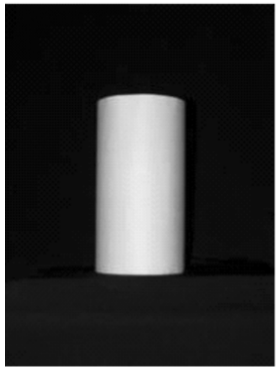
3D IMAGING METHODS FROM COMPUTER VISION

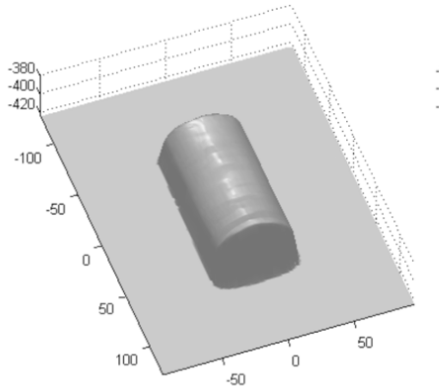
STRUCTURE FROM X OR SHAPE FROM X

Computer vision techniques for computing 3D structure

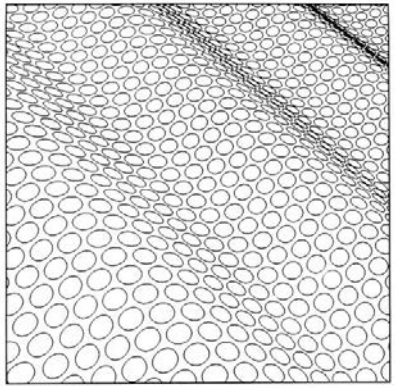
- **Shading**
- **Focus/defocus**
- **Texture**

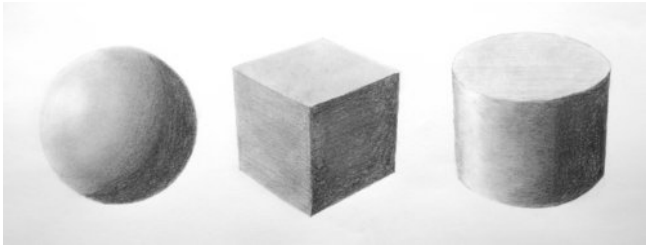






(a) (b)

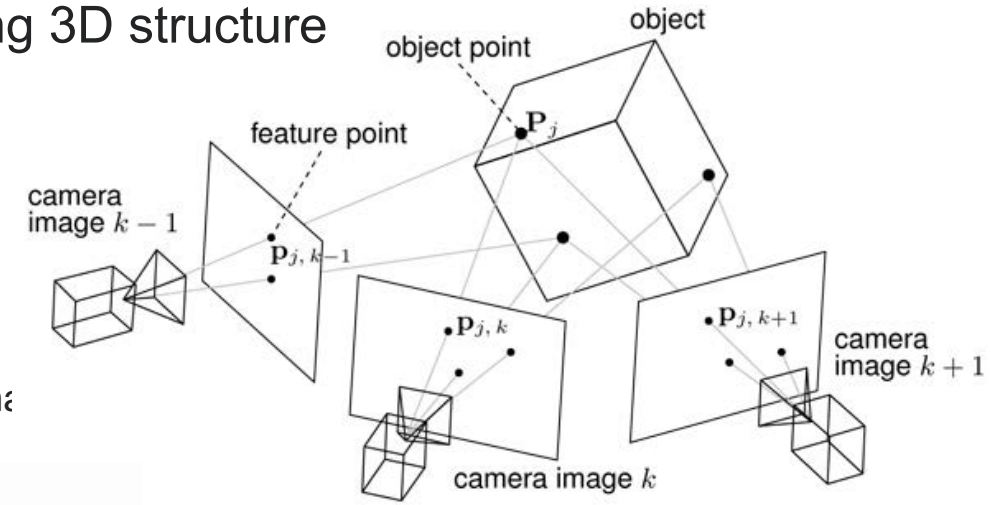


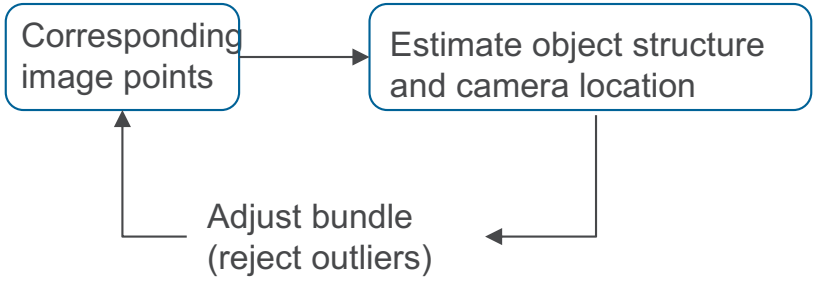


STRUCTURE FROM X OR SHAPE FROM X

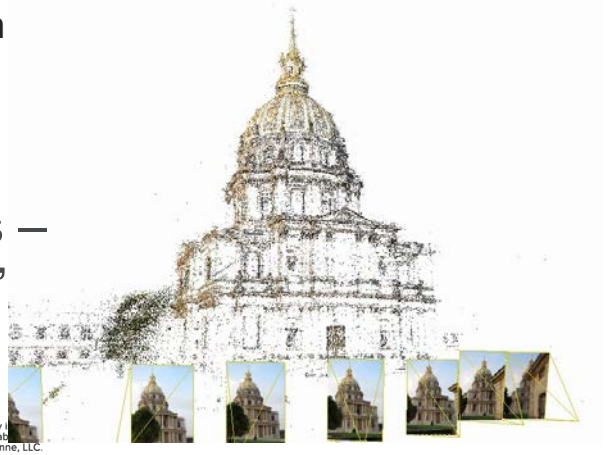
Computer vision techniques for computing 3D structure

- Shading
- Focus/defocus
- Texture
- **Multiview (Stereo or Motion)**
  - Requires:
    - Correspondences (Feature points in images tha correspond to the same physical point)
    - Camera Calibration





Point clouds – not “objects”

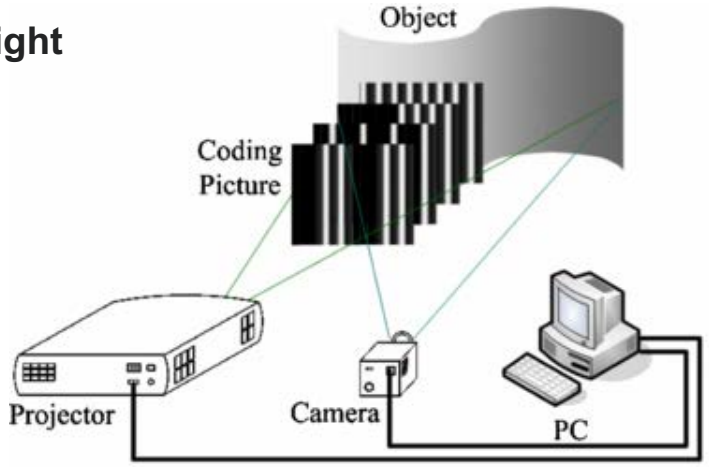


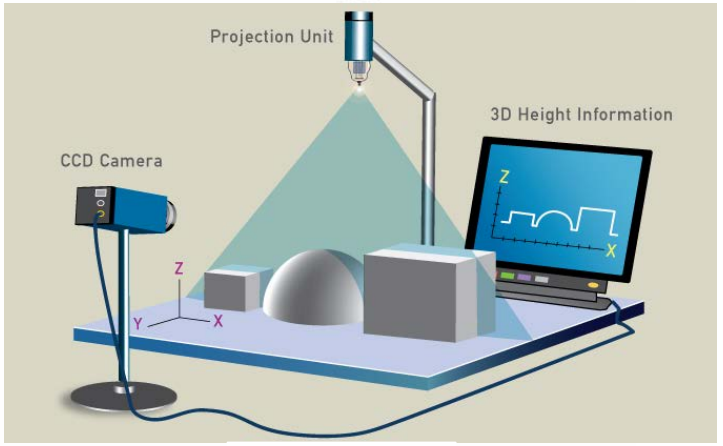
STRUCTURE FROM X OR SHAPE FROM X

Computer vision techniques for computing 3D structure

- Shading
- Focus/defocus
- Texture
- Multiview/Stereo
- **Structured light**

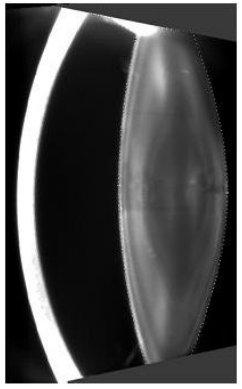
david3d.com

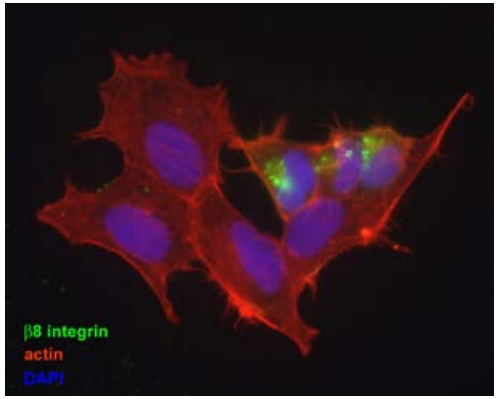


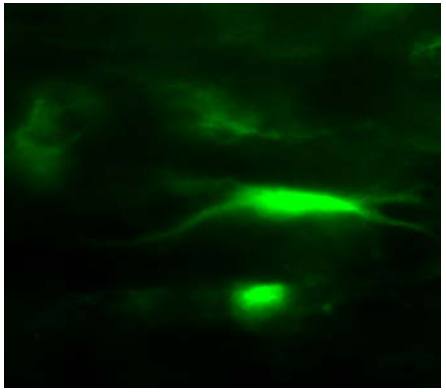


APPLICATION IN LIFE SCIENCES (AND MATERIALS)?

- what can we use from 40+ years of computer vision ?
  - Focus
  - Multiple views
  - Use structured “light” (or other electromagnetic energy, ultrasound, x-ray etc).
  - Still have correspondence problem
    - Life sciences: stains, fluorescent proteins, quantum dots, etc.

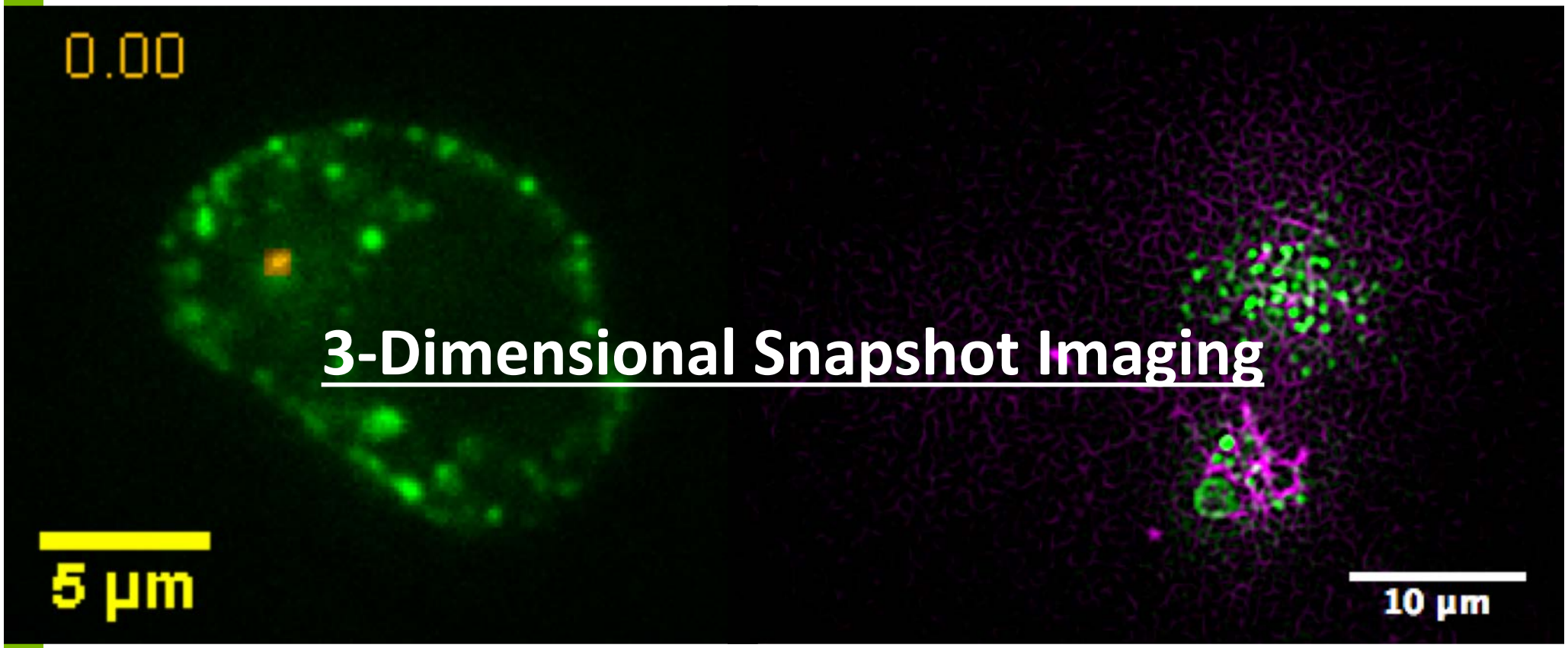






MULTIFOCAL MICROSCOPY (MFM) FOR 3D SNAPSHOT VOLUMETRIC IMAGING

INVESTIGATION OF FAST 3D BIOLOGICAL PROCESSES: TIME VS Z COMPROMISE

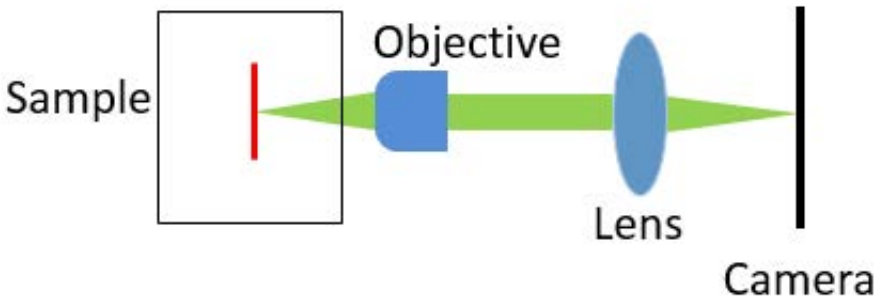


2D movie of insulin granules in MIN6 cells

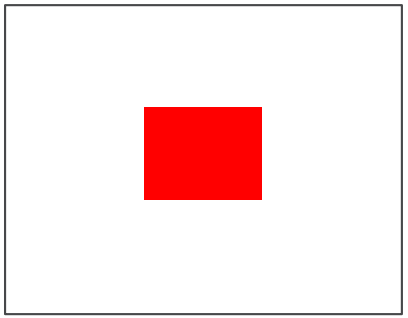
z-stack of insulin granules and microtubules

CONVENTIONAL MICROSCOPE

Conventional Microscope



On camera:

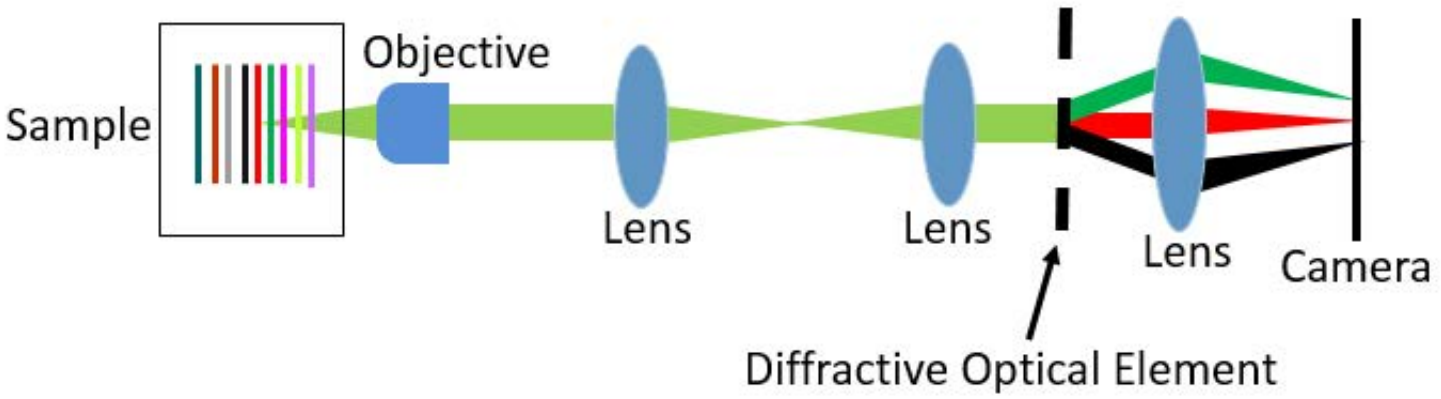


A single focal plane is in-focus

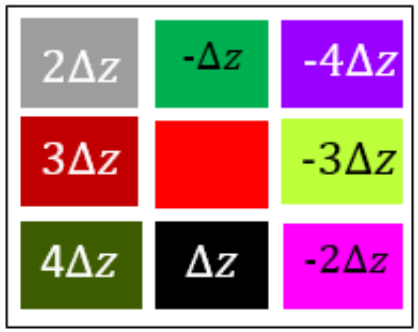
MULTI-FOCAL MICROSCOPE (MFM)

Simultaneously images 9 or 25 focal planes separated by Δz (tunable)
Each sub-image is a conventional widefield image

Conventional Microscope + MFM Modality

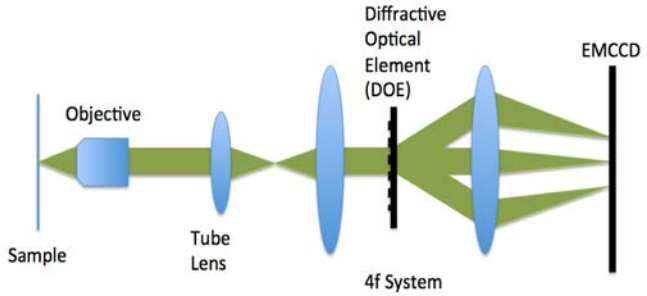


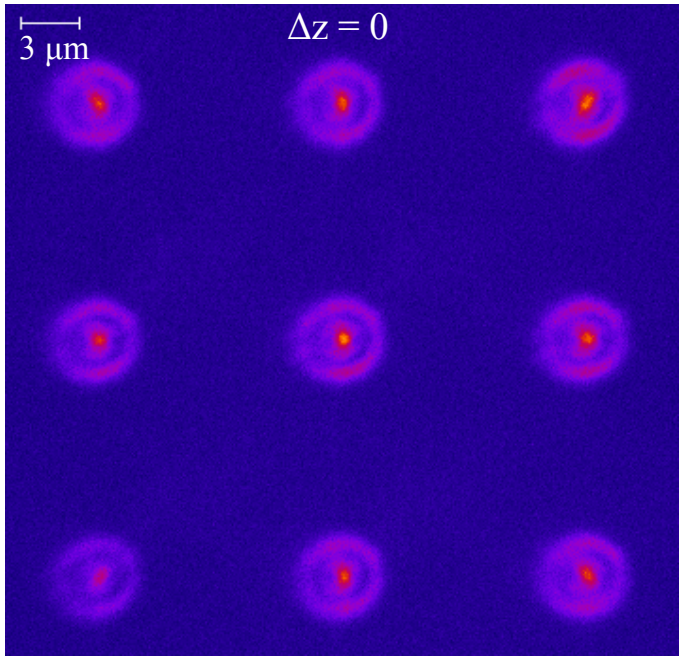
On camera:



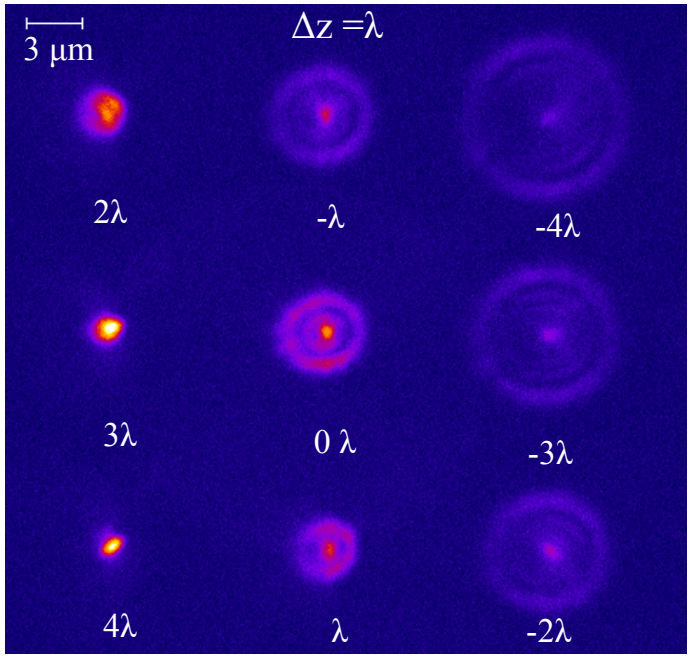
Multiple planes simultaneously

MULTI-FOCAL MICROSCOPY



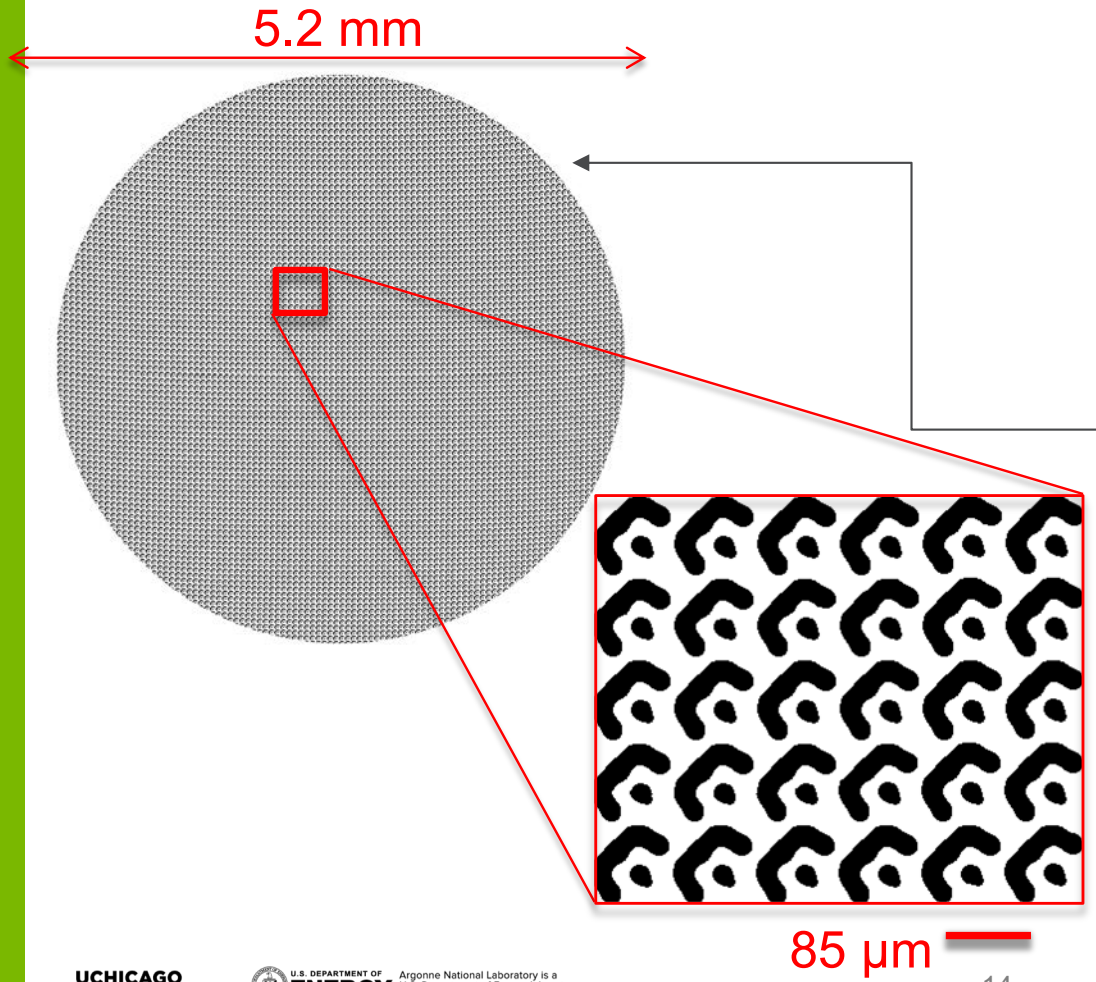


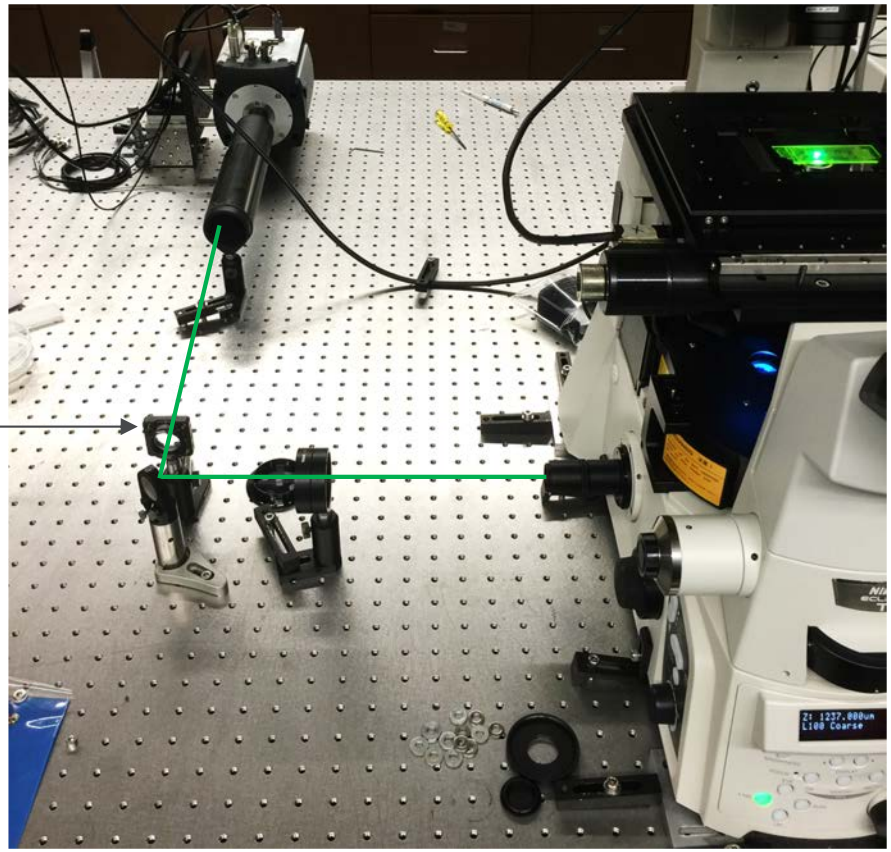
Wide field (conventional)

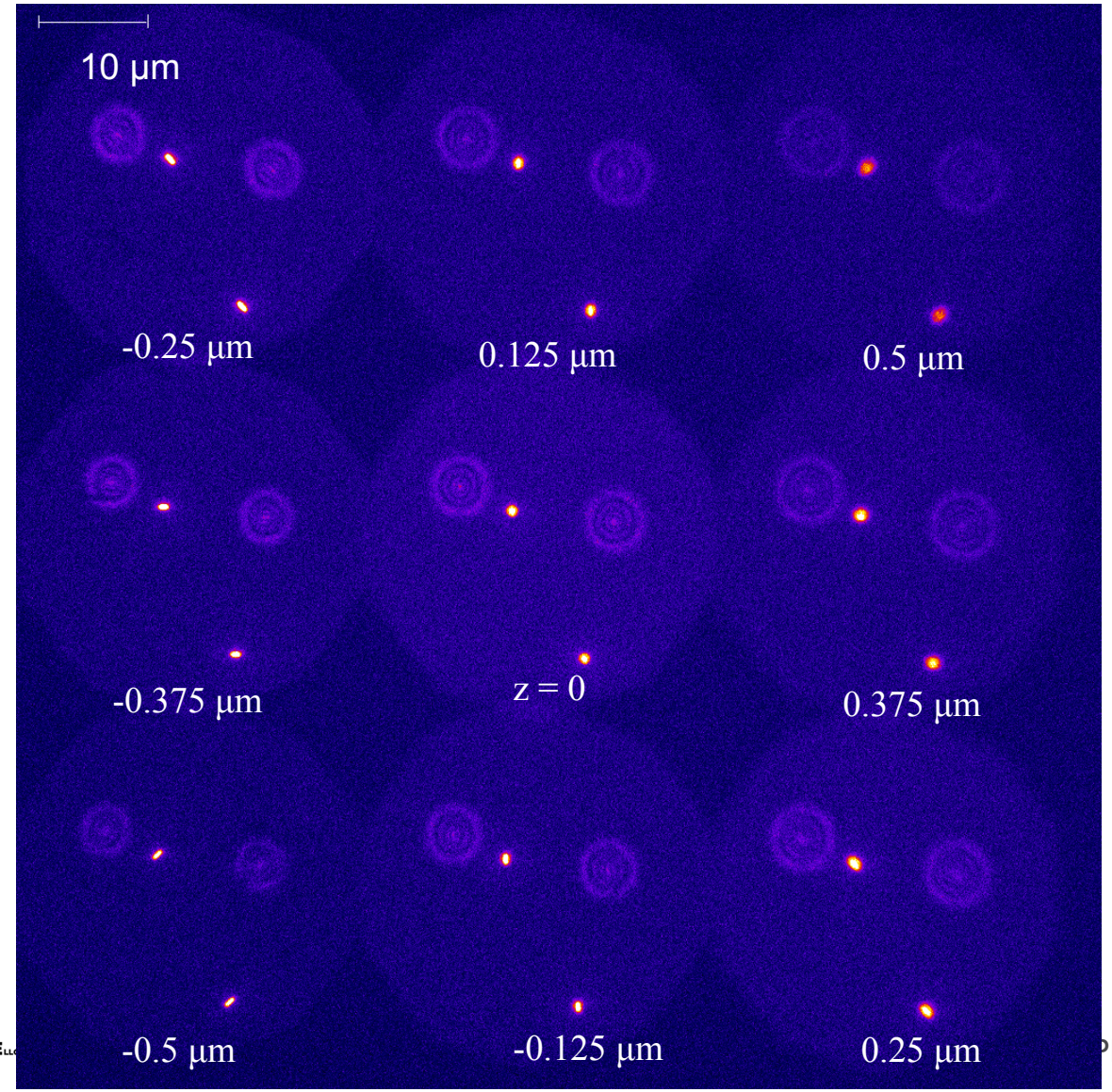


MFM image of a single ~170 nm fluorescent bead

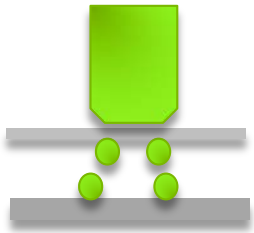
MFM W/DIFFRACTIVE OPTICAL ELEMENT

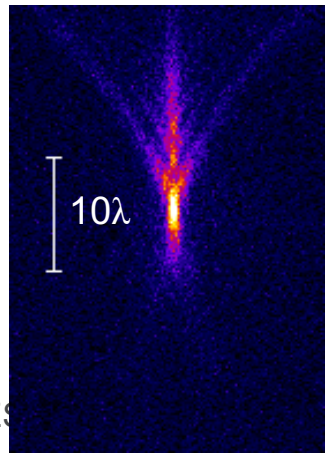




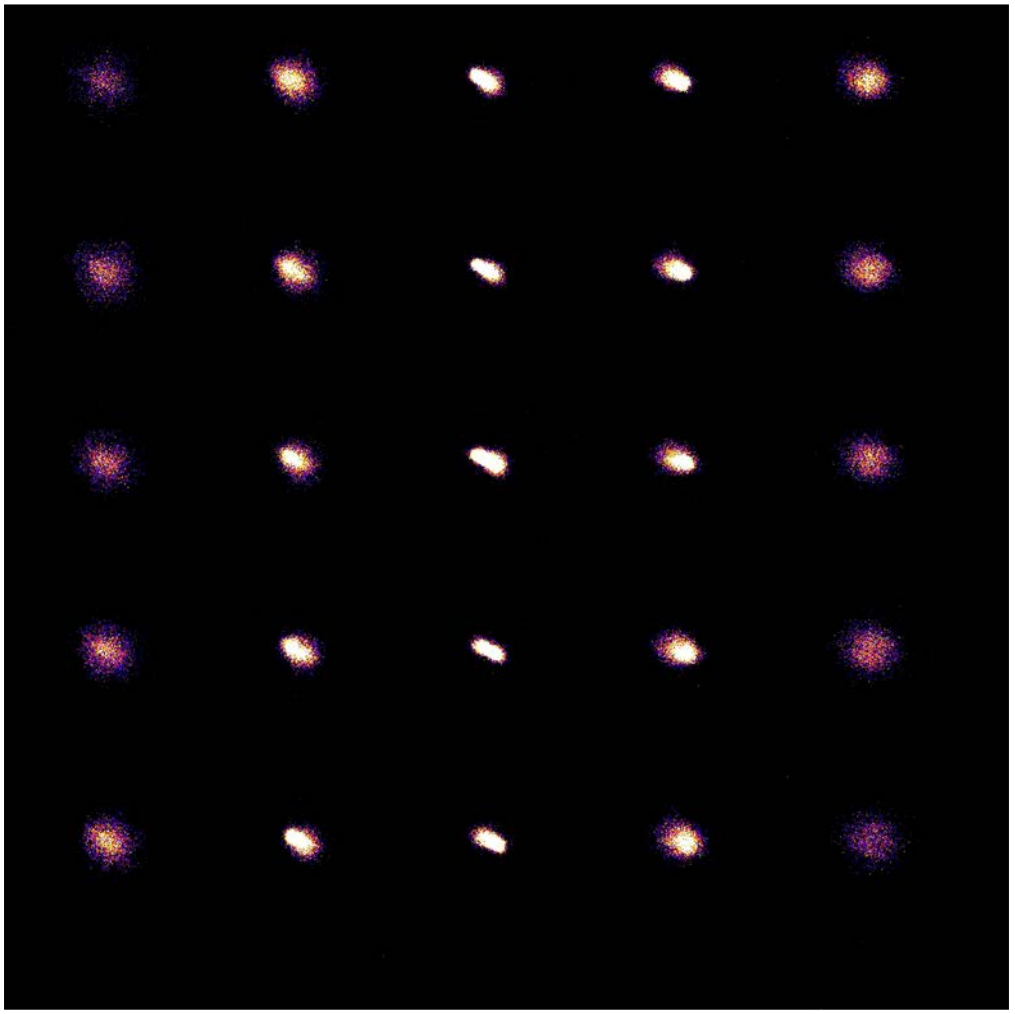


MFM imaging of fluorescent beads using physical DOE





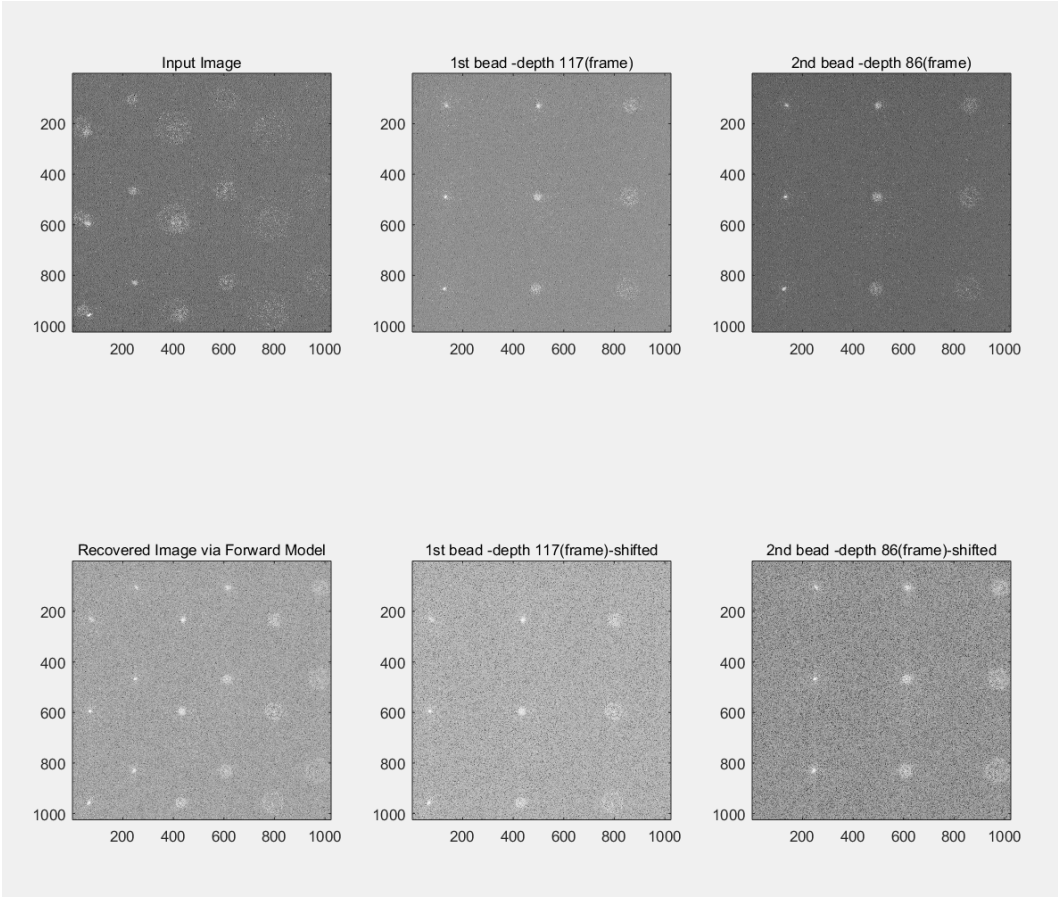
MFM VIDEO OF TUMBLING PSEUDOMONAS



COMPUTATIONAL METHODS FOR RECONSTRUCTING 3D FROM MFM IMAGES

MULTIFOCAL MICROSCOPY – 3D RECONSTRUCTION

- Brute force approach
  - beads



PARTICLE TRACKING

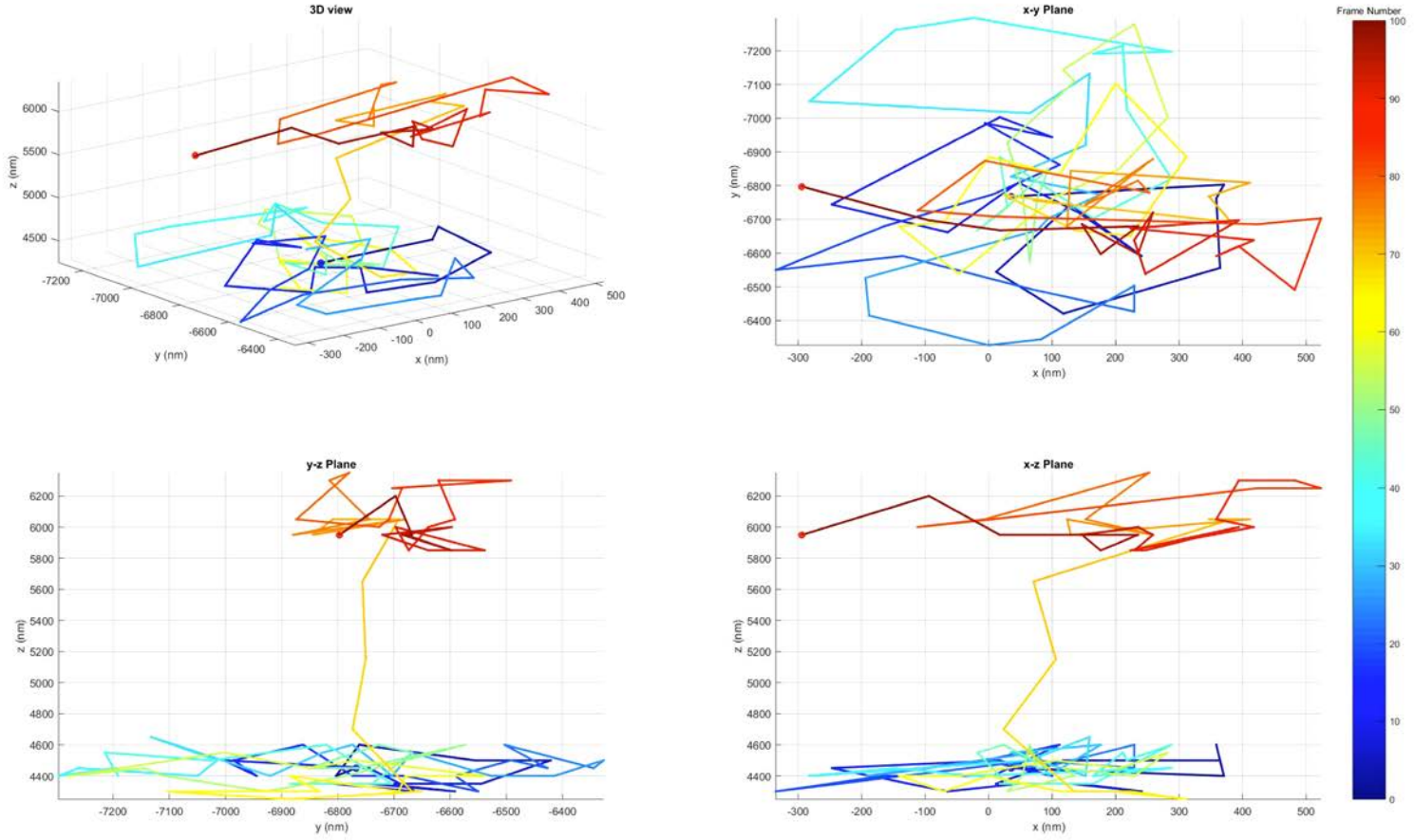
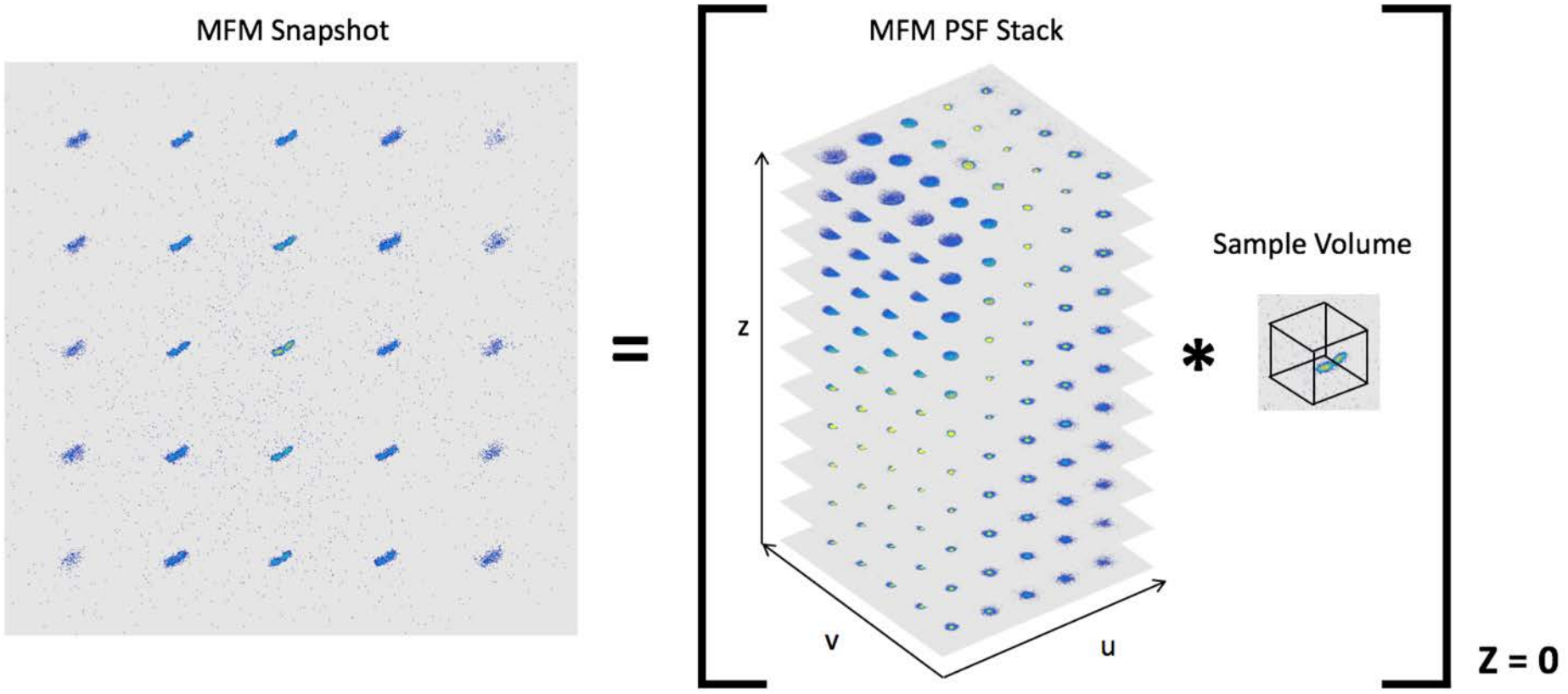
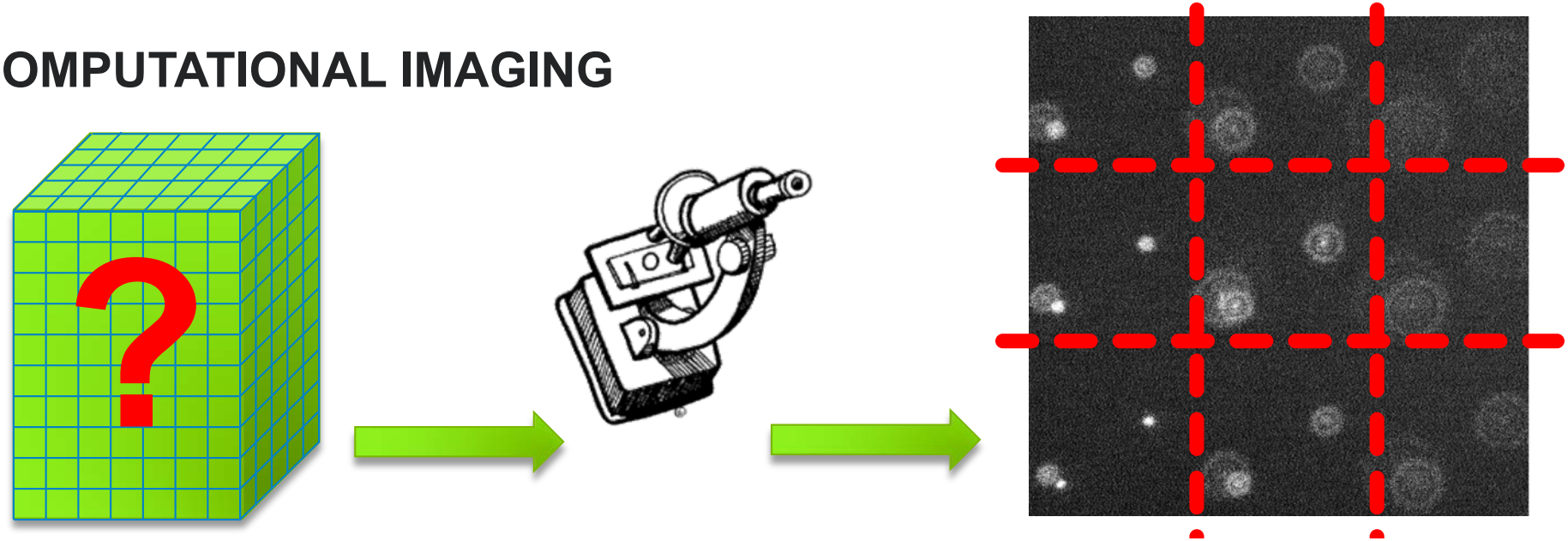


IMAGE FORMATION



COMPUTATIONAL IMAGING



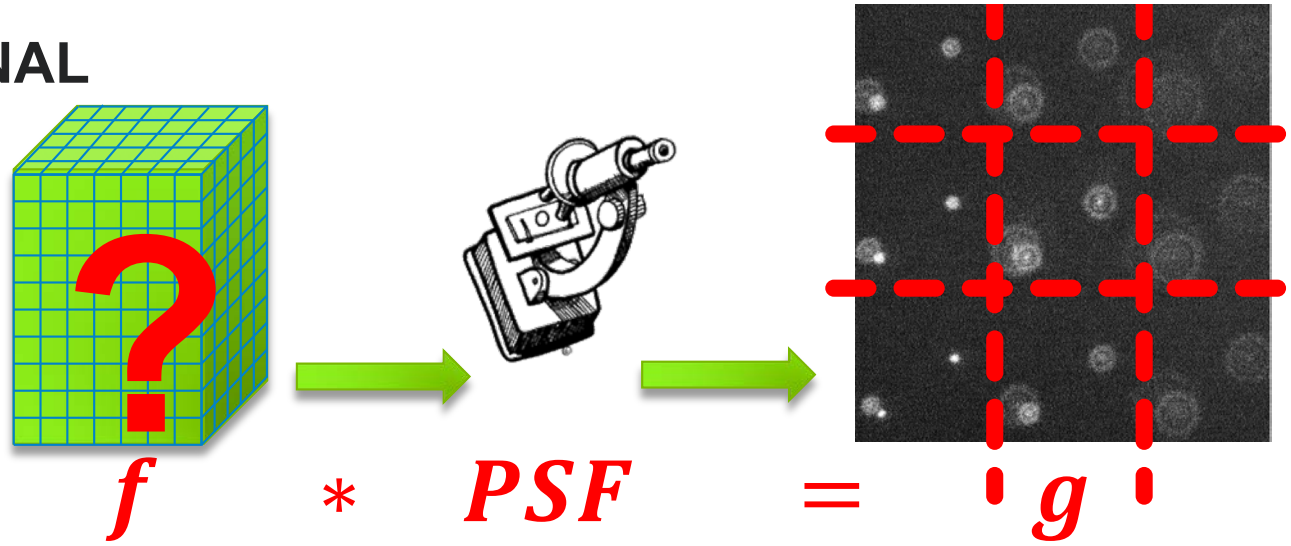
3D object

Microscope

2D Image

$$f * PSF = g$$

COMPUTATIONAL IMAGING

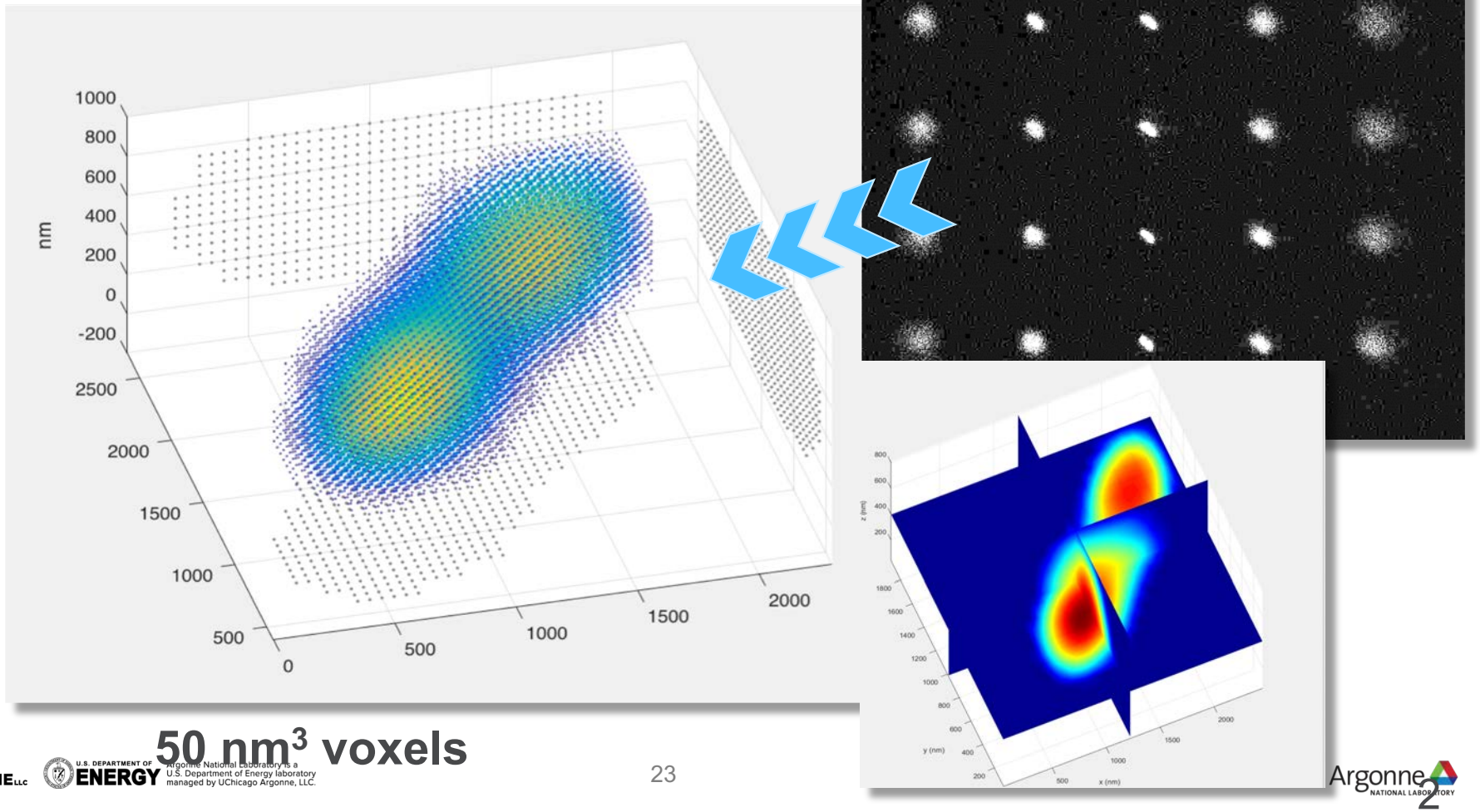


$f \quad * \quad PSF \quad = \quad g$

1. Update best guess for f (or make an initial guess if just starting)
2. Test current candidate solution for two measures of solution fitness:
   a. good facsimile of measured image g?
   b. satisfies constraints based on prior knowledge (e.g. smooth, sparse, point-like, smooth gradient)?
3. Repeat from (1) if current candidate is not good enough

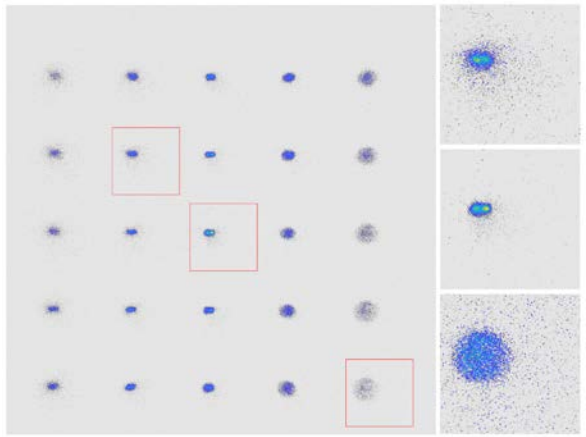
Our 3D reconstruction is the final f

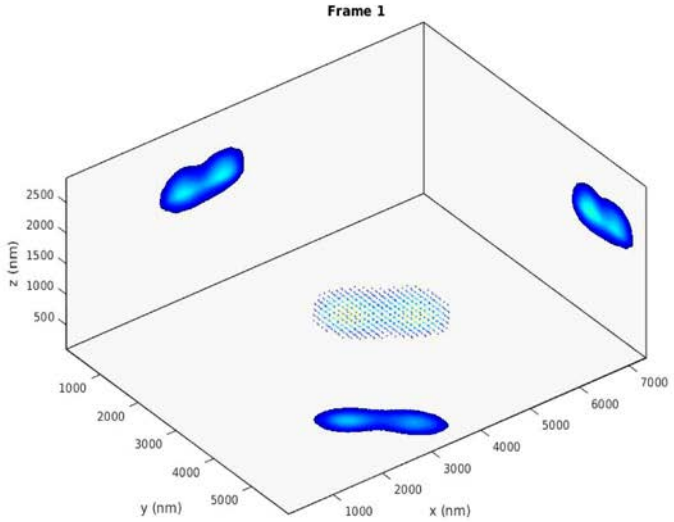
EXTENDED OBJECT RECONSTRUCTION

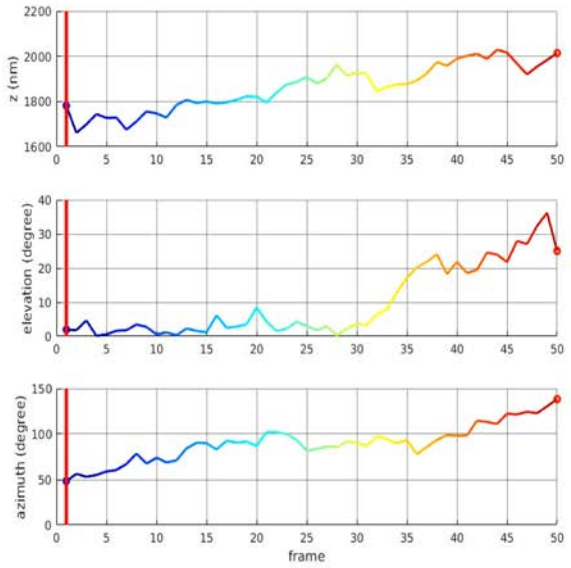


50 nm^3 voxels

MFM 3D MOVIE

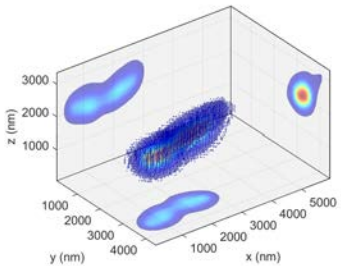



Frame 1
z (nm)
y (nm)
x (nm)

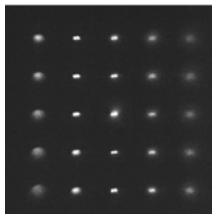

z (nm)
elevation (degree)
azimuth (degree)
frame

3D RECONSTRUCTION VALIDATION

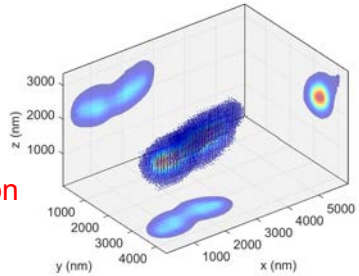
Multiple-focal Microscope (MFM) of Bacterium

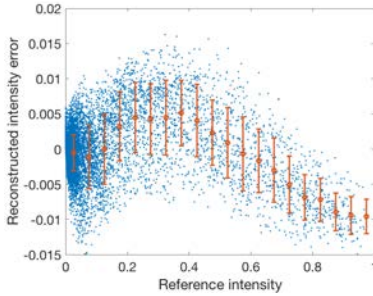


Sensing



Reconstruction



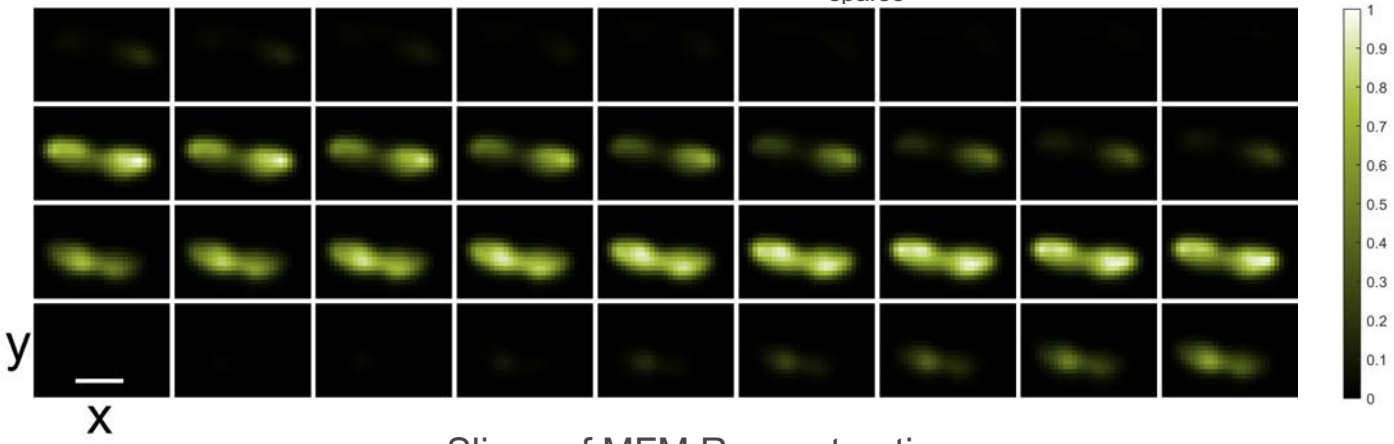


3D Confocal Stack

2D Captured by MFM

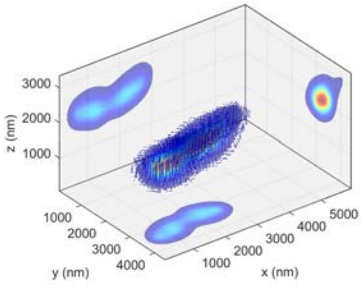
MFM Reconstruction $PSNR_{sparse}$=47.33dB

Voxel-by-voxel Comparison

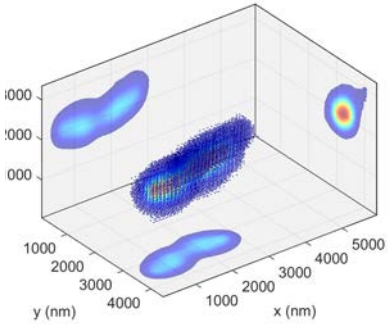


z-Slices of MFM Reconstruction

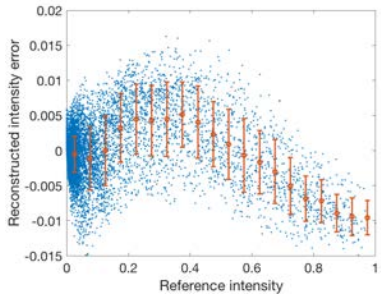
DOUBLE LOBE BACTERIUM VERIFICATION



Confocal

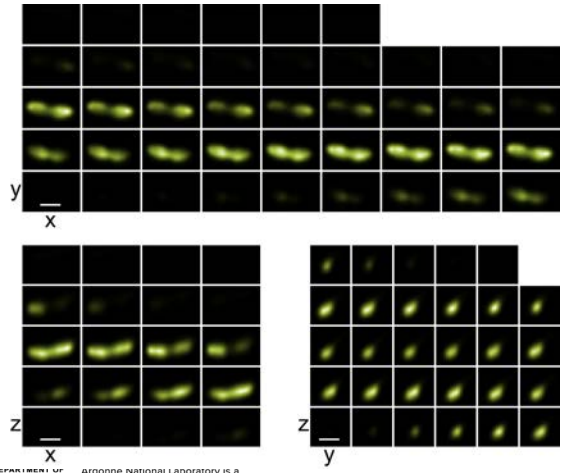


MFM Recons. PSNR_sparse=47.33dB

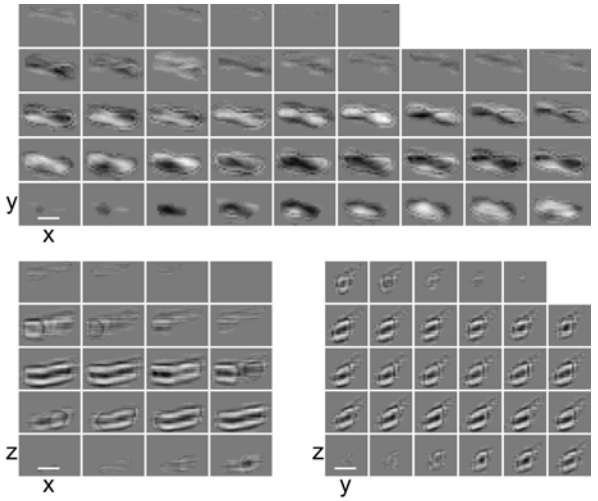


Voxel-by-voxel Comparison

MFM Reconstruction Unfolded

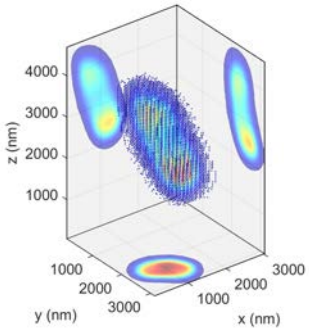


Colorbar

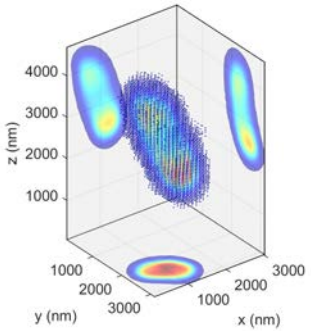


MFM Reconstruction Error

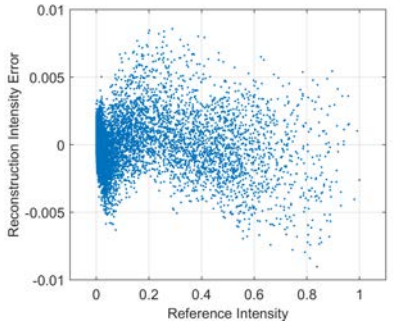
LONG Z BACTERIUM VERIFICATION



Confocal

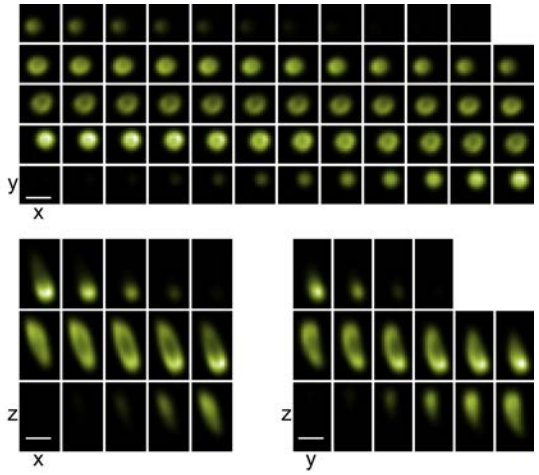


MFM Recons. PSNR sparse=53.77dB

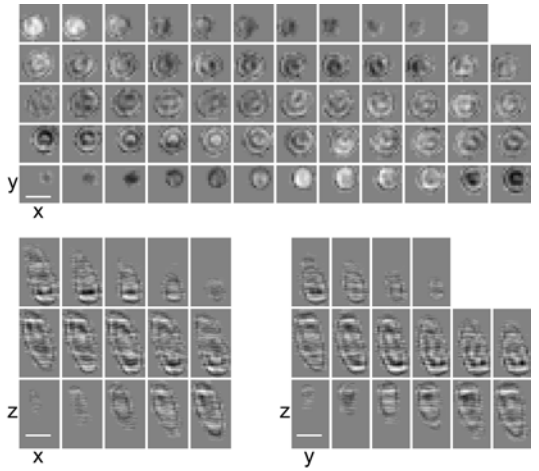


Voxel-by-voxel Comparison

MFM Reconstruction Unfolded

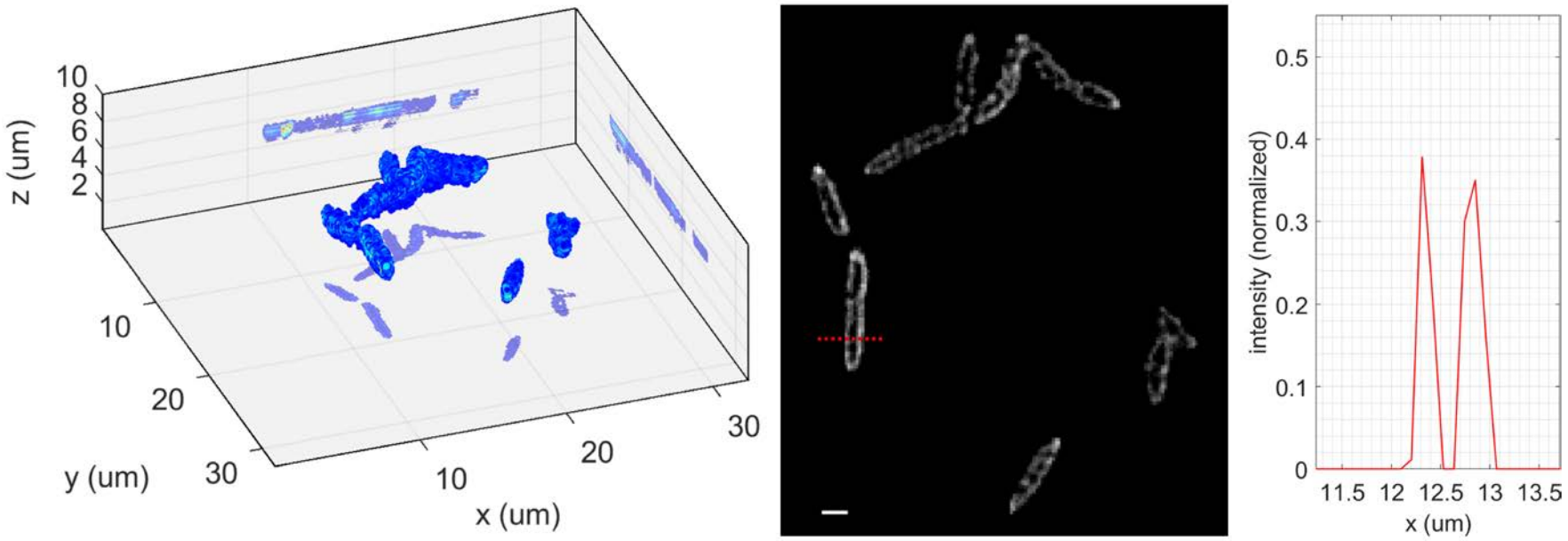


Colorbar

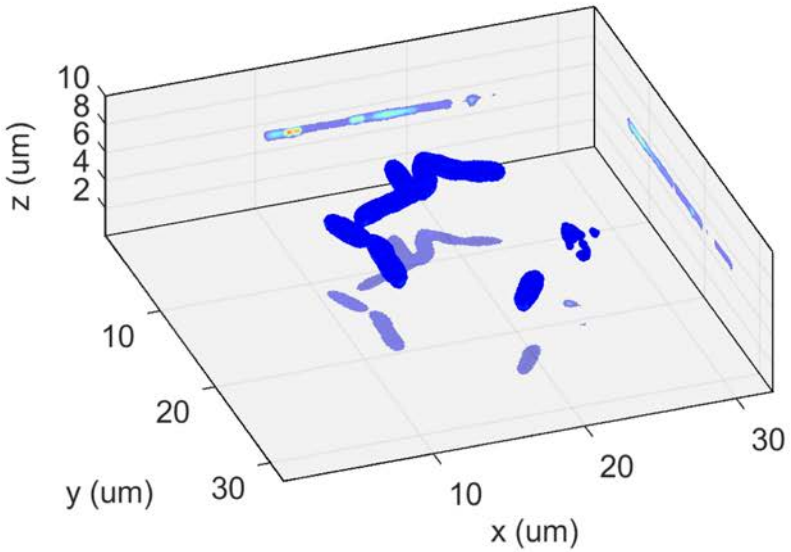


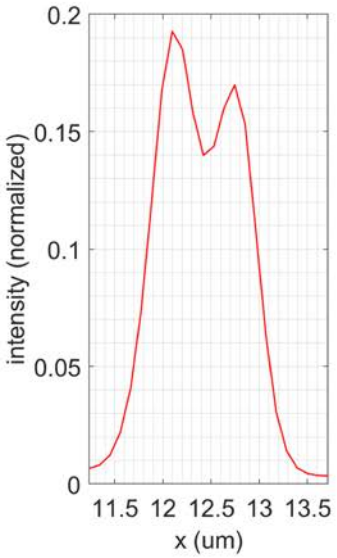
MFM Reconstruction Error

RECONSTRUCTION FROM SINGLE SNAPSHOT MFM (0.5S)

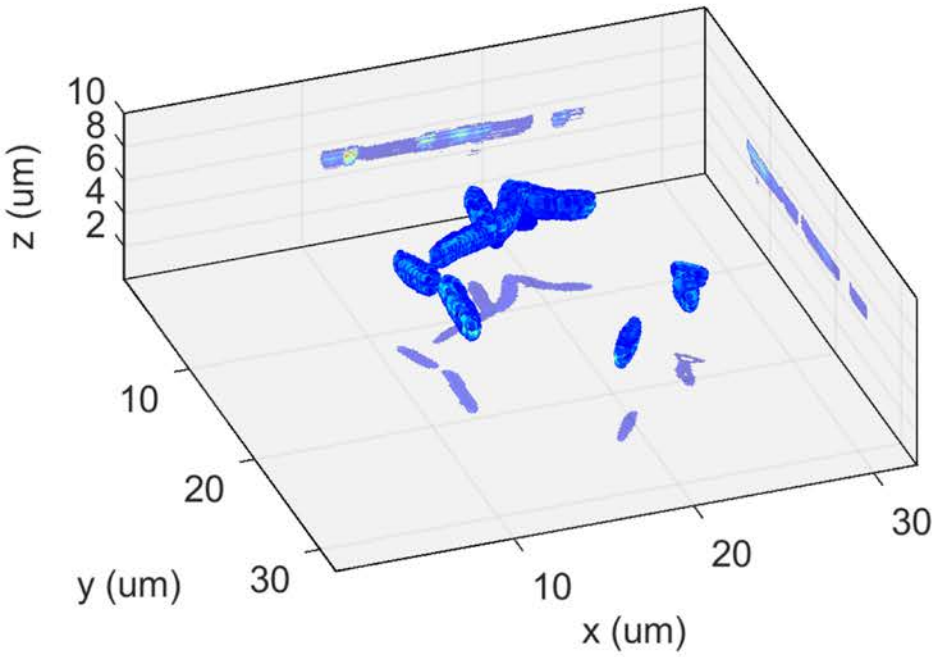


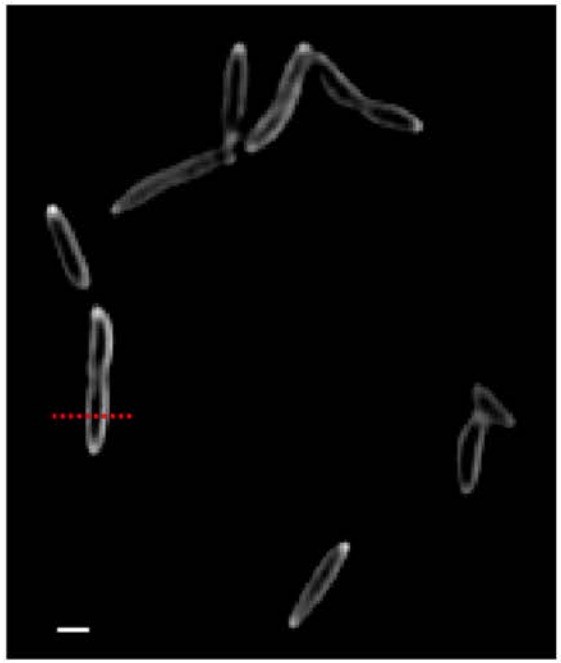
SPINNING DISC CONFOCAL MICROSCOPY (10 S)

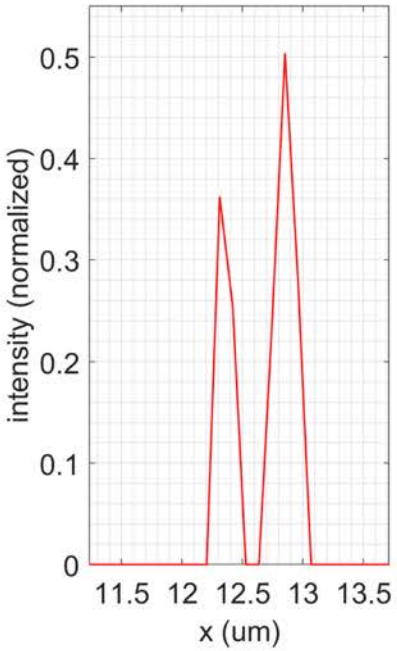




RECONSTRUCTION FROM AVERAGING MULTIPLE FRAMES

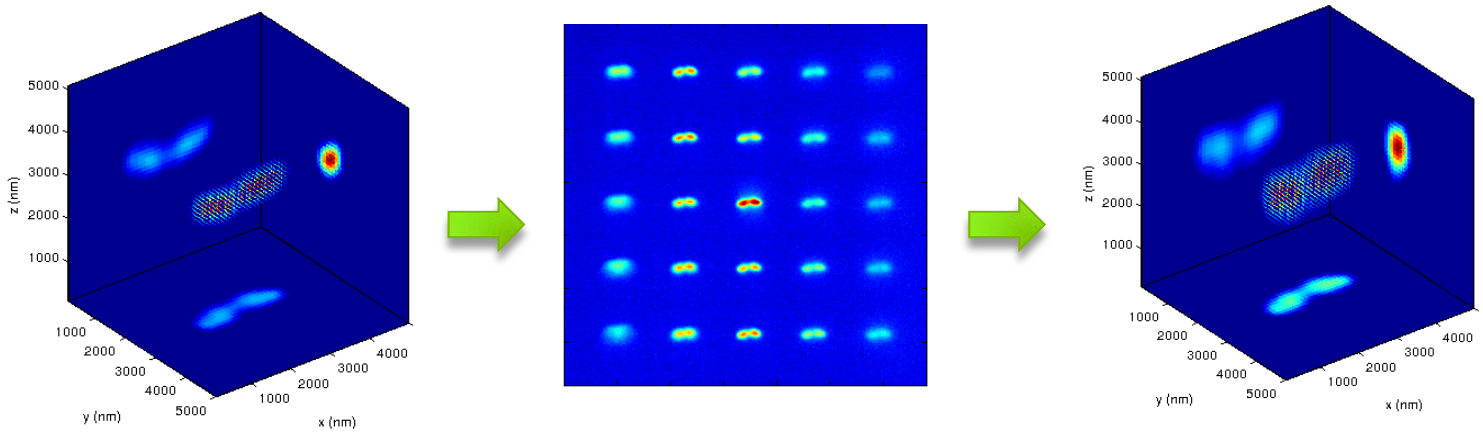






4D MFM

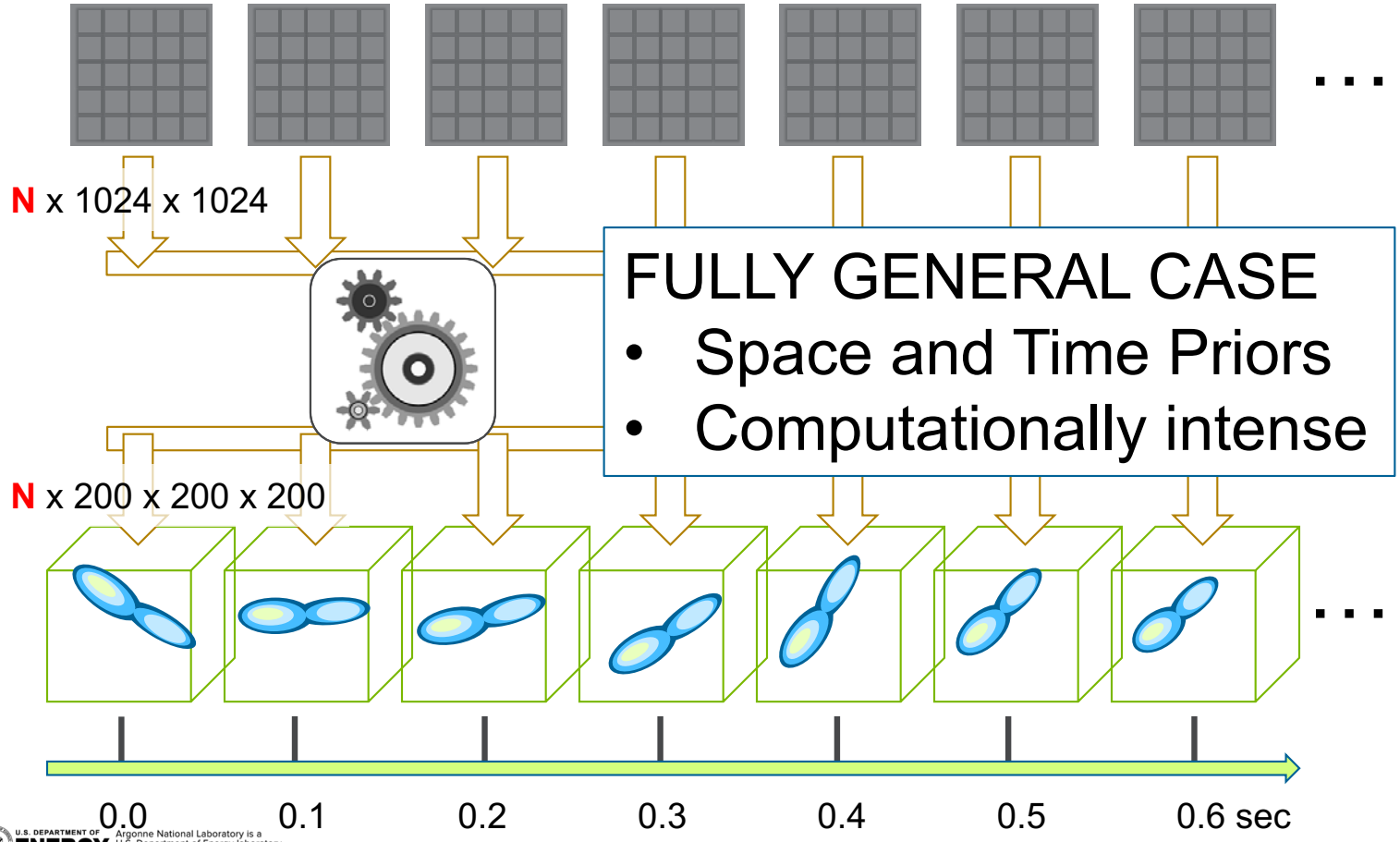
MFM IMAGING MODEL & RECONSTRUCTION (SINGLE FRAME)



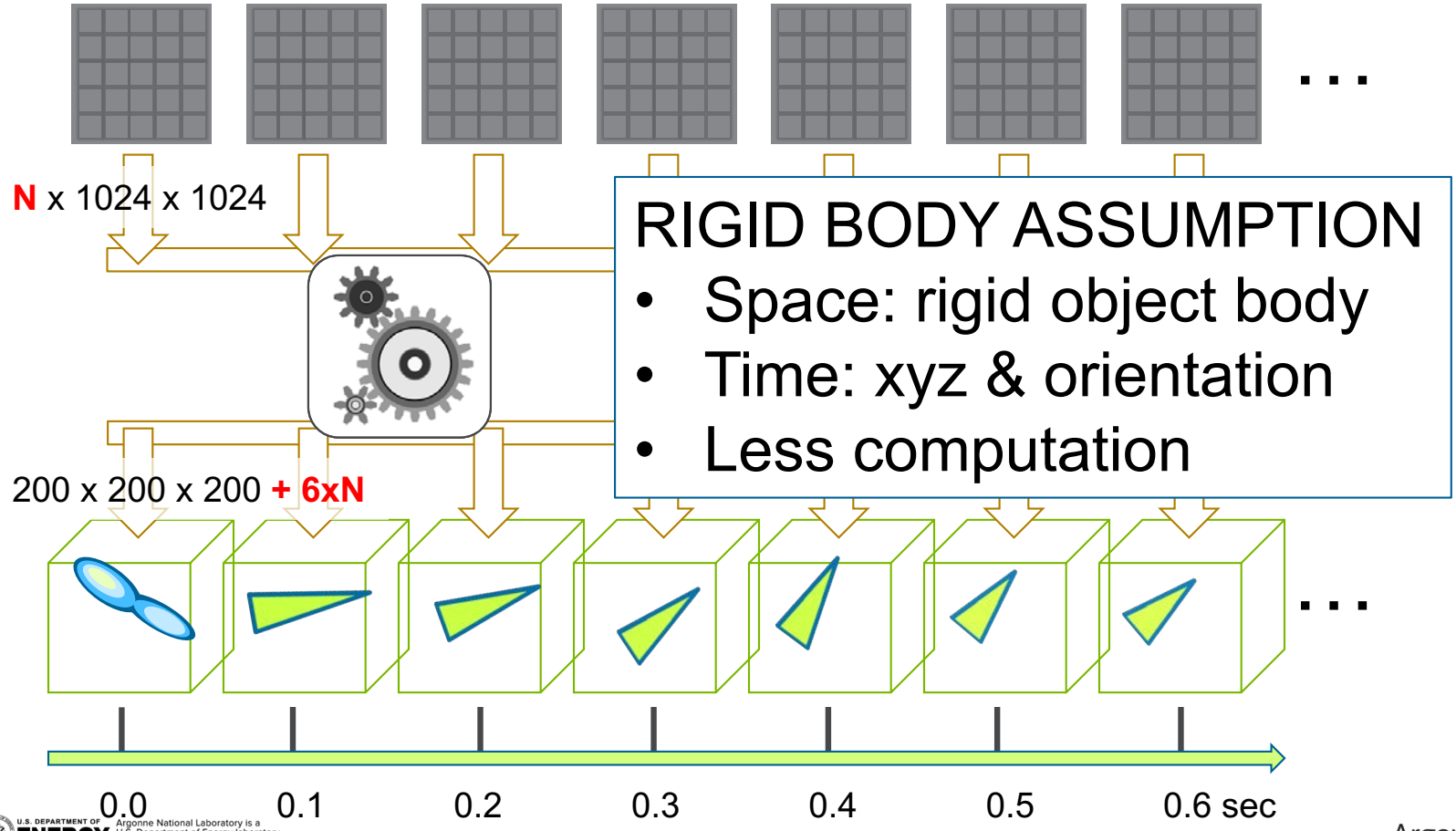
$$\mathbf{g} = \mathbf{H}\mathbf{f} + \boldsymbol{\epsilon}$$

$$\hat{\mathbf{f}} = \arg\min_{\mathbf{f}} \|\mathbf{g} - \mathbf{H}\mathbf{f}\|_2^2 + \lambda\Phi(\mathbf{f}) \quad \text{subject to } \mathbf{f} \geq 0$$

MFM AND THE 4TH DIMENSION



MFM AND THE 4TH DIMENSION



MULTIPLE-FRAME MFM RECONSTRUCTION

- Batch approach

$$\text{For } k = l-m, \cdots, l+m$$

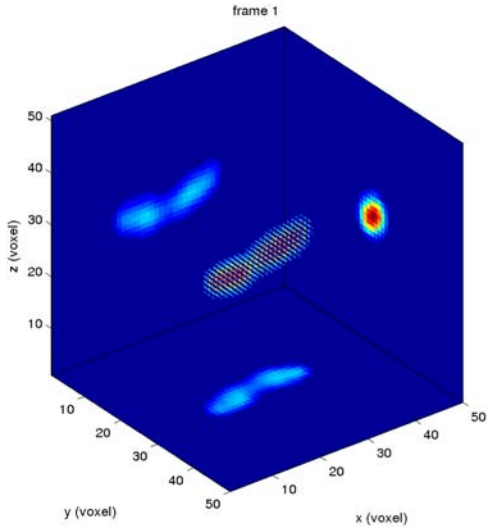
$$\mathbf{g}_k = \mathbf{H}\mathbf{M}_{l,k}(\boldsymbol{\alpha}_{l,k})\mathbf{f}_l + \boldsymbol{\epsilon}_{l,k}$$

$$\{\hat{\mathbf{f}}_l, \hat{\boldsymbol{\alpha}}_{l,k}\} = \arg \min_{\mathbf{f}_l \geq 0, \boldsymbol{\alpha}_{l,k}} \sum_{k=l-m}^{l+m} \|\mathbf{g}_k - \mathbf{H}\mathbf{M}_{l,k}(\boldsymbol{\alpha}_{l,k})\mathbf{f}_l\|_2^2 + \lambda\Phi(\mathbf{f}_l) + \omega \sum_{k=l-m}^{l+m} \|\boldsymbol{\alpha}_{l,k}\|_2^2$$

- Recursive approach

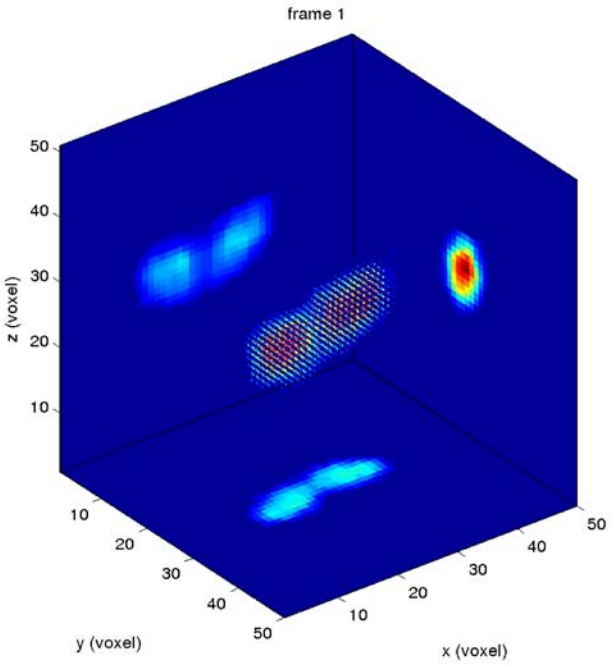
$$\{\hat{\mathbf{f}}_k, \hat{\boldsymbol{\alpha}}_{k-1,k}\} = \arg \min_{\mathbf{f}_k \geq 0, \boldsymbol{\alpha}_{k-1,k}} \|\mathbf{g}_k - \mathbf{H}\mathbf{f}_k\|_2^2 + \lambda\Phi(\mathbf{f}_k) + \eta\|\mathbf{f}_k - \mathbf{M}_{k-1,k}(\boldsymbol{\alpha}_{k-1,k})\mathbf{f}_{k-1}\|_2^2$$

SIMULATION

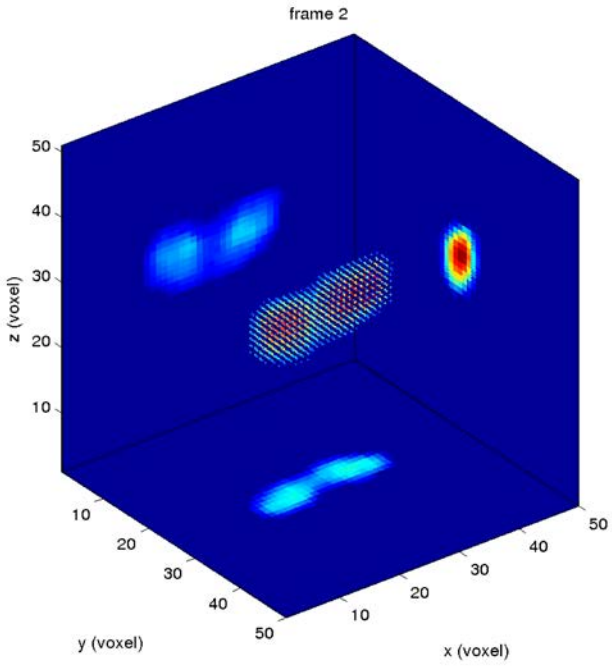


- Object
  - Bacteria image from confocal microscopy
  - Movement: rotation + translation
  - Total frames: 30
- MFM measurement
  - PSF: scaled measured PSF
  - Noise: additive Gaussian noise

MFM RECONSTRUCTION

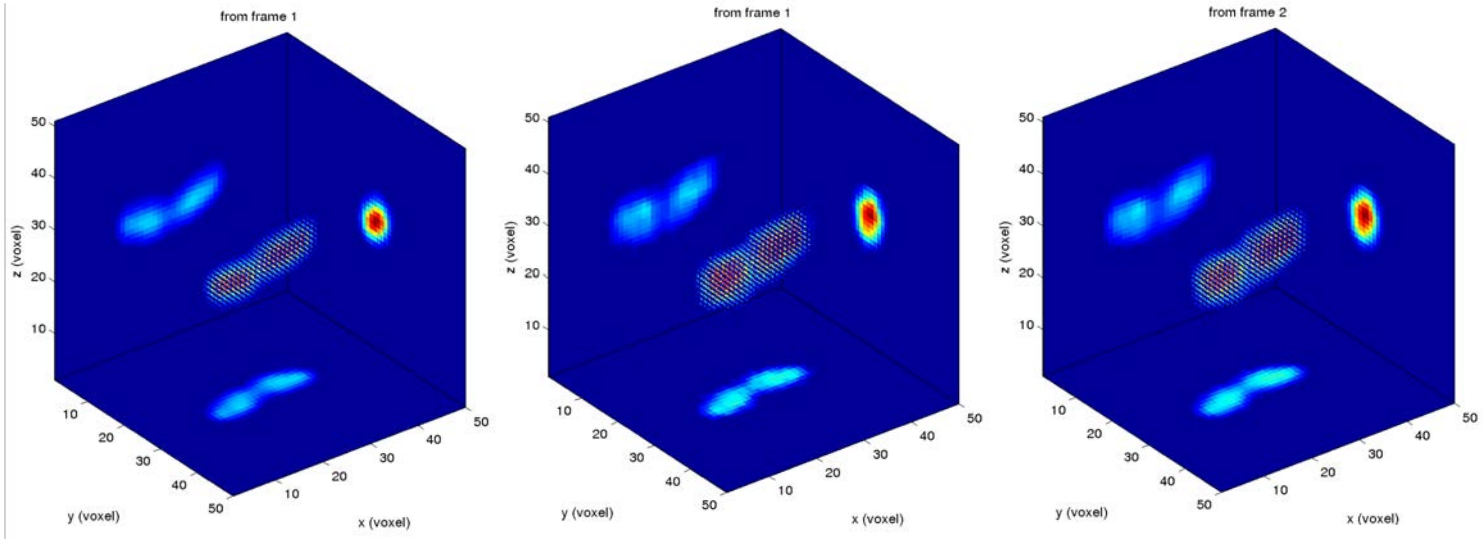


Single-frame reconstruction
Average PSNR: 36.61 dB



Multiple-frame recursive
Average PSNR: 39.67 dB

MFM RECONSTRUCTION

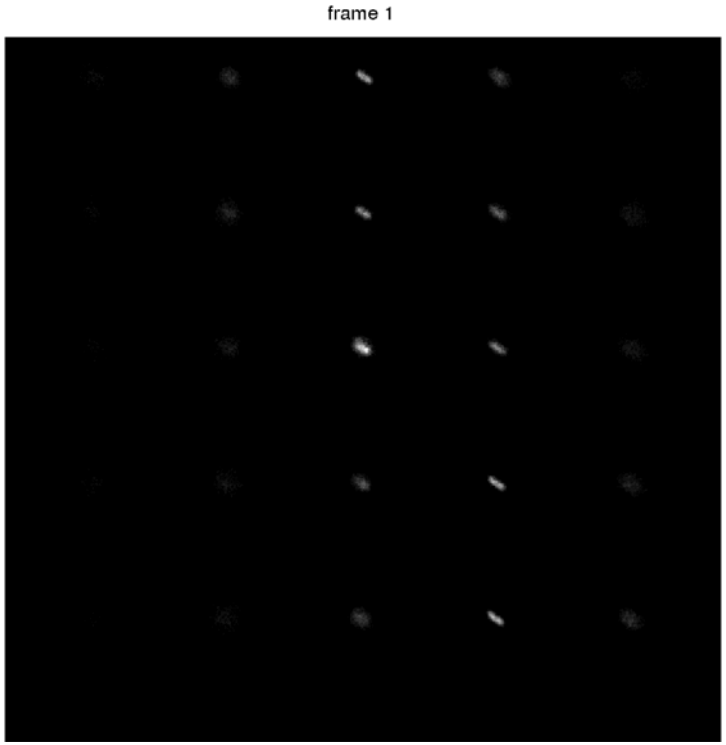


Ground truth

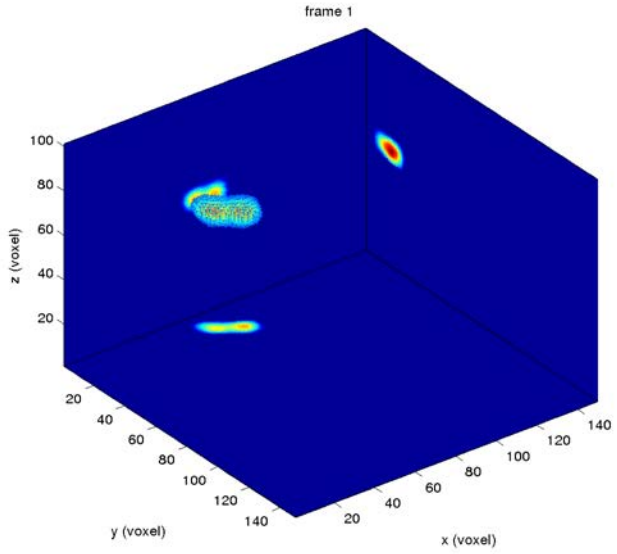
Single-frame reconstruction
Average PSNR: 36.61 dB

Multiple-frame recursive
Average PSNR: 39.67 dB

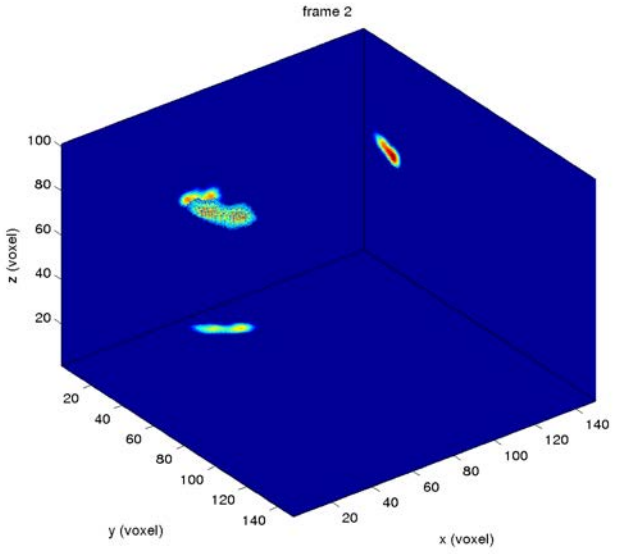
EXPERIMENTS - MFM MEASUREMENT



EXPERIMENTAL RESULTS

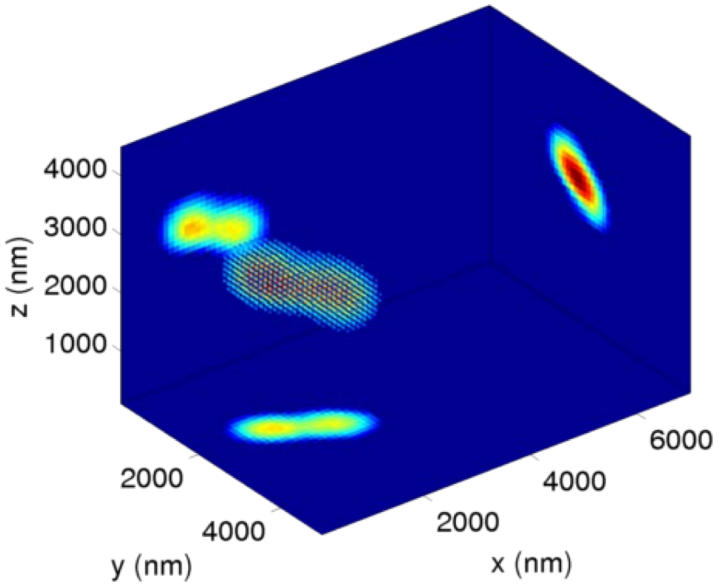


(a) Single-frame reconstruction

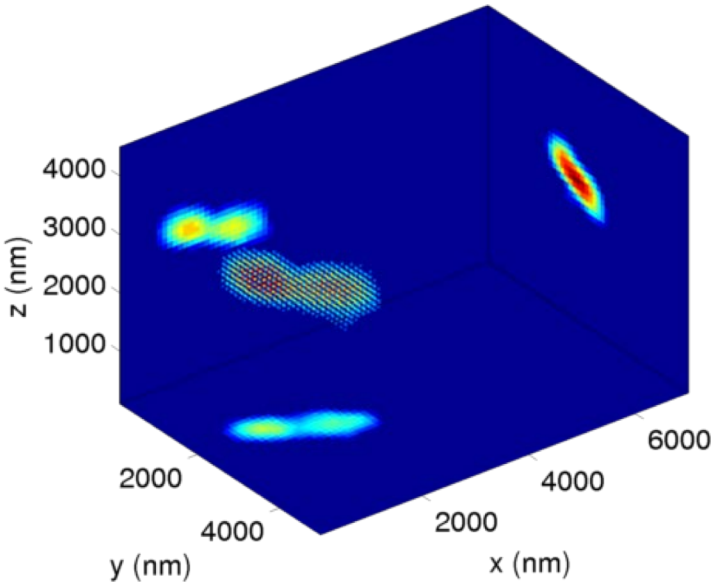


(b) Multiple-frame recursive

EXPERIMENTAL RESULTS – FRAME 9

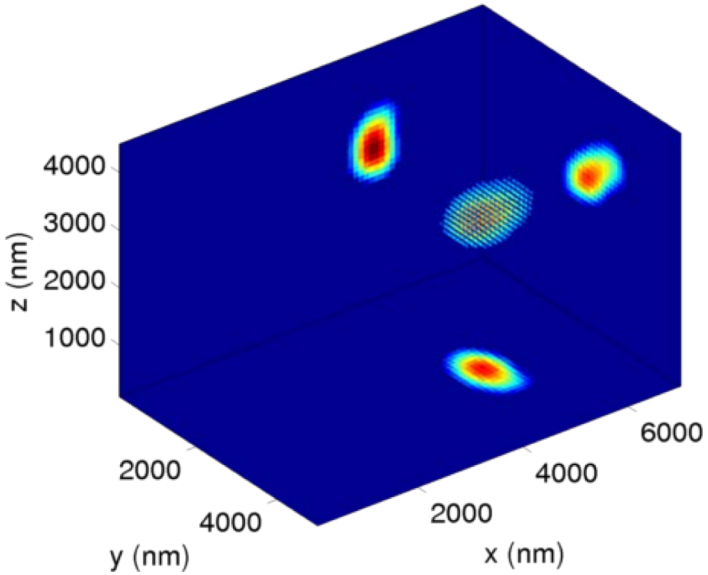


(a) Single-frame reconstruction

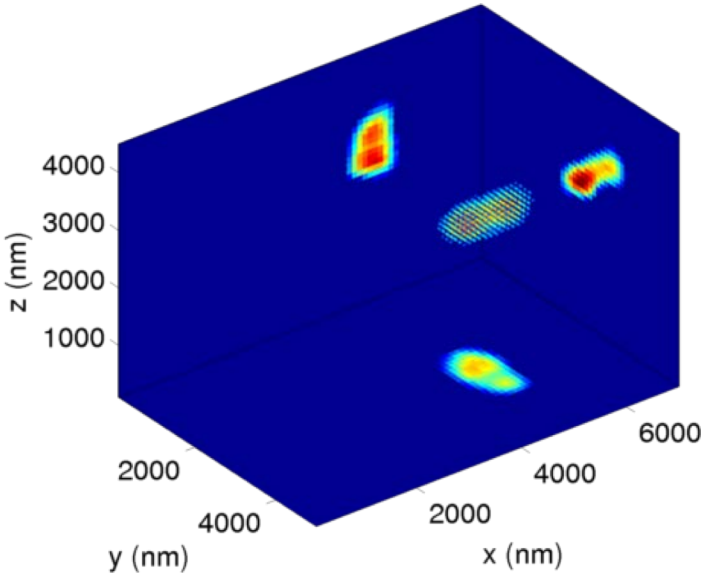


(b) Multiple-frame recursive

EXPERIMENTAL RESULTS – FRAME 42



(a) Single-frame reconstruction



(b) Multiple-frame recursive

MFM IN ACTION

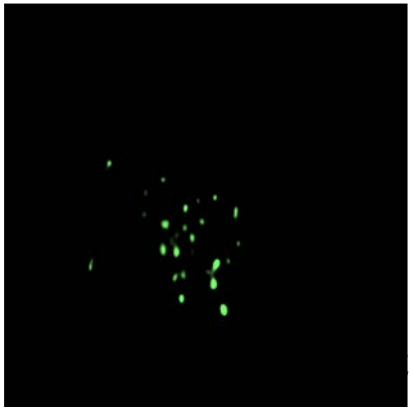
MFM OF INSULIN LABELED WITH MCHERRY IN MIN6

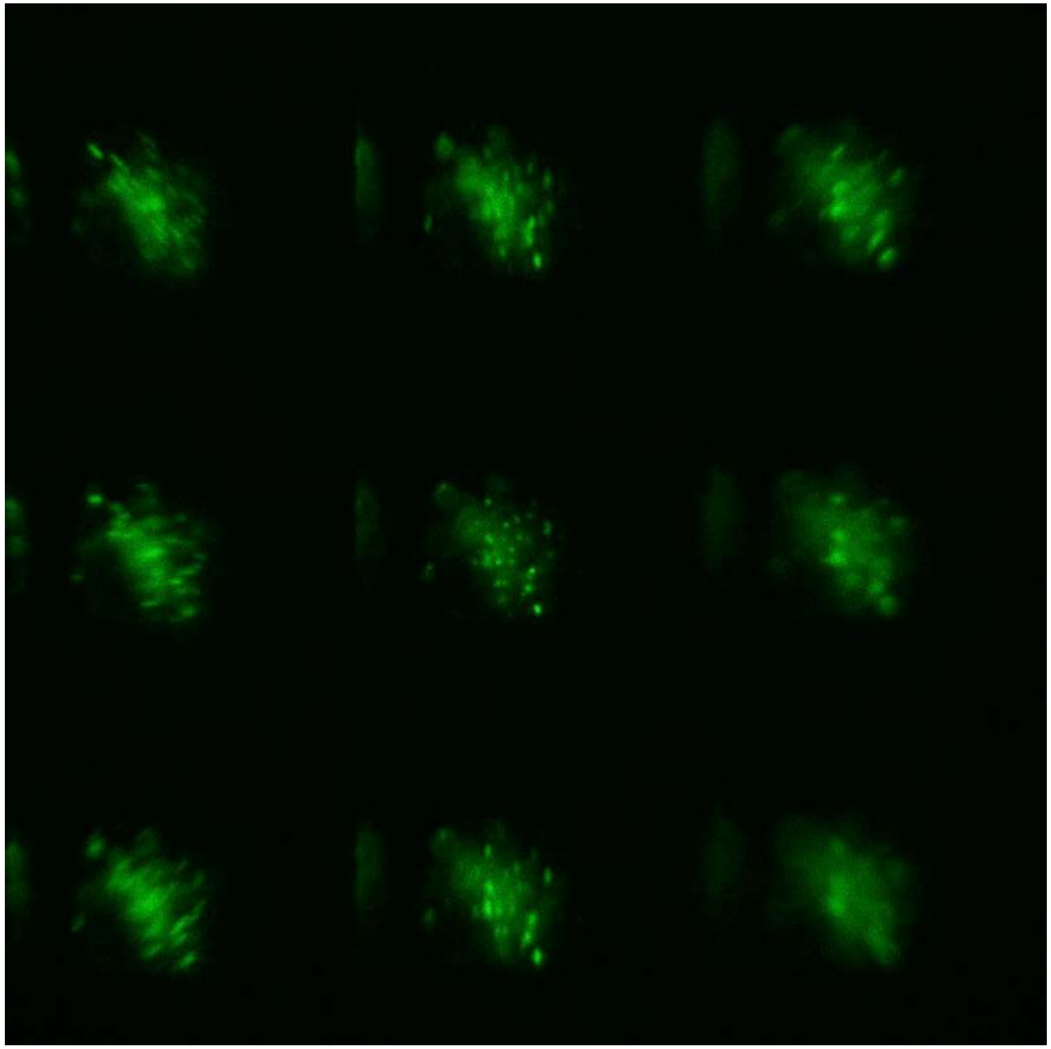
mCherry-labeled insulin granules in MIN6 sublines

- MIN6: mouse insulinoma 6 (popular pancreatic beta-cell line)

Exposure time:100ms

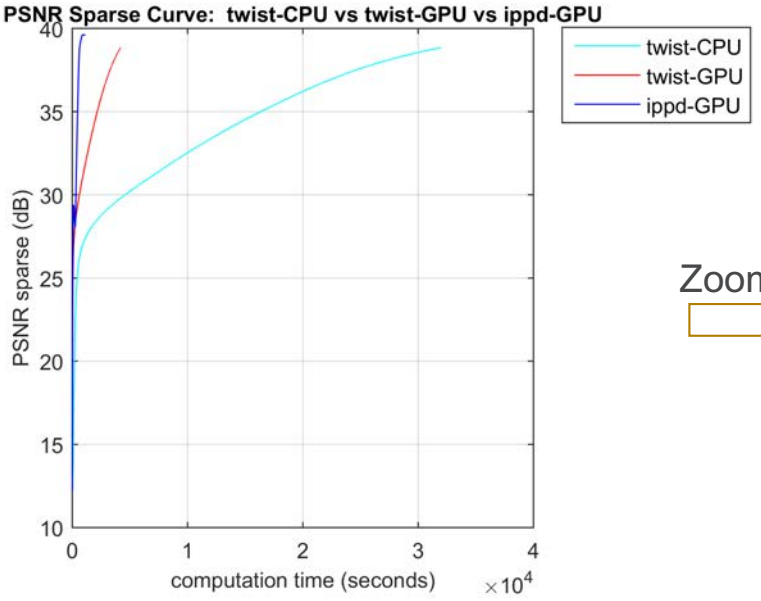
10 frames/s



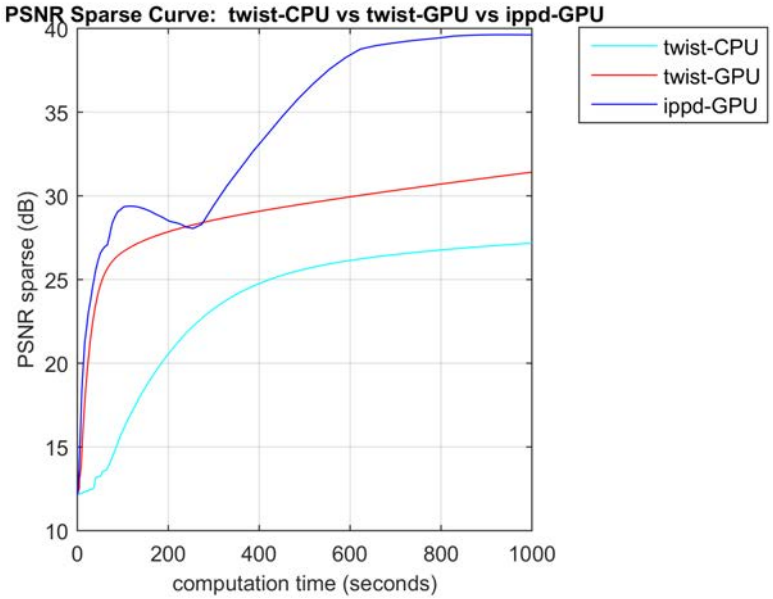


COMPUTATIONAL IMPROVEMENTS

FASTER ALGORITHMS USING GPU & NEW INTERIOR POINT METHOD (IPM)



Zoom in



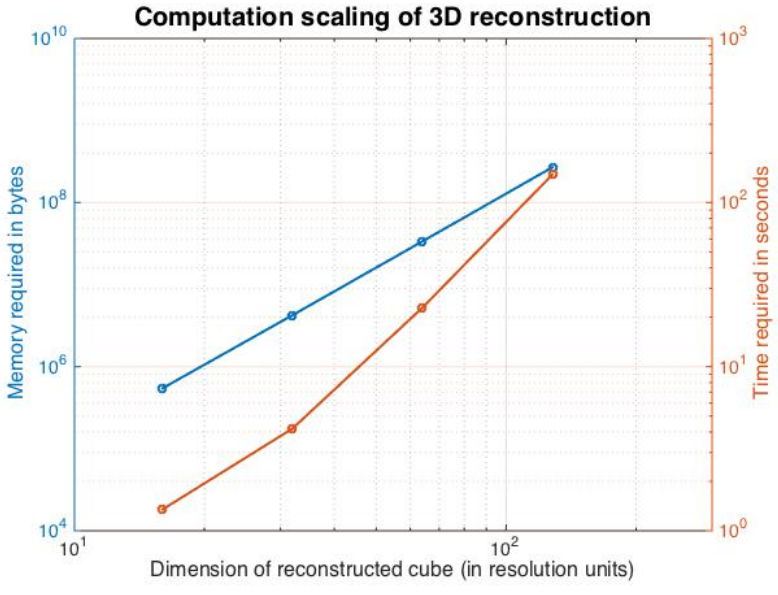
our 50x speedup Combine GPU & IPM
GPU 8x and IPM 6x speed up in 2017.09

PARALLEL ANALYSIS

Provided by Mark Hereld

- Motivations
  - Organizing repetitive tasks
  - Run many interlinked computations automatically and efficiently
  - Speed
- Applications to our problem
  - Synthetic data generation
  - Performance characterization
  - Algorithm development & tuning
  - Real-time reconstruction

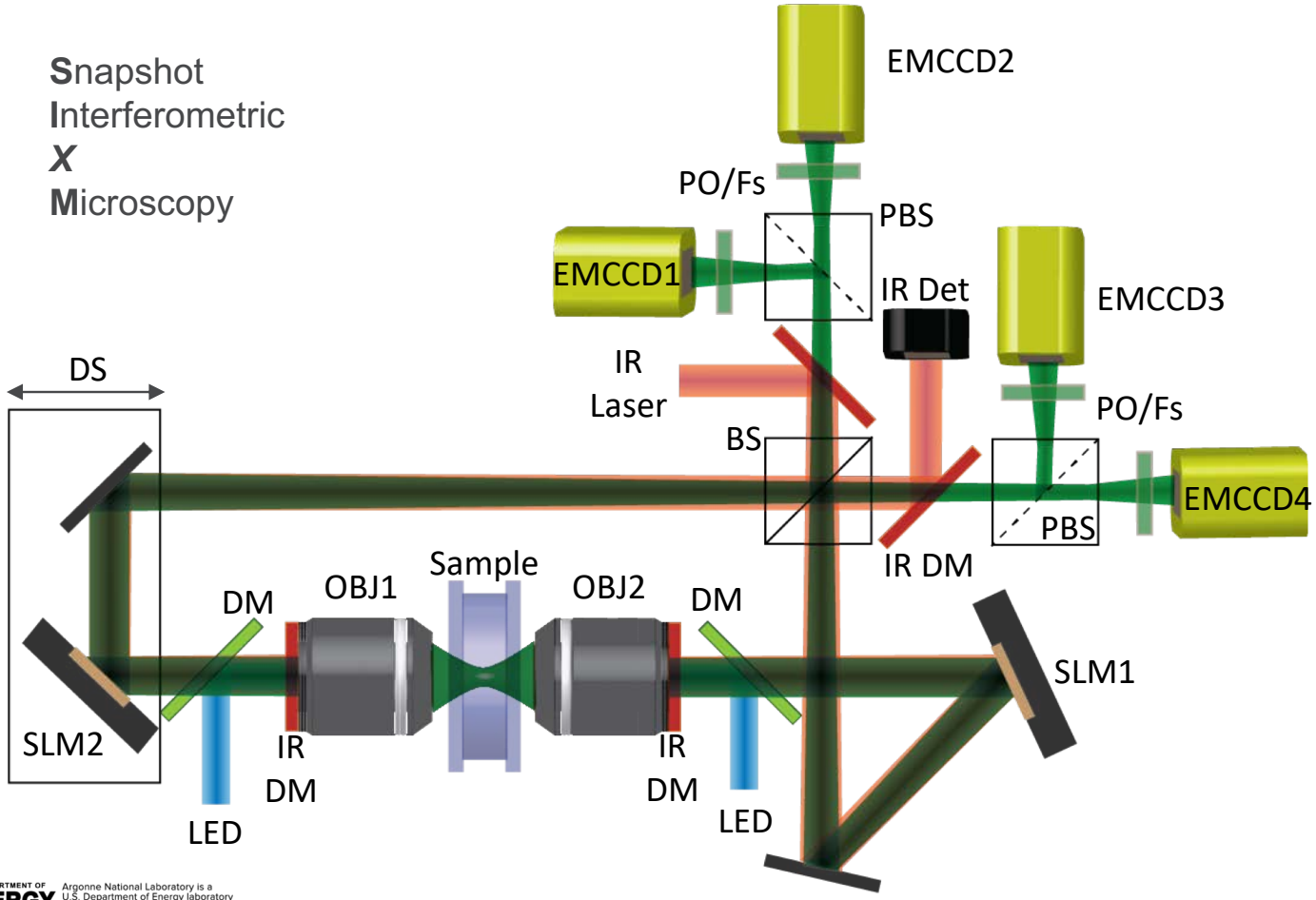
- PROGRESS
  - Running 3D reconstructions on cluster
  - Basic performance



WIP: ALTERNATE IMAGING METHODS FOR 3D

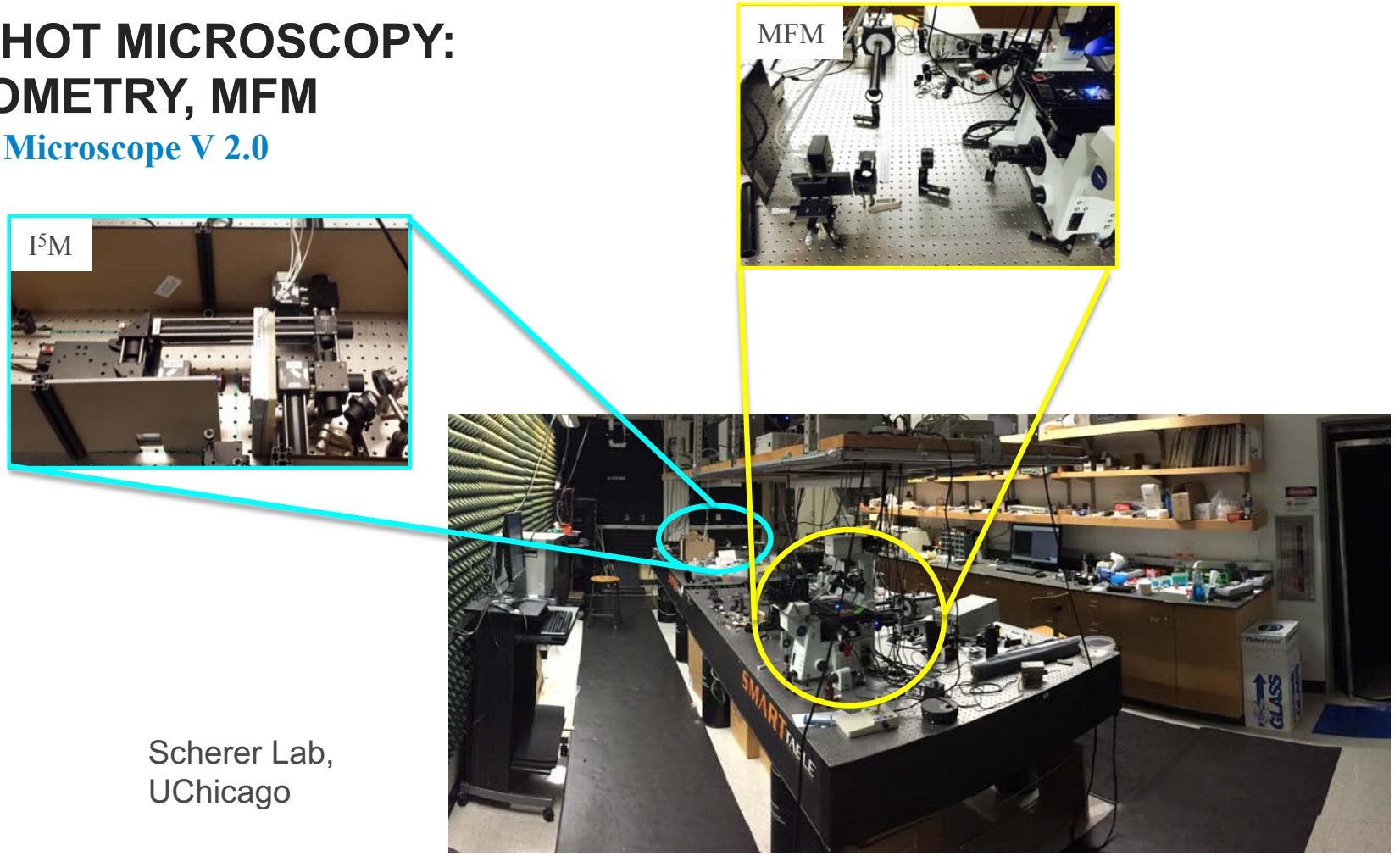
OPTICAL SETUP: 3D-SIXM

Snapshot
Interferometric
X
Microscopy



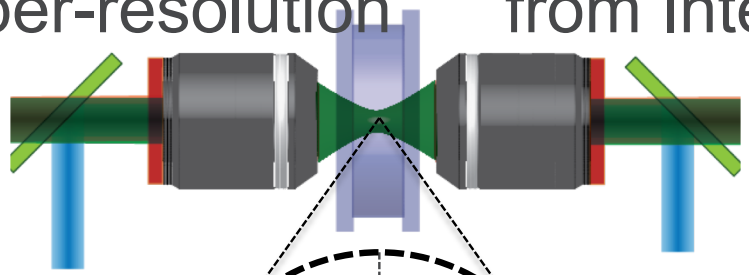
3-D SNAPSHOT MICROSCOPY: INTERFEROMETRY, MFM

$I^{2/5}M$ Microscope V 2.0



Scherer Lab,
UChicago

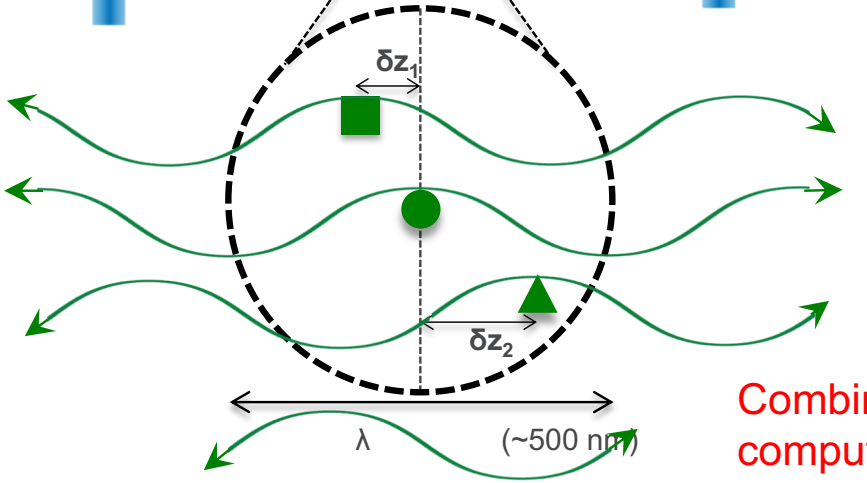
Axial super-resolution from Interferometry



Axial direction
z-axis

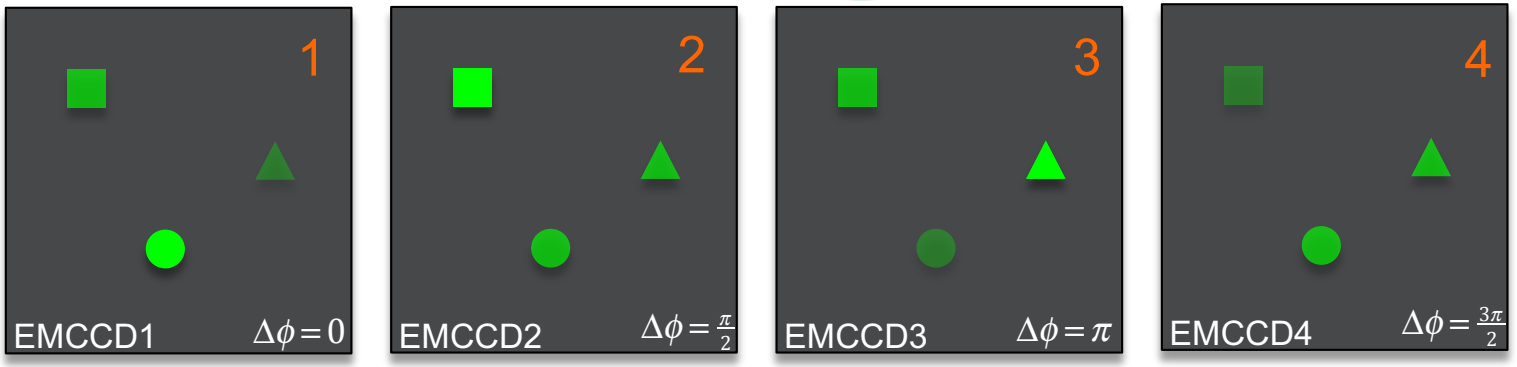
Phase shift related to emitter position

δz_1

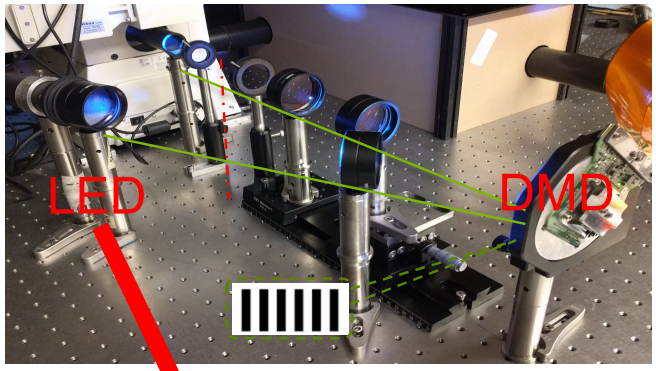


Phase maps
=>
intensity
on detectors

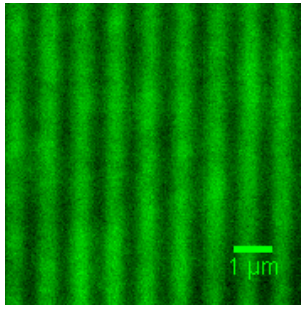
Combine 1-4 by computational imaging



STRUCTURED ILLUMINATION MICROSCOPE

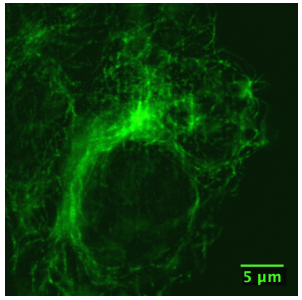


illumination

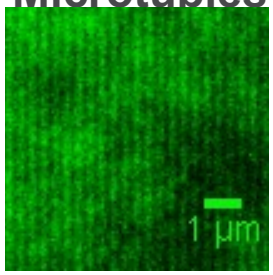


Period:1um

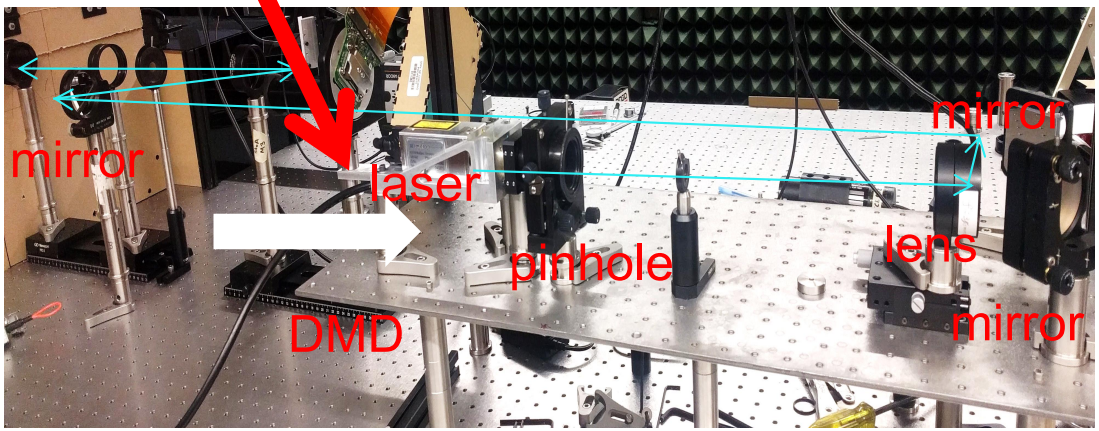
sample



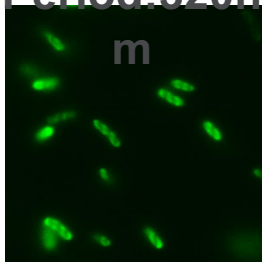
Microtubles



Period:320n
m



Periplasm
cell



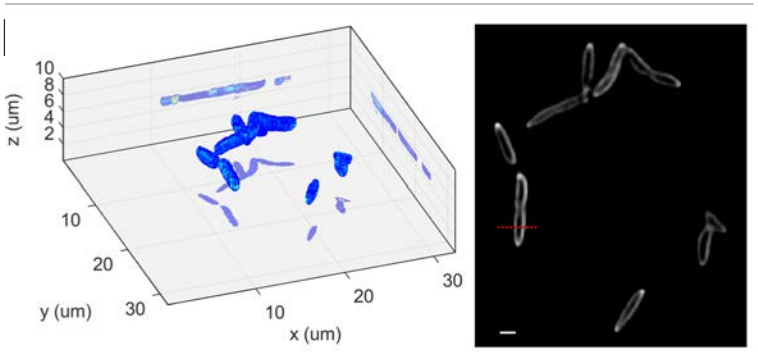
CLOSING

3D VOLUME SNAPSHOT IMAGING

- Current technique:
  - Captures 3D at frame rate of detector
    - Able to image tumbling cells
    - Resolution sufficient for periplasm (voxels ~50 nm^3)

Inside the cell?

- Need to combine techniques to get resolution (s
  observe celluar processes



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EXASCALE COMPUTING PROJECT

THANK YOU!


U.S. DEPARTMENT OF
ENERGY
Office of
Science


National Nuclear Security Administration