

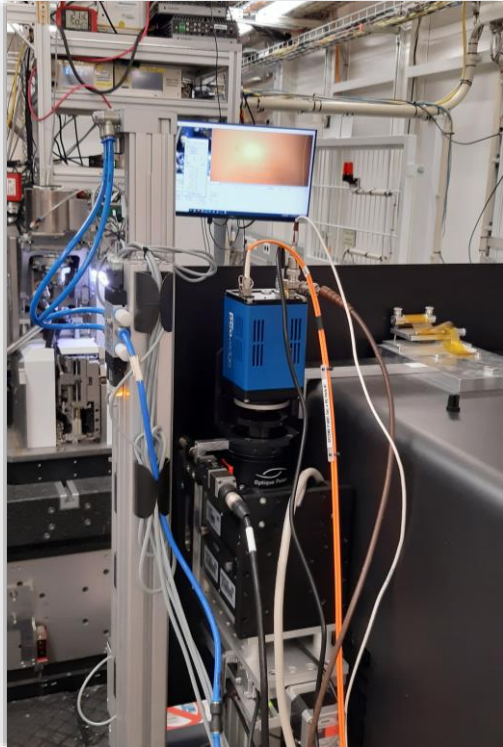
From Raw Data to Tomographic Reconstruction in 30s

Marina Nikolova, EMBL

NOBUGS, 2024

Frame Tripping
at the EMBL P14 Beamline

HiTT at P14

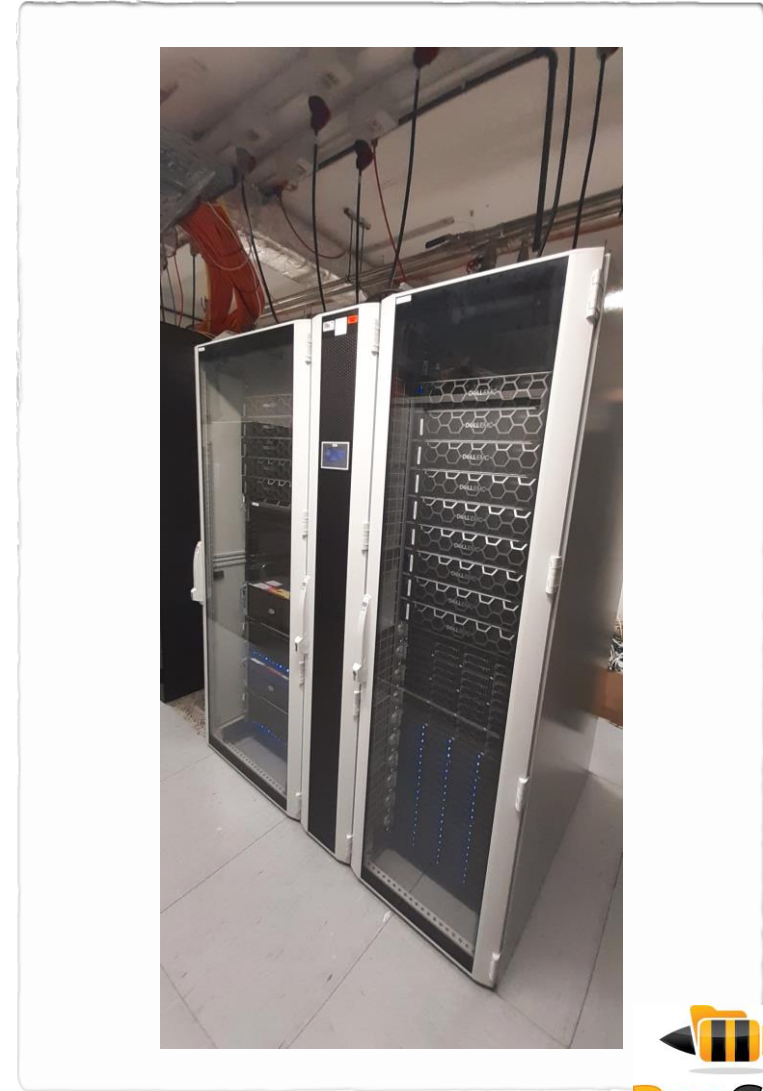


Data Acquisition

PCO
Camera
Server

Arapaho

PCO Edge Camera
4 MP @ 100Hz
Kaya Driver, Ubuntu 22.04



P12
P13
P14
TREXX



Samples

FOV 1.2 mm

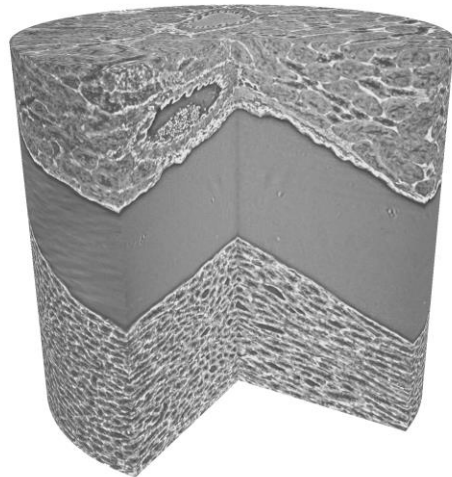
Tissue

Plants

Insects

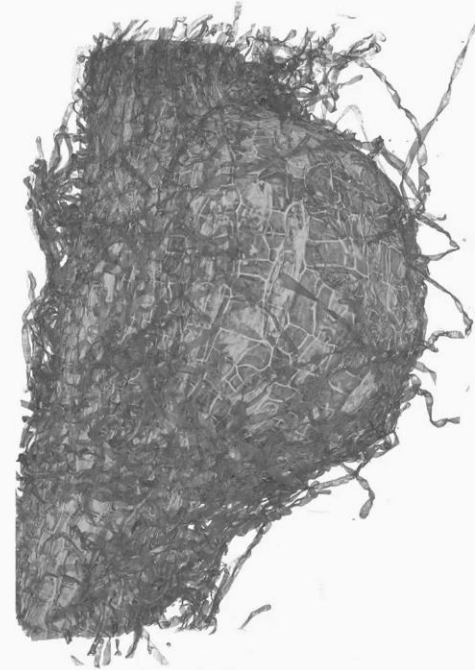
Plankton

...



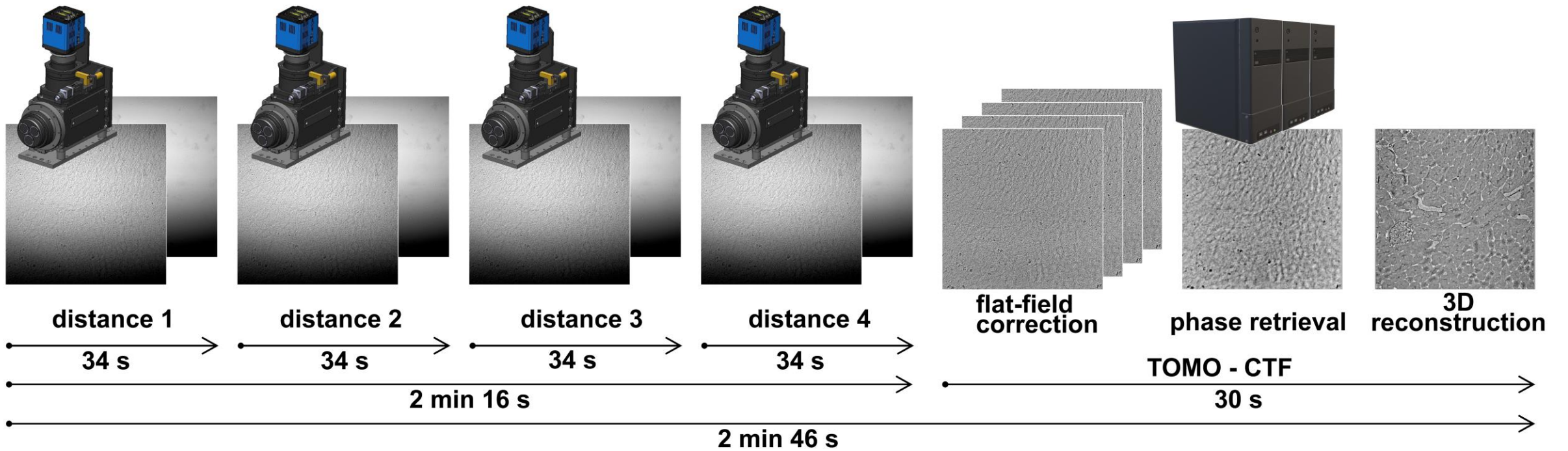
Formalin Fixed Paraffin Embedded Mouse Kidney

Plant Root Nodule

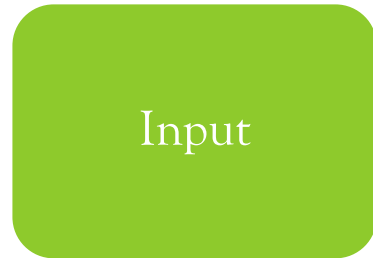


Data Courtesy of Jonas Albers
in Collaboration with the University of Aarhus

Data Acquisition and Reconstruction Timeline



TOMO-CTF



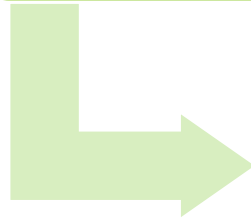
- Parameters File
- Arguments

```
ENERGY= 18.0001536104
PIXELSIZE= 0.650
DISTANCES= 0.073000, 0.077000, 0.083000, 0.092000,
FLATAVG = 3
ROI = 0, 8, 2048, 2040
BETADELTA= 0.1
ZEROCOMP= 0.1
PADDING= 200
ROTATION-AXIS-GUESS= 249
OFFSET-Y-360= 0
PREFIX= tomo_111_d1_1_,tomo_111_d2_1_,tomo_111_d3_1_,tomo_111_d4_1_
PREFIX-FF = _ff_tomo_111_d1_1_,ff_tomo_111_d2_1_,ff_tomo_111_d3_1_,ff_tomo_111_d4_1_
```



- Crop
- Divide by Average of 3 Best Matches

```
Tag 1200: 0.987608,0.987929,0.987967,0.988117,0.988214,0.987805,0.987216,0.988093,0.987900,0.988210,0.986738,0.988037,0.988108,0.988017,0.988079,0.988148,0.988065,0.988198,0.987612,0.988262,0.987455,0.986171,0.987514,0.988020,0.988138,0.988137,0.988163,0.988131,0.988202,0.988224,0.987858,0.987787,0.988217,0.987855,0.987905,0.988141,0.987154,0.987501,0.988138,0.987863,0.988214,0.987815,0.988215,0.987945,0.988124,0.988027,0.988029,0.988126,0.988180,0.986611,0.987129,0.988235,0.987320,0.988152,0.988149,0.988028,0.987412,0.988231,0.987223,0.988211,0.987727,0.987878,0.986723,0.988193,0.987457,0.988139,0.988165,0.987112,0.986712,0.988087,0.988257,0.988181,0.988141,0.988120,0.988093,0.987928,0.988075,0.987986,0.988186,0.987465,0.987738,0.988235,0.988017,0.988039,0.988147,0.987506,0.988158,0.988045,0.985670,0.988105,0.988246,0.988156,0.986438,0.987751,0.985784,0.988205,0.987938,0.987716,0.986056,0.987609
Tag 1201: 19,70,90
```



- Shifts/Filter
- Pad
- Contrast Transfer Function Algorithm on 4 Distances



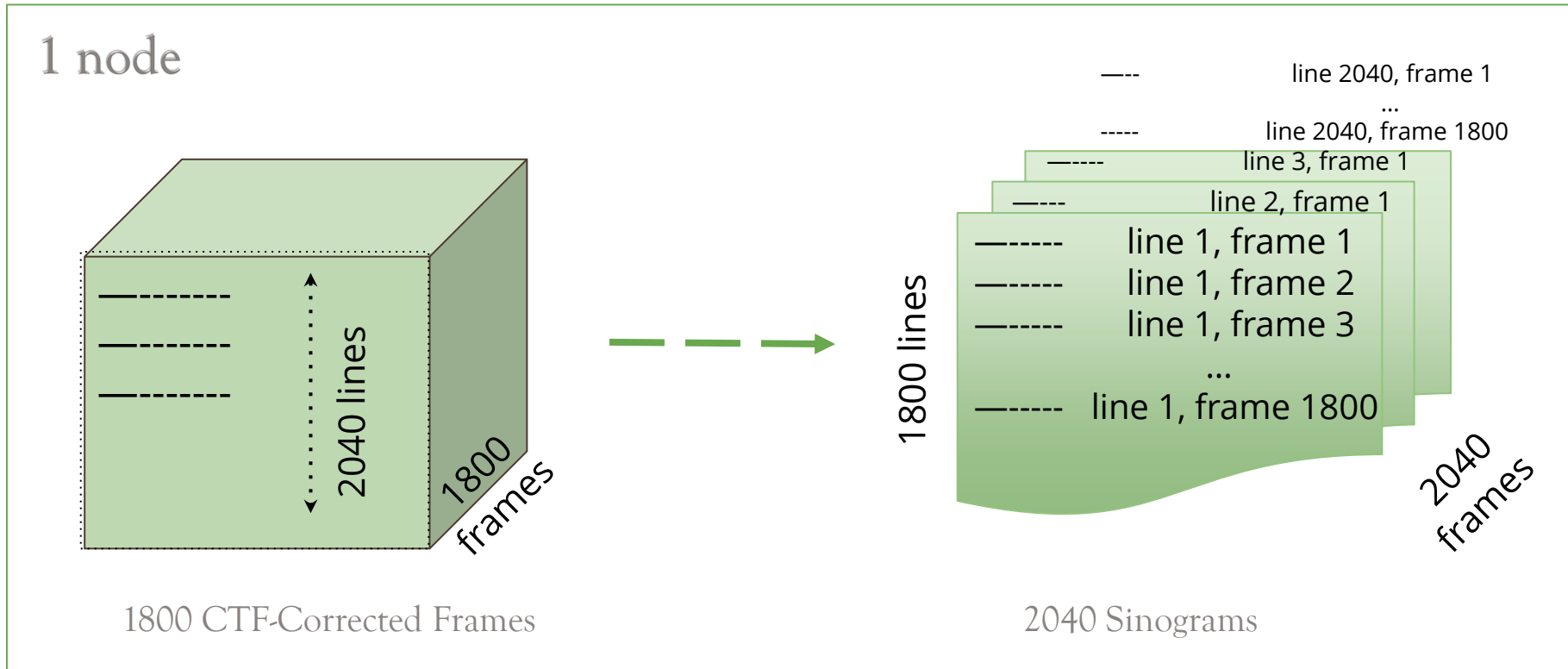
- Rotation Center
- Store as Sinogram
- TomoPy Gridrec/Mask

Cloetens et al. (1999) J. Phys. D: Appl. Phys. 32, A145.

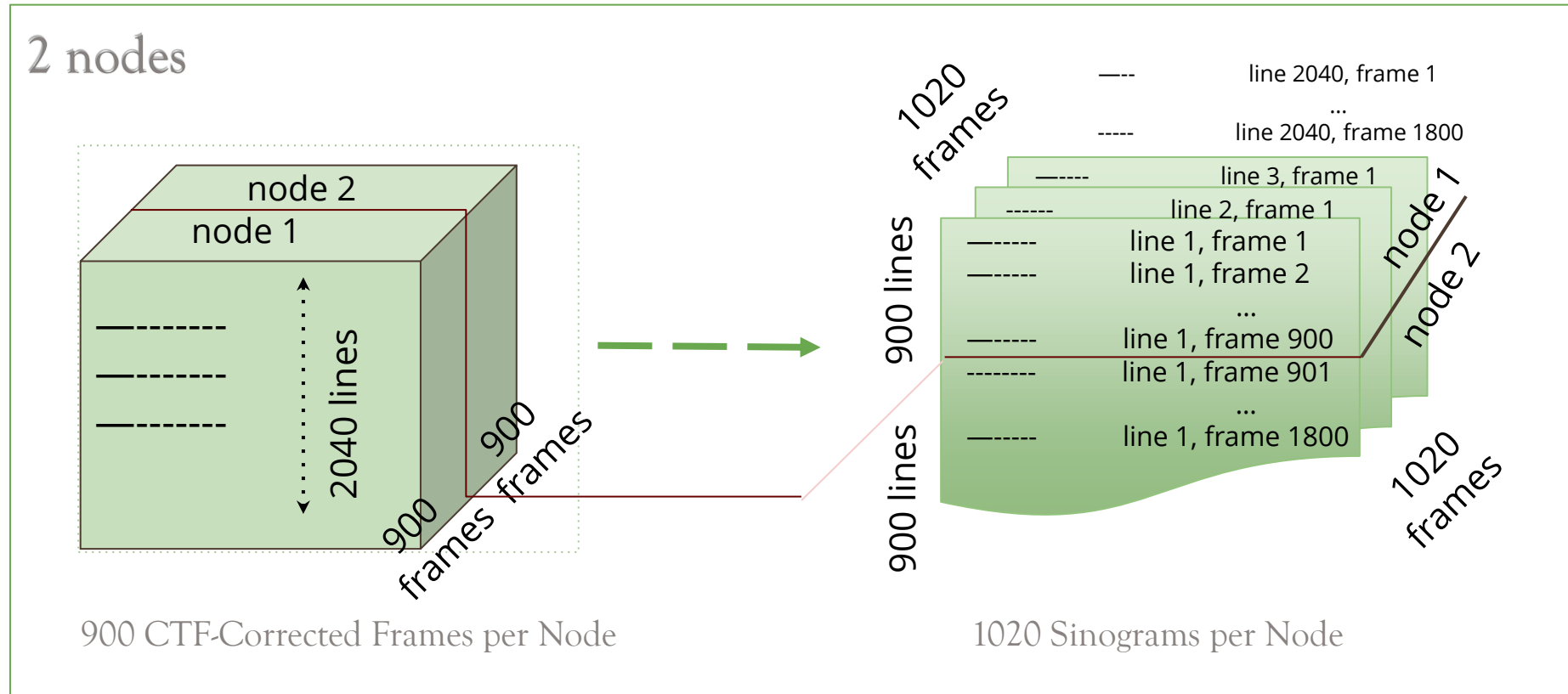
Zabler, et al. (2005). Review of Scientific Instruments 76, 073705.

Gürsoy D, et al. (2014) Journal of Synchrotron Radiation, 21(5):1188-1193.

CTF-Corrected Frames → Input to Reconstruction



CTF-Corrected Frames → Input to Reconstruction



Parallelization

Posix Threads

- ◇ Processing Threads
- ◇ Disk-Writing Threads
- ◇ Threads for Node-to-Node Data Sending
- ◇ Intermediate Result Synchronization Threads



MPI

- ◇ Cluster Node Allocation via Slurm salloc ~exclusive
- ◇ 1 MPI Process per Cluster Node
- ◇ Remote Memory Access via Exposed Windows
- ◇ Partially Assembled Sinograms in Local Memory Window
- ◇ In-place Sinogram Writes on Remote Node via MPI_Put
- ◇ Node Synchronization Points: MPI Windows Creation, Rotation Center Determination, CTF Generation, Log File Disk Writes

Live Performance

Collection Type: **Single** 180°

4 x 1810 Projections, 4 x 100 Flat Fields


Raw Frame Dimensions: 2048 x 2048

Raw Input Data Size: 60 GB

Default Output Size (CTF + Reconstruction): 60 GB

1 Node, 88 Cores: 65s

2 Nodes, 176 Cores: 45s

 4 Nodes, 352 Cores: 30s

DECTRIS Cloud, 1 Lightspeed Node, 192 Cores: 30s

with RAM Reads/Writes

} with BeeGFS
Reads/Writes

1947.418u	144.025s	0:26.30	7952.2%
1450.622u	153.482s	0:34.14	4698.5%
1368.075u	135.959s	0:48.04	3130.7%
1228.699u	141.451s	0:38.34	3573.6%
1481.687u	123.528s	0:29.77	5392.0%
1306.430u	161.879s	0:42.71	3437.8%
1332.300u	163.034s	0:34.91	4283.3%
1767.404u	146.732s	0:26.69	7171.7%
1347.893u	141.530s	0:43.86	3395.8%
1172.188u	165.633s	0:40.99	3263.7%
1826.316u	147.984s	0:27.82	7096.6%
1792.632u	137.073s	0:26.27	7345.6%
1468.754u	173.374s	0:30.70	5348.9%
1738.469u	159.184s	0:27.48	6905.5%
1308.559u	156.443s	0:30.05	4875.1%
1359.292u	176.165s	0:32.63	4705.6%
1817.899u	130.557s	0:25.90	7522.9%
1428.294u	139.220s	0:30.15	5199.0%
1311.082u	177.116s	0:35.00	4251.9%
1707.092u	142.276s	0:26.19	7061.3%
1803.599u	134.438s	0:27.14	7140.8%
1761.240u	160.219s	0:27.93	6879.5%
1815.836u	114.503s	0:25.42	7593.7%
1313.402u	167.891s	0:43.08	3438.4%
1385.540u	163.961s	0:36.91	4198.0%
1771.703u	118.744s	0:26.05	7256.9%
1449.743u	130.852s	1:04.25	2460.0%
1241.453u	191.231s	1:19.27	1807.3%

More Challenging Case: Full Beamline Load
P13 (Eiger16M) / P14 XIMG Queued Collections

Extended Field of View

Collection Type: Single 360°

4 x 3610 Projections, 4 x 100 Flat Fields

Overlap approx. 450 pixels

Process 2 Projections at a Time

Additional Operations:

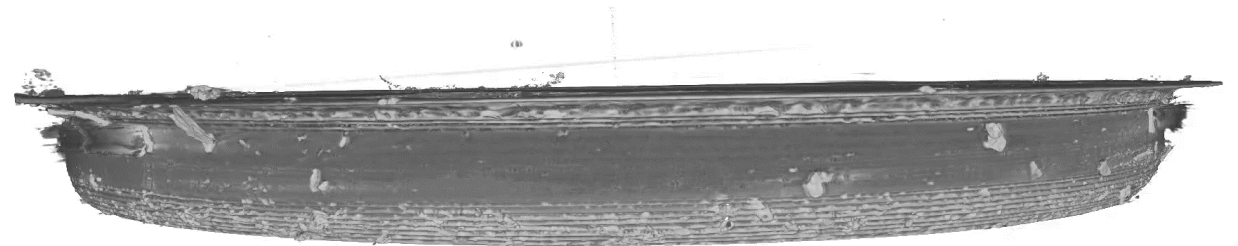
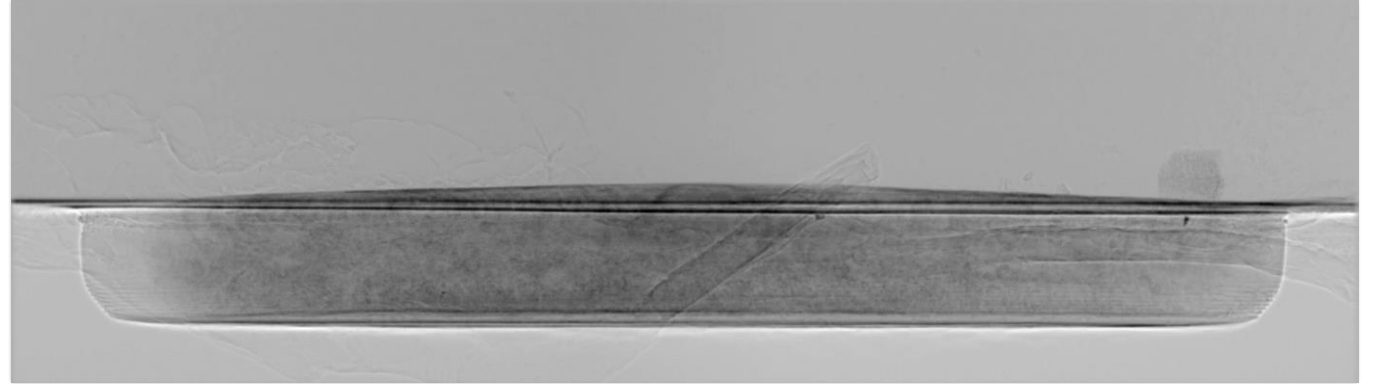
Find Shift between Frames in 180° Pair

Flip 1 Frame

Glue

Mask to Apply Cutouts

Heavy Metal Stained, Resin Embedded Plankton Sample from EMBL TREC



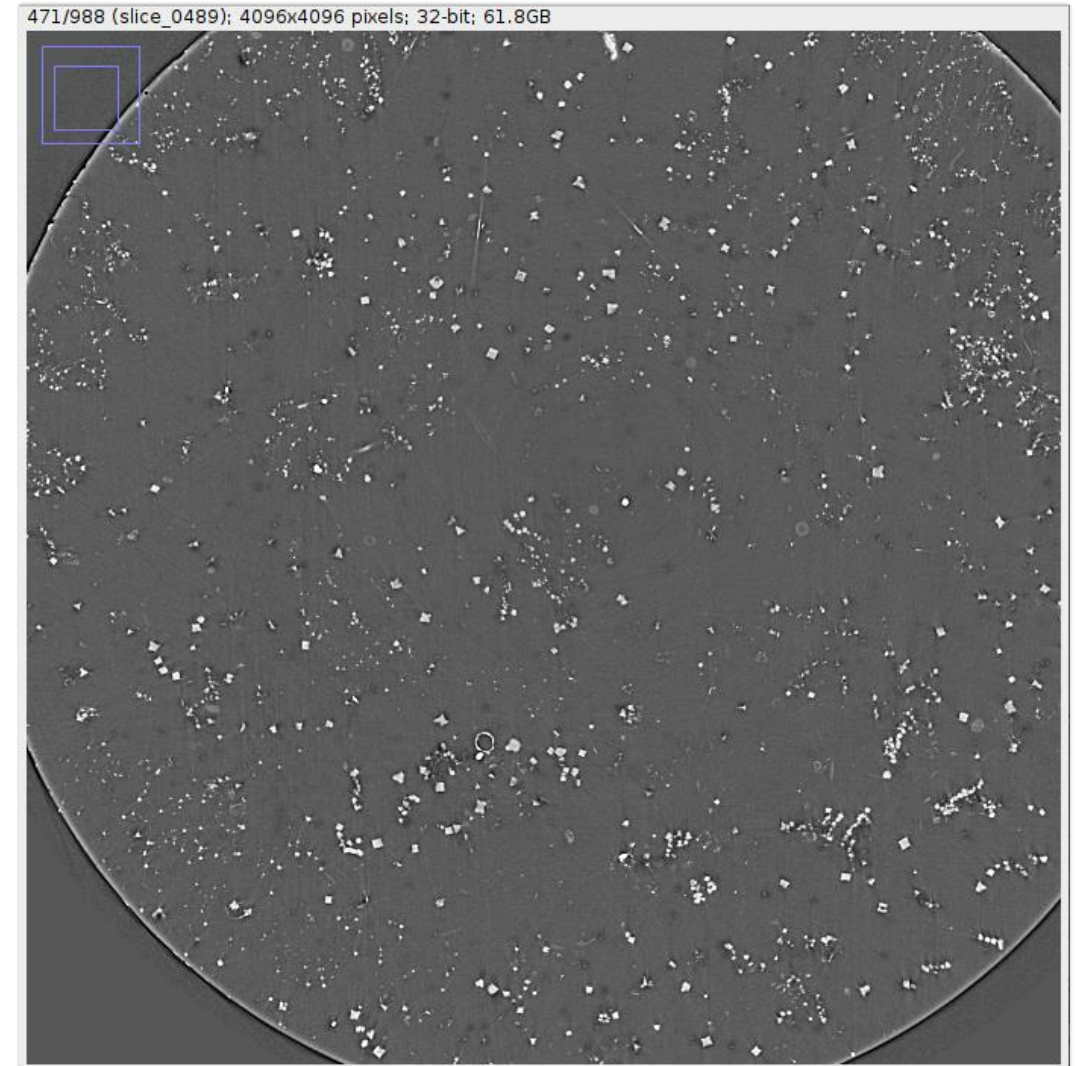
Data Courtesy of Angelika Svetlove

Extended Field of View

Collection Type: Single 360°

4 x 3610 Projections, 4 x 100 Flat Fields

Raw Frame Dimensions	2048 x 2048	2048 x 1024
Raw Input Data Size	116 GB	56 GB
Default Output Size CTF, Glued CTF, Reconstruction	240 GB	119 GB
1 Node, 88 Cores	150s	90s
2 Nodes, 176 Cores	95s	57s
4 Nodes, 352 Cores	70s	38s

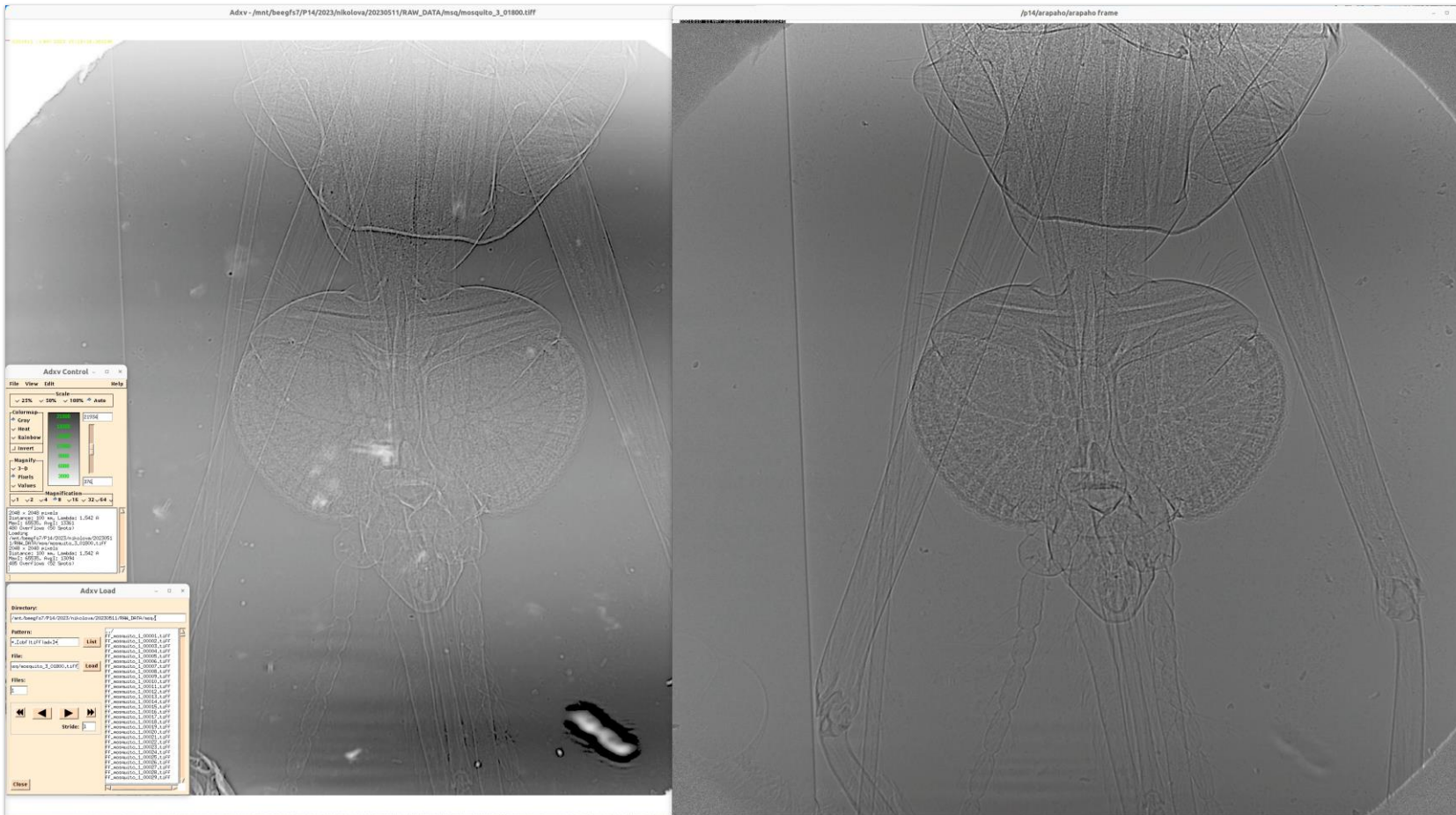


Reconstructed Slice, EMBL TREC Sample

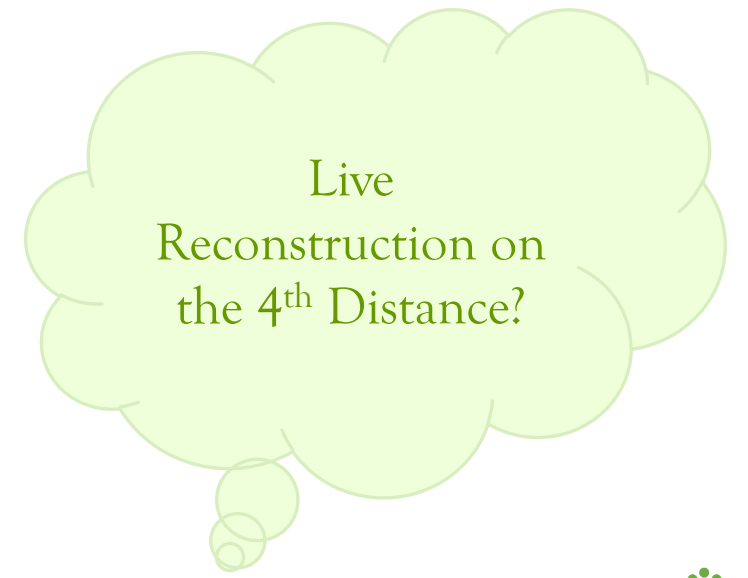
Live Viewers

Mosquito
Nedal Darif EMBL Heidelberg
Recording @ 11 fps

Viewer	Data Format	Source	Display Rate
ADXV	Raw Tiff Files	Read from BeeGFS	25 fps
FFC Viewer	Flat-Field Corrected JPEGs	Received over TINE	23 fps



Albers J, Nikolova M, ... Bourenkov G and Duke E.
High Throughput Tomography (HiTT) on EMBL
Beamline P14 on PETRA III. Journal of Synchrotron
Radiation (2024). DOI: 10.1107/S160057752300944X



Summary and Outlook

- ◆ 30s Reconstruction for Single 180° Collections
- ◆ 70s Reconstruction for Extended Field of View 360° Collections
- ◆ Challenging: Queued 180° Collections
- ◆ Yet More Challenging: Queued Extended Field of View 360° Collections
- ◆ Can Stitching be Automated and Fast?
- ◆ How about Compression?
- ◆ Is our Extended Field of View 360° Scan Under-sampled for Gridrec?

Acknowledgements

◆ **Gleb Bourenkov**

◆ **X-Ray Imaging Team**

◆ Jonas Albers

◆ Angelika Svetlove

◆ Mathew Lawson

◆ Ksenia Denisova

◆ Fabio de Marco

◆ Elizabeth Duke

EMBL Hamburg IT

Andrea d'Amato

Eduard Avetisyan

Eniola Fadare

EMBL Hamburg Instrumentation

Stefan Fiedler and Team

Thomas R. Schneider

Maxim Polikarpov

DECTRIS

Max Burian

Pascal Störzbach