Preprocessing with ScipionTomo

Spanish Research Council

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CSIC
Consejo Superior de Investigaciones Científicas

NYSBC

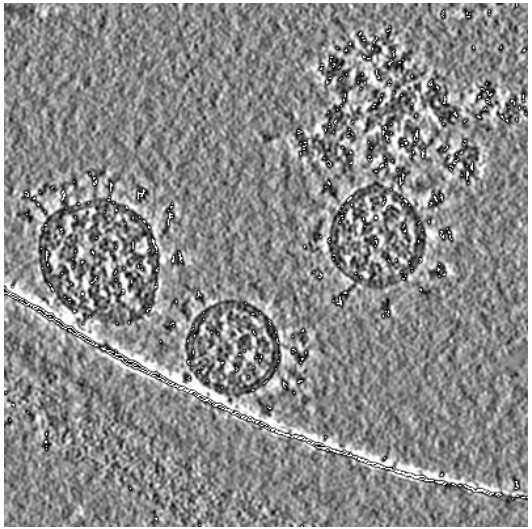
instruct ES

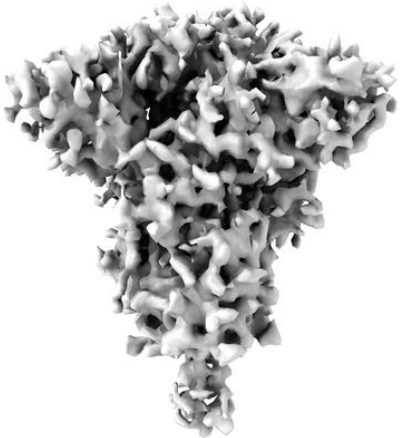
Contents

- What is Scipion?
- Preprocessing workflows
- Image processsing in streaming demonstration

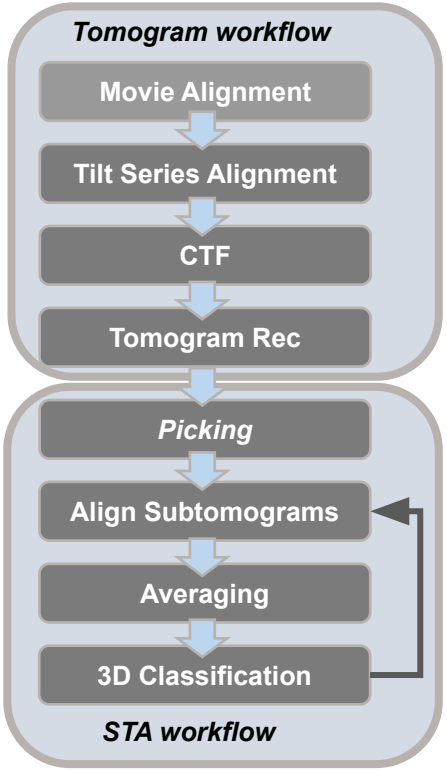
What is Scipion?

There is a huge software offer, which one should I use?



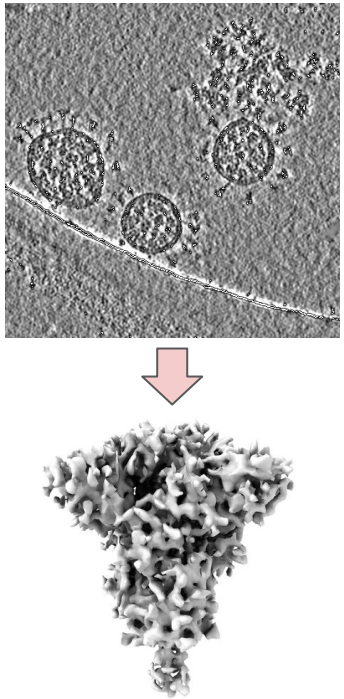


Workflow



What is Scipion?

There is a huge software offer…, which one should I use?



Software Package X

Package X

Release: 2021

Attributes:

Speed

Reliability

Usability

Pros

Good at Classification

Cons

Bad at particle Picking

Installation

Easy to install

Graphical Interface

No. Command line

Interoperability

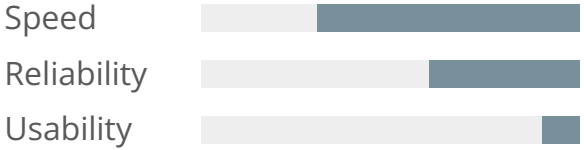
Easy to migrate results to other software

Software Package Y

Package Y

Release: 2020

Attributes:



Pros

Good at particle Picking

Cons

Bad at Classification

Installation

Complex to install

Graphical Interface

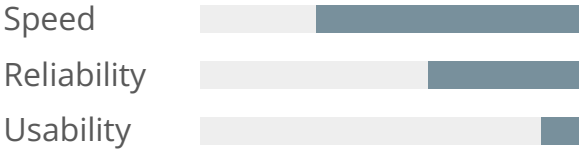
Yes

Interoperability

Limited

Which one to choose?

Attributes:



Pros

Good at particle Picking

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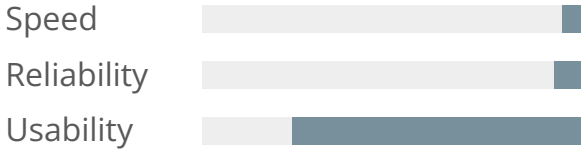
Bad at Classification

Attributes:



Pros

Good at Classification

Cons

Bad at particle Picking

What software should I use?

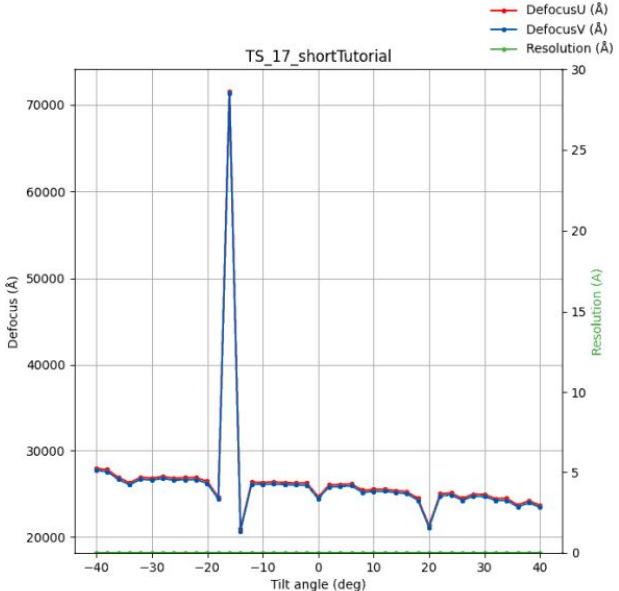
- Some softwares are designed for the whole pipeline
- Others are designed for specific steps of the pipeline
- To use both implies a price to pay in:
  - **Traceability**
  - **Time consuming**
  - **Data conversion**
  - **Risk of human errors**
  - **Comparison between Software**

How reliable is the estimation of the software I choose?

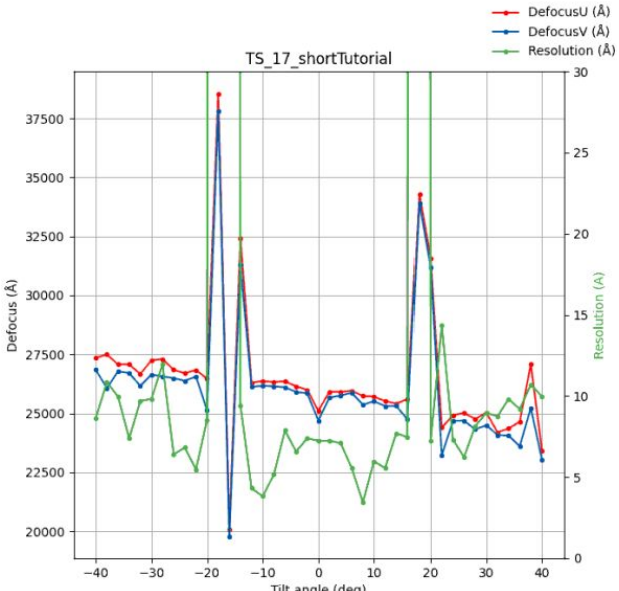
Usually software package present a single algorithm per step

For instance, CTF estimation

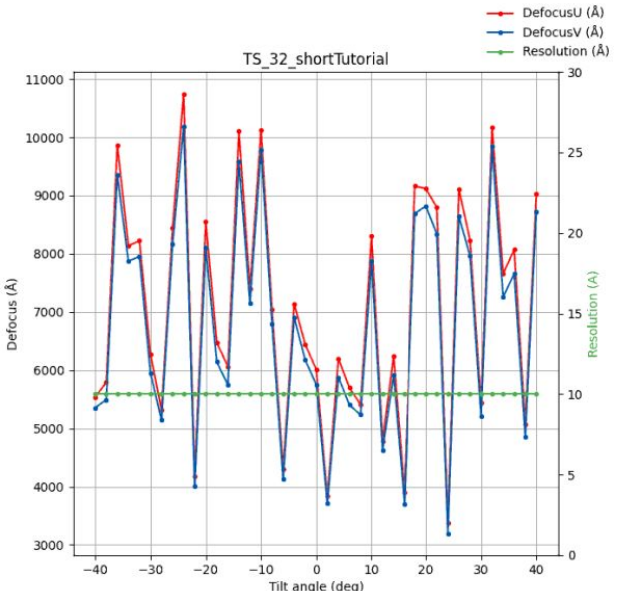
Software A



Software B



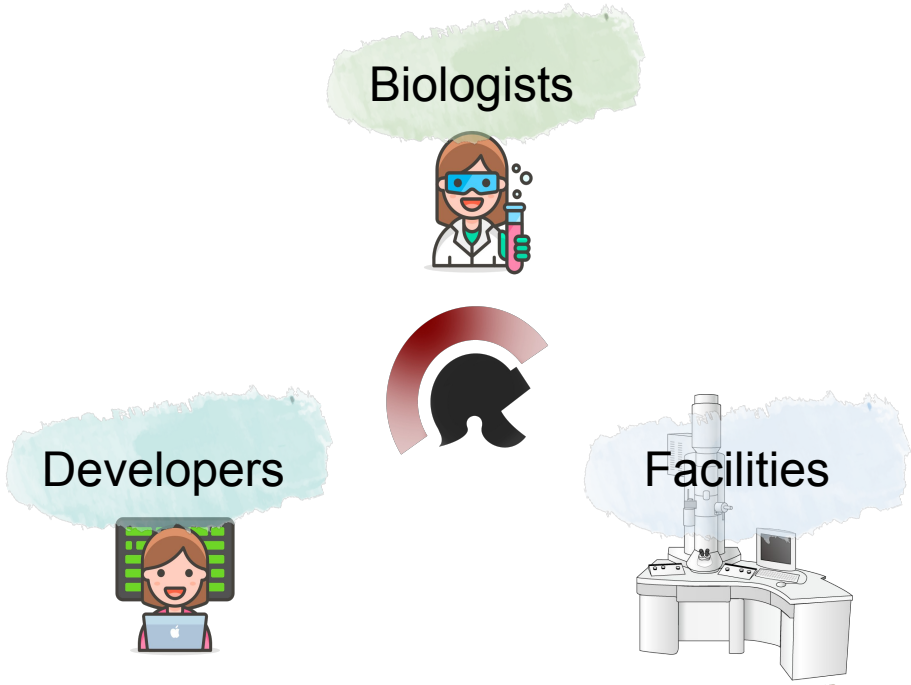
Software C



What Scipion is

An integrative framework

- Software packages
- Visualization tools
- Workflow engine
- Communication standards
- Thought for users



Currently Scipion integrates…

The plugins do not modify the original software, only provide tools to interact with the original software

Some Tomography plugins

IMOD

DYNAMO

MEMBRAIN

TOMO3D

GCTF

ARETOMO

CRYOCARE

ISONET

WARP

XMIPP

NOVACTF

MOTIONCORR2

GAPSTOP

DEEPFINDER

CRYOLO

EMAN2

RELION5

FIDDER

CTFFIND

IMOD

TOMOSEGMEMTV

MANAGEMENT

TOMOVIZ

CHIMERAX

Tomography plugins

Tilt Series Movies alignment	Xmipp	Motioncorr3	Warp			
CTF estimation	IMOD	cisTEM	Gctf	EMAN 2.3	Warp	
Tilt Series alignment	IMOD	tomo3d	EMAN 2.3	AreTomo	Warp	
Tomo reconstruction	IMOD	NovaCTF	tomo3d	AreTomo	EMAN 2.3	
Denoising	tomo3d	CRYOCARE	Isonet			
Picking	EMAN 2.3	Dynamo	DEEPFINDER TOMOGRAPHY	PySeg	GAPSTOP™	
Alignment	EMAN 2.3	Dynamo	RELION	Xmipp		
Heterogeneity	EMAN 2.3	Dynamo	RELION	Xmipp	PySeg	
*Other tools: visualization, segmentation, quality, annotation, pruning, consensus....	Xmipp	tomoviz	TomoSegMemTV	DEEPFINDER TOMOGRAPHY	MemBrain	#team tomo Fidder

Tomo rec

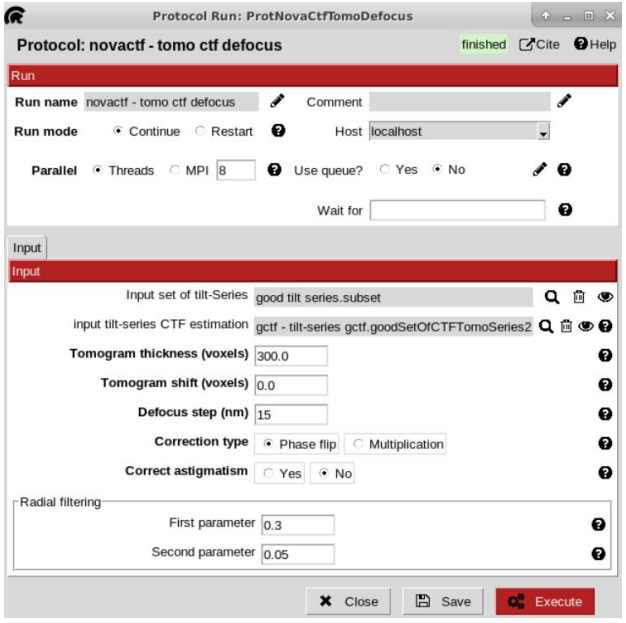
STA

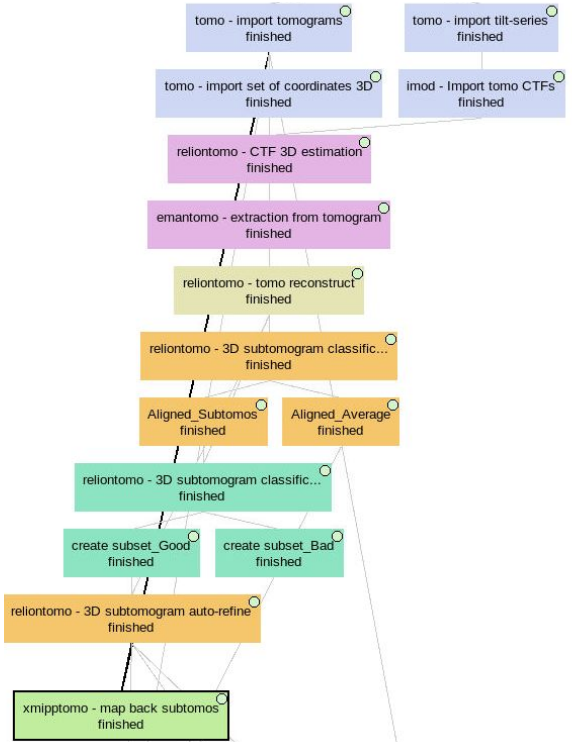
Other

Traceability, connectivity and communications stands

Tracking all processing steps and their parameters

Automatic conversion between data formats





Visualization tools

New developed viewers

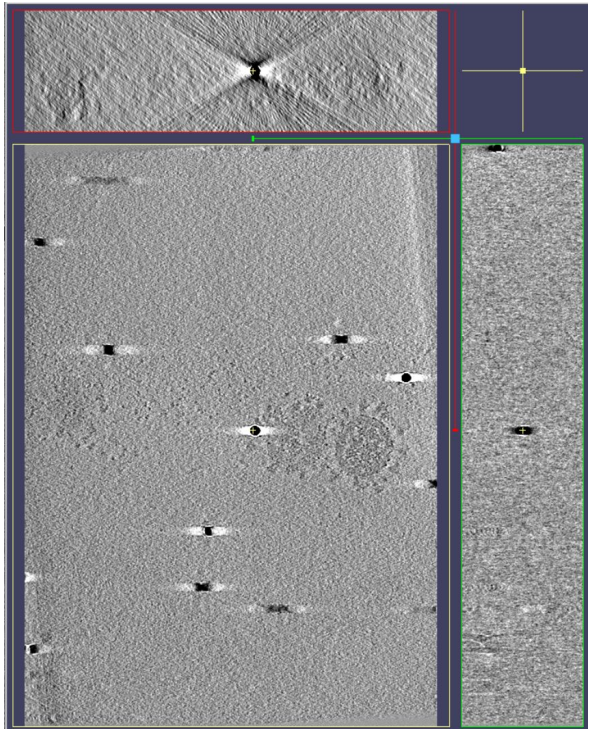
- METADATA-VIEWER
- TOMOVIZ
- XMIPP
- CTF VIEWER

Others from the installed packages

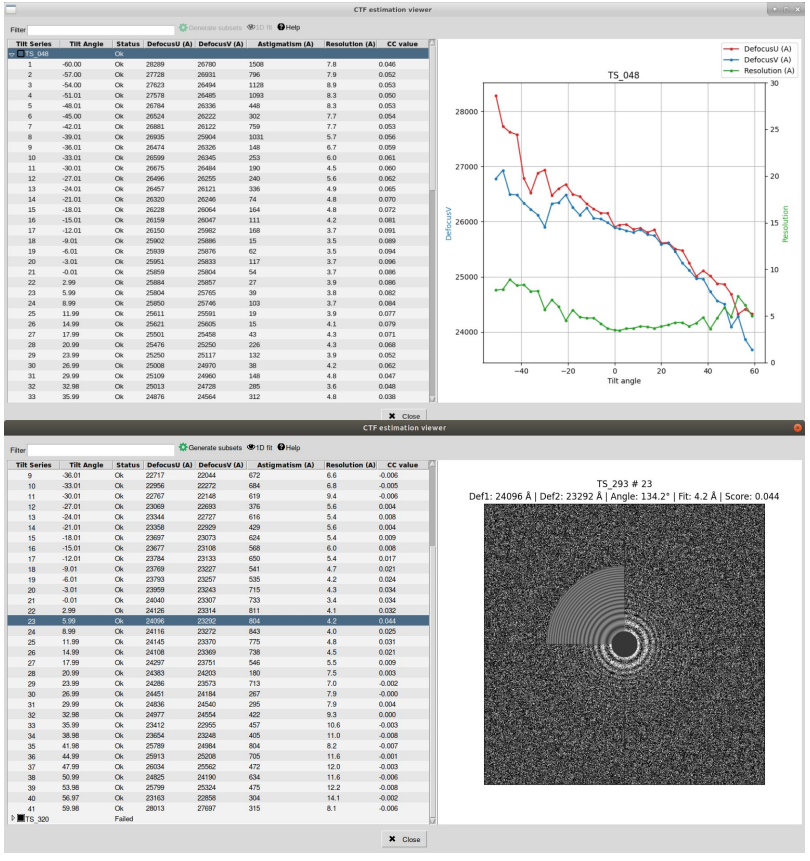
- 3DMOD
- DYNAMO
- NAPARI
- DEEPFINDER
- EMAN
- CHIMERA

Visualization tools

3DMOD

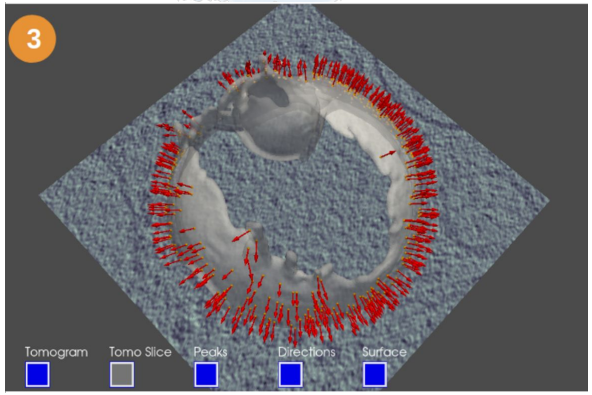


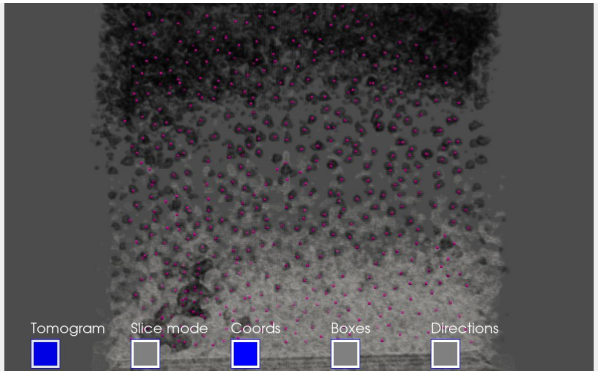
CTF VIEWER



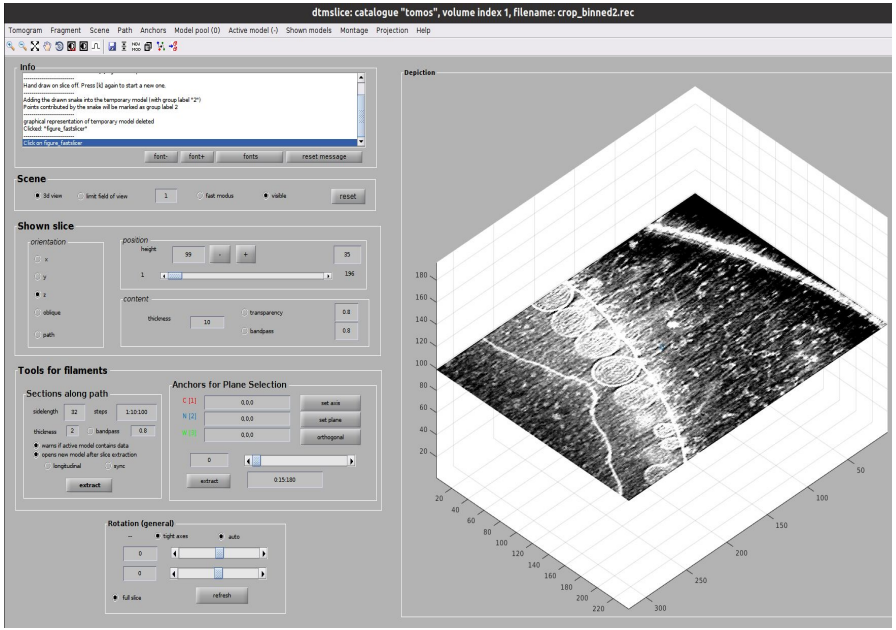
Visualization tools

TOMOVIZ

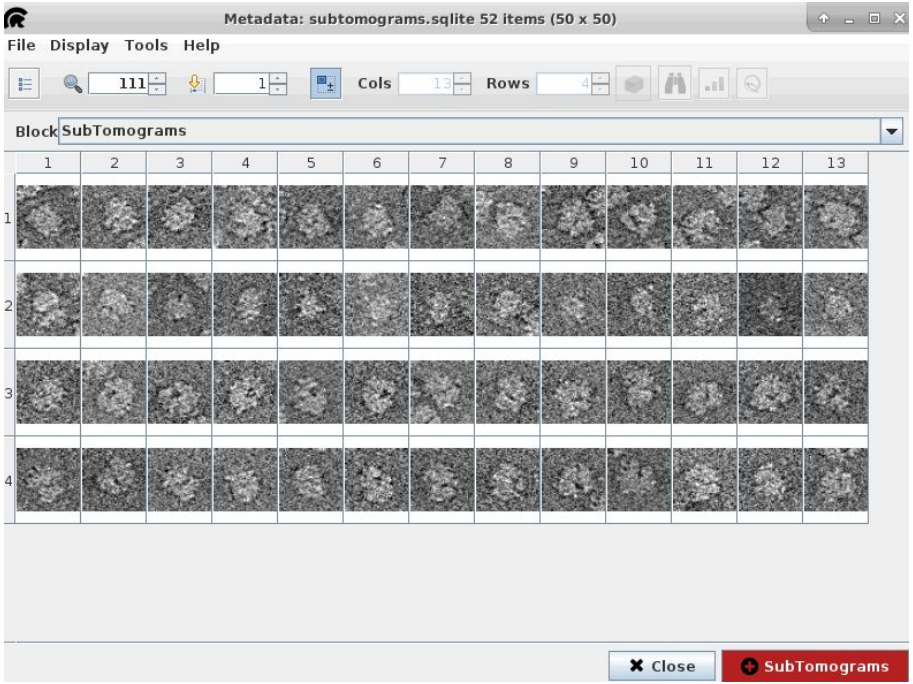


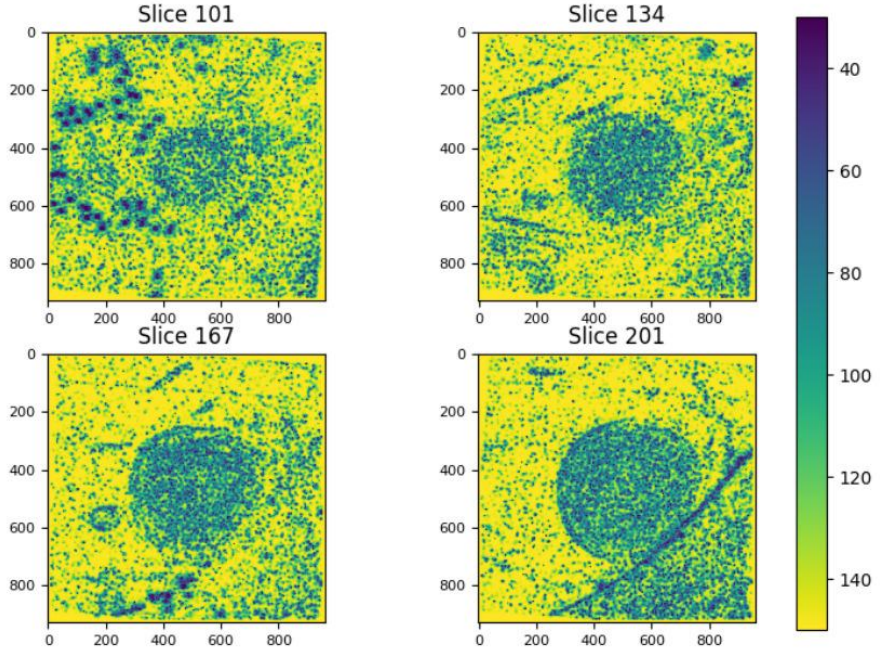


DYNAMO

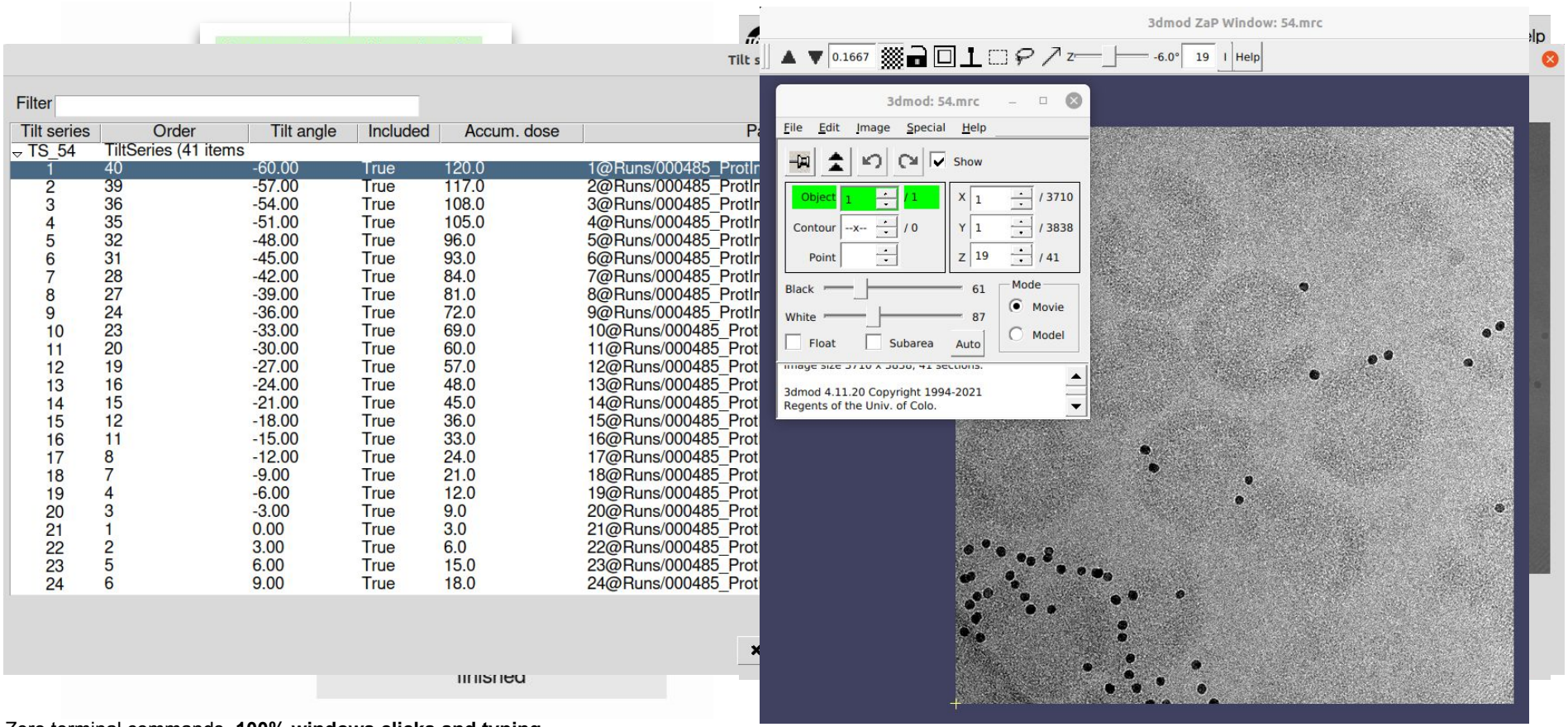


Visualization tools



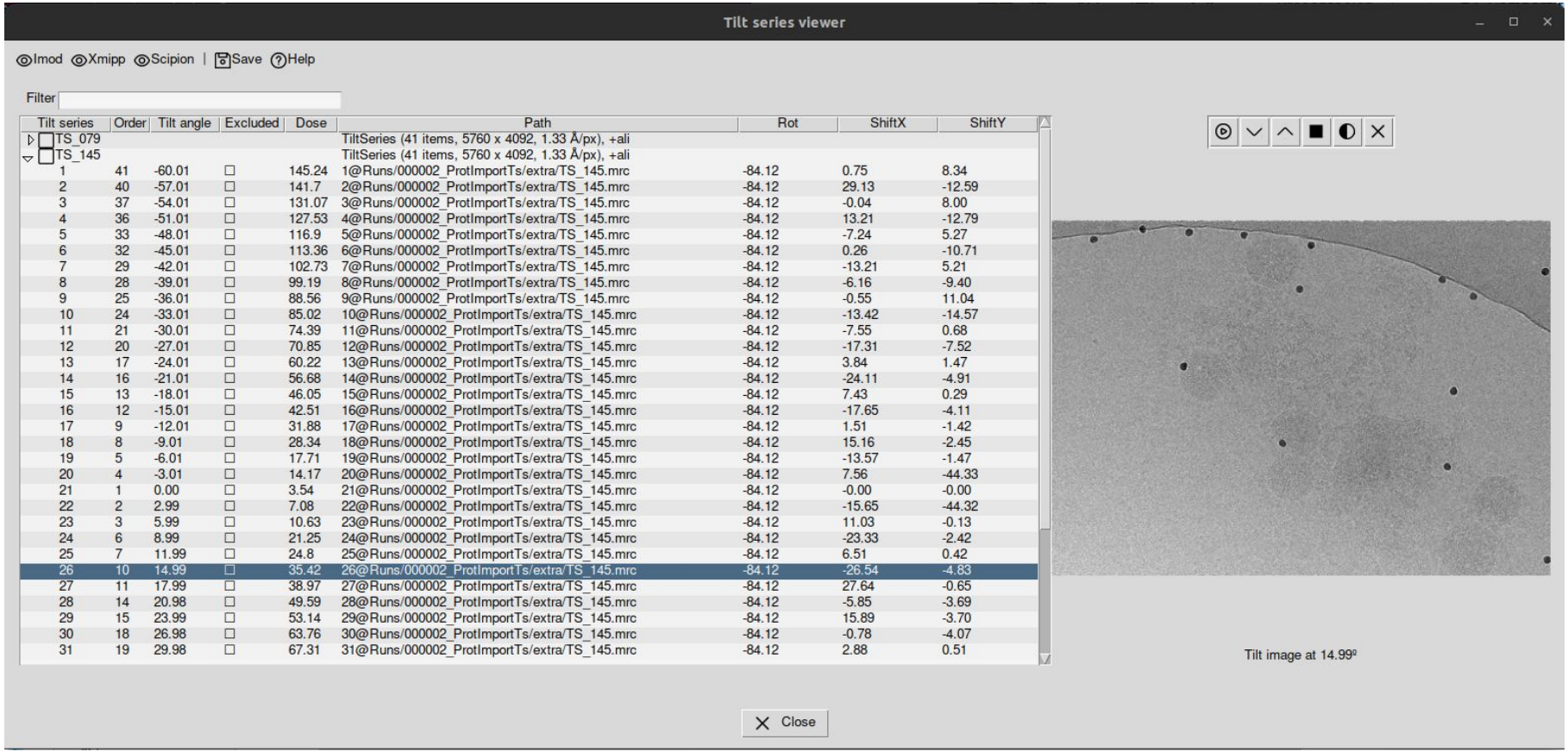


Example I: Importing Tilt series, visualization with Imod



Zero terminal commands. **100% windows clicks and typing.**

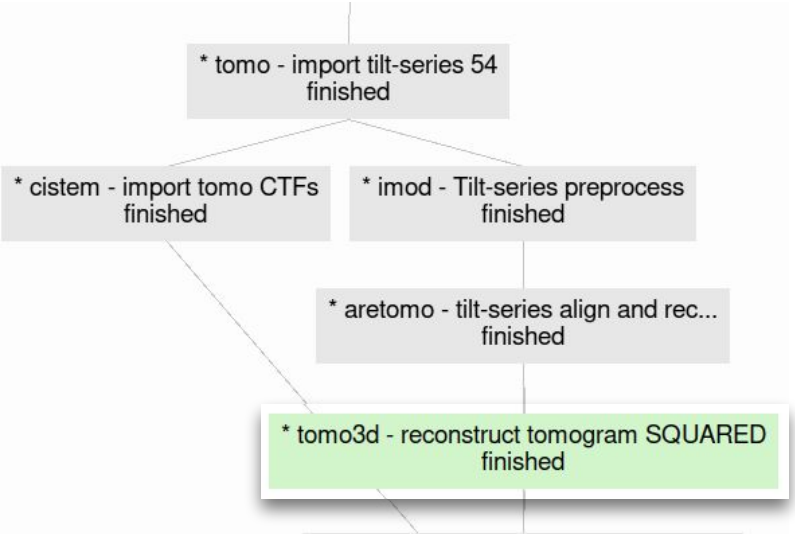
Example II: Aretomo, visualization with ScipionTomo viewer

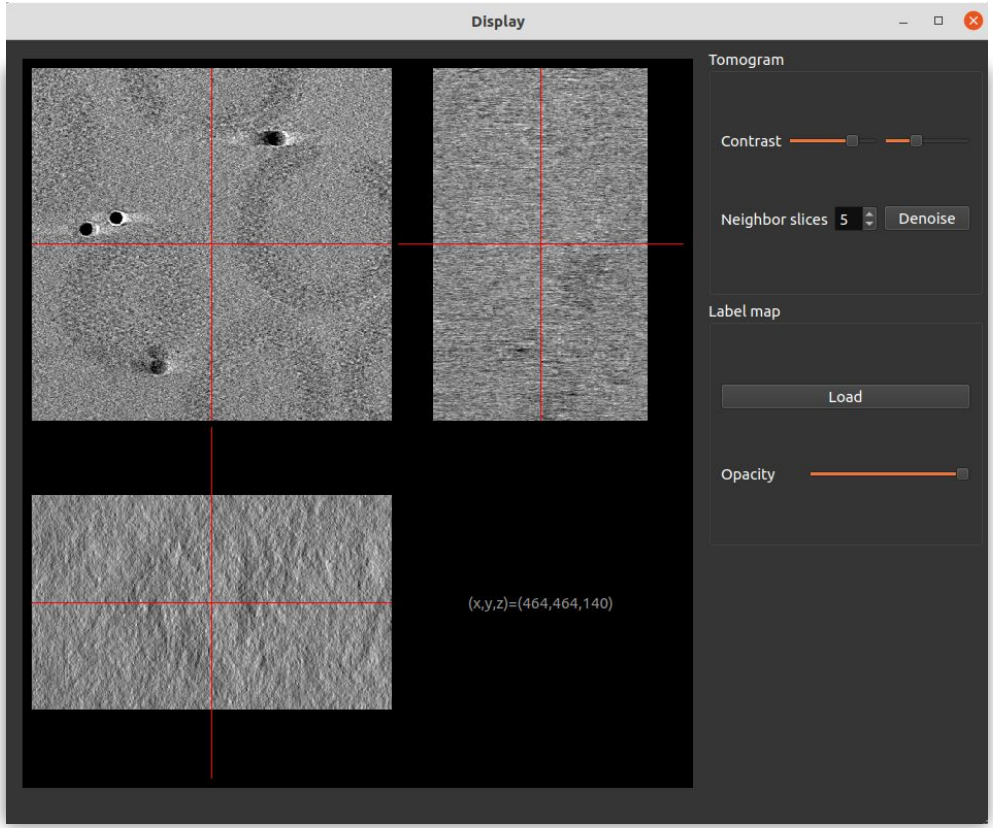


Tilt series	Order	Tilt angle	Excluded	Dose	Path	Rot	ShiftX	ShiftY
TS_079					TiltSeries (41 items, 5760 x 4092, 1.33 Å/px), +ali			
TS_145					TiltSeries (41 items, 5760 x 4092, 1.33 Å/px), +ali			
1	41	-60.01	☐	145.24	1@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	0.75	8.34
2	40	-57.01	☐	141.7	2@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	29.13	-12.59
3	37	-54.01	☐	131.07	3@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-0.04	8.00
4	36	-51.01	☐	127.53	4@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	13.21	-12.79
5	33	-48.01	☐	116.9	5@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-7.24	5.27
6	32	-45.01	☐	113.36	6@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	0.26	-10.71
7	29	-42.01	☐	102.73	7@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-13.21	5.21
8	28	-39.01	☐	99.19	8@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-6.16	-9.40
9	25	-36.01	☐	88.56	9@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-0.55	11.04
10	24	-33.01	☐	85.02	10@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-13.42	-14.57
11	21	-30.01	☐	74.39	11@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-7.55	0.68
12	20	-27.01	☐	70.85	12@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-17.31	-7.52
13	17	-24.01	☐	60.22	13@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	3.84	1.47
14	16	-21.01	☐	56.68	14@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-24.11	-4.91
15	13	-18.01	☐	46.05	15@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	7.43	0.29
16	12	-15.01	☐	42.51	16@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-17.65	-4.11
17	9	-12.01	☐	31.88	17@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	1.51	-1.42
18	8	-9.01	☐	28.34	18@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	15.16	-2.45
19	5	-6.01	☐	17.71	19@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-13.57	-1.47
20	4	-3.01	☐	14.17	20@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	7.56	-44.33
21	1	0.00	☐	3.54	21@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-0.00	-0.00
22	2	2.99	☐	7.08	22@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-15.65	-44.32
23	3	5.99	☐	10.63	23@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	11.03	-0.13
24	6	8.99	☐	21.25	24@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-23.33	-2.42
25	7	11.99	☐	24.8	25@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	6.51	0.42
26	10	14.99	☐	35.42	26@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-26.54	-4.83
27	11	17.99	☐	38.97	27@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	27.64	-0.65
28	14	20.98	☐	49.59	28@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-5.85	-3.69
29	15	23.99	☐	53.14	29@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	15.89	-3.70
30	18	26.98	☐	63.76	30@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	-0.78	-4.07
31	19	29.98	☐	67.31	31@Runs/000002_ProtImportTs/extra/TS_145.mrc	-84.12	2.88	0.51

Zero terminal commands. **100% windows clicks and typing.**

Example III: Tomogram rec. with tomo3d, visualization with DeepFinder





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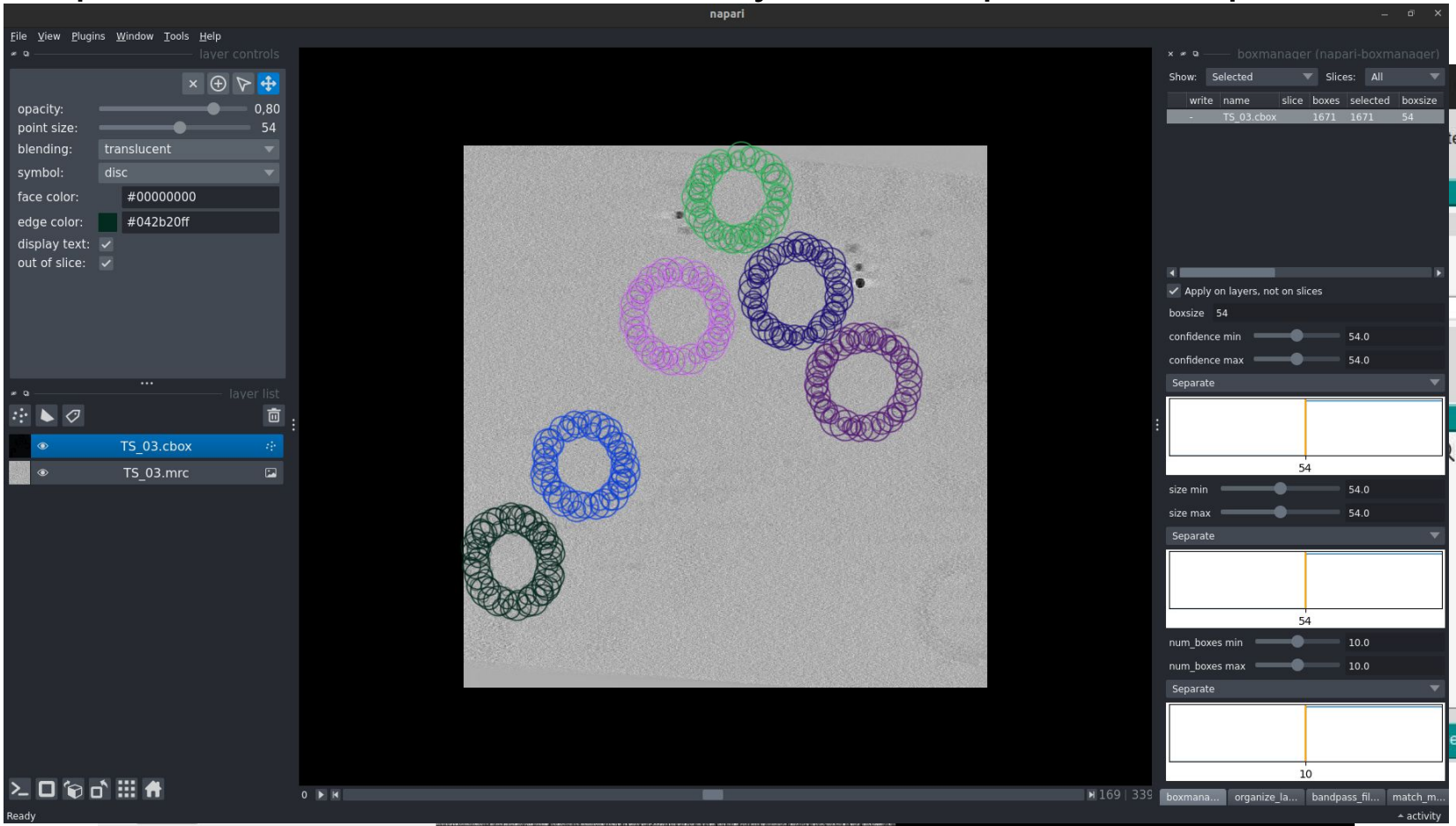
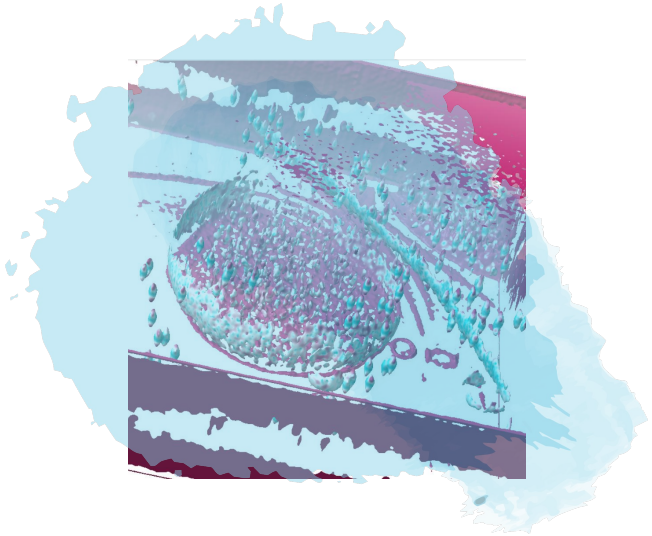
Example I: 3D coordinates, vis. with Dynamo, Napari and Napari



In demo: Pre-processing workflow



From movies to tomograms

USERS:
Standard Image processing

FACILITIES
Image processing in streaming

Information

- Scipion’s doc site: https://scipion-em.github.io/docs/release-3.0.0/index.html
- Youtube channel: https://www.youtube.com/user/BiocompWebs/videos
- Biocomputing unit: http://biocomputingunit.es/
- Discord : https://discord.gg/ErchZ9sJfW