

Preprocessing with ScipionTomo

Spanish Research Council

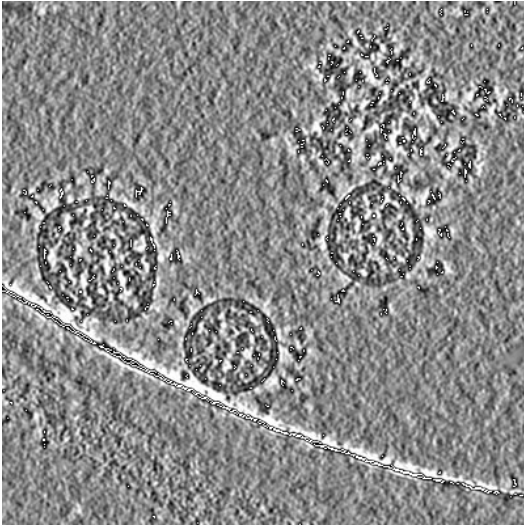
March 31th-April 4th 2025

Contents

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

What is Scipion?

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



Workflow

Tomogram workflow

Movie Alignment



Tilt Series Alignment



CTF



Tomogram Rec



Picking



Align Subtomograms



Averaging



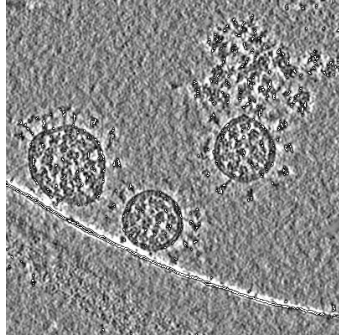
3D Classification



STA workflow

What is Scipion?

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



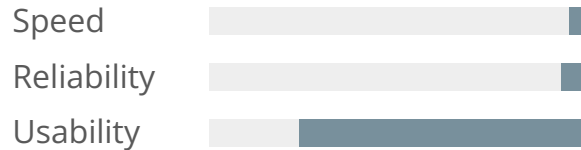
Software Package X



Package X

Release: 2021

Attributes:



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

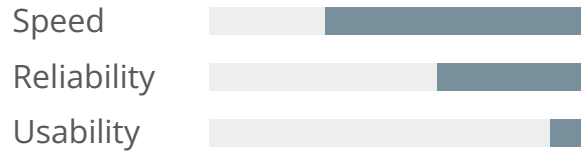
Software Package Y



Package Y

Release: 2020

Attributes:



Pros

Good at particle Picking



Cons

Bad at Classification



Installation

Complex to install



Graphical Interface

Yes

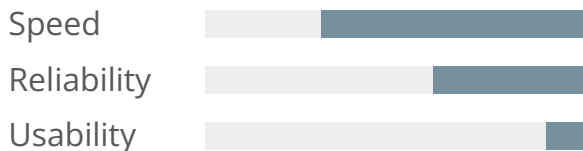


Interoperability

Limited

Which one to choose?

Attributes:



Pros



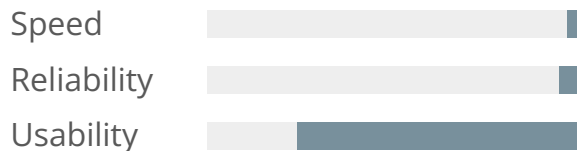
Good at particle Picking

Cons



Bad at Classification

Attributes:



Pros



Good at Classification

Cons

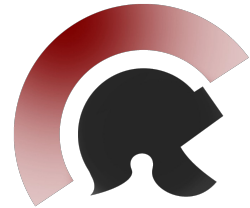


Bad at particle Picking



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**



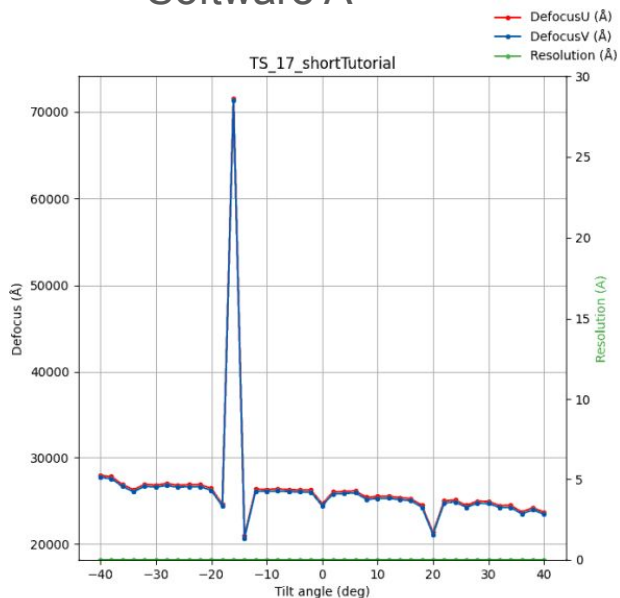
The user

How reliable is the estimation of the software I choose?

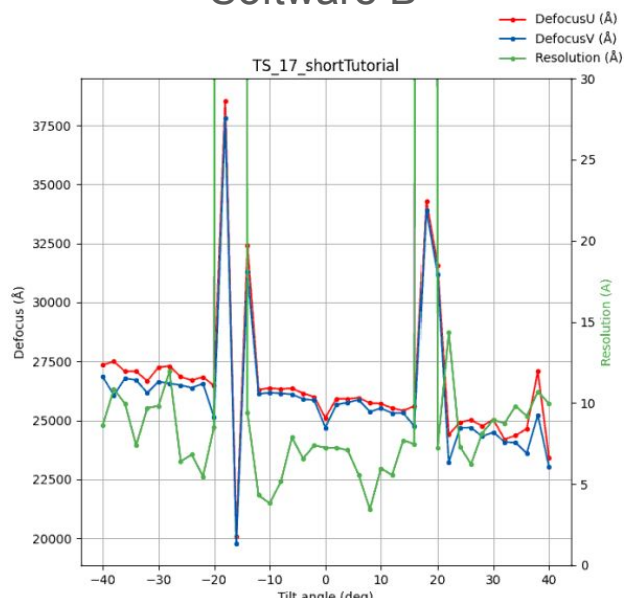
Usually software package present a single algorithm per step

For instance, CTF estimation

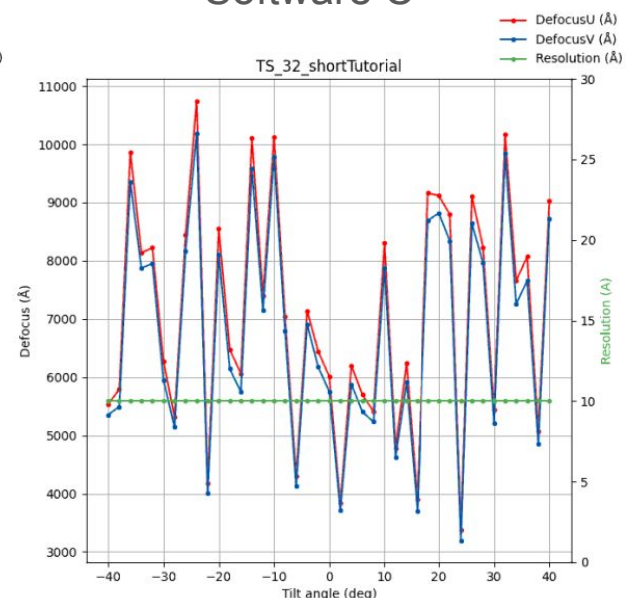
Software A



Software B



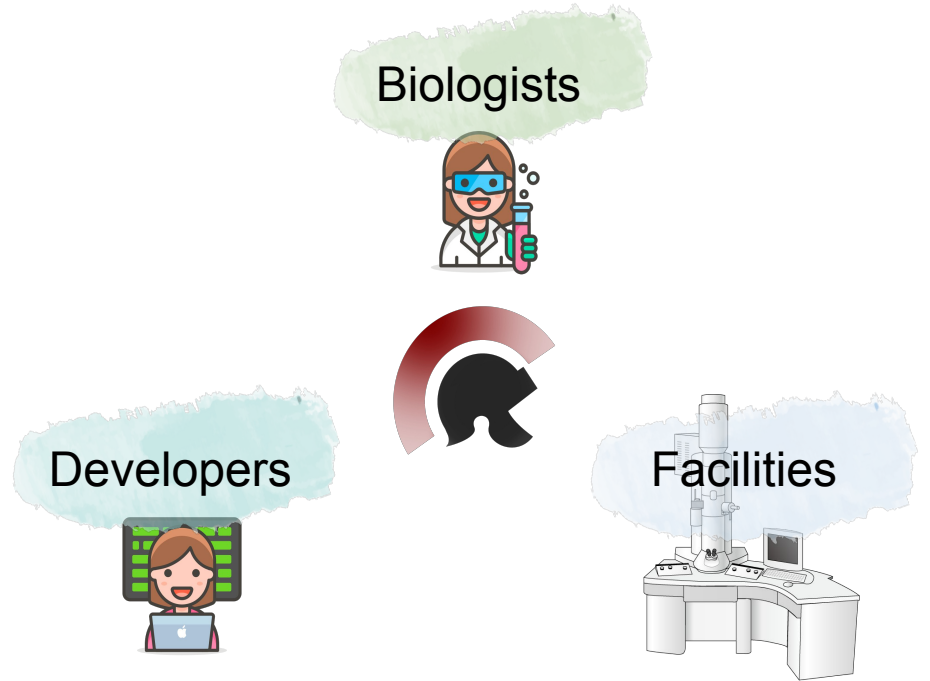
Software C



What Scipion is

An integrative framework

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



Currently Scipion integrates...

+ 100 plugins

Between SPA, tomography and modelling



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

DEEPPINDER

CRYOLO

EMAN2

RELION5

FIDDER

CTFFIND

IMOD

TOMOSEGMENTV

MANAGEMENT

TOMOVIZ

CHIMERAX

Tomography plugins

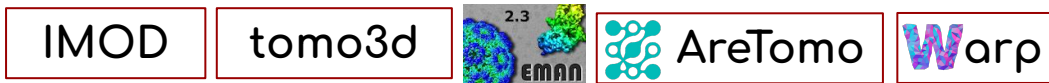
Tilt Series Movies alignment



CTF estimation



Tilt Series alignment



Tomo reconstruction



Denoising



Picking



Alignment



Heterogeneity



*Other tools: visualization, segmentation, quality, annotation, pruning, consensus....



rec Tomo

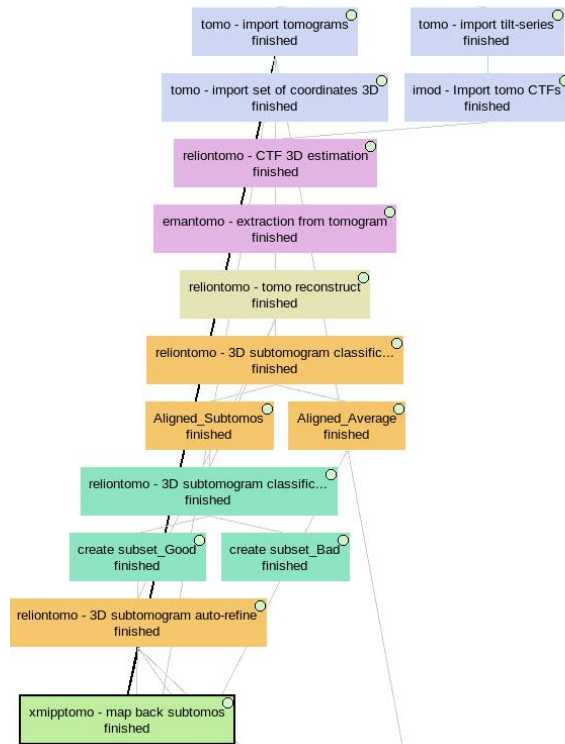
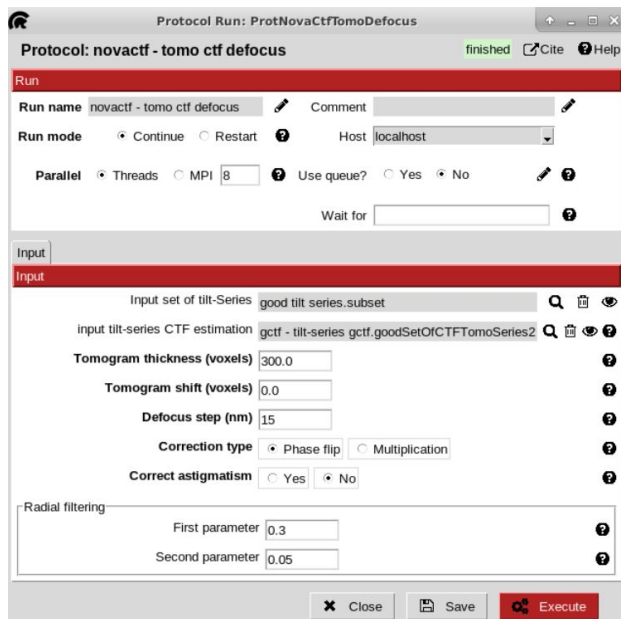
STA

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

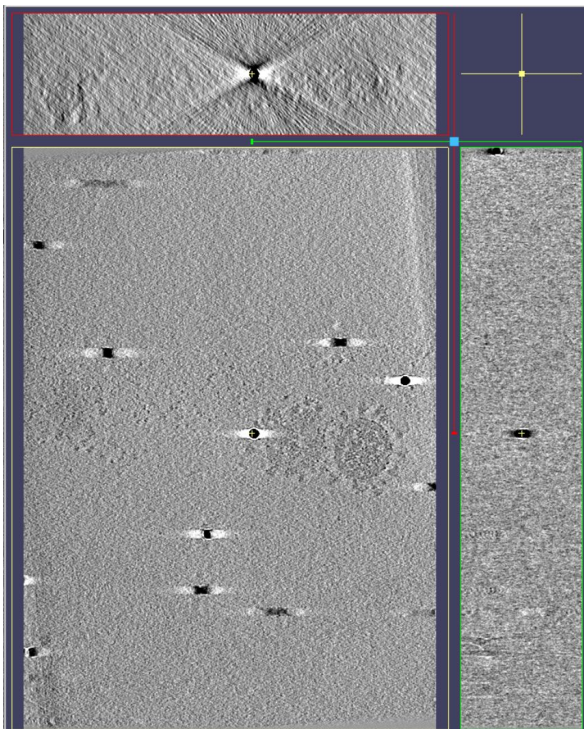
DEEPPINDER

EMAN

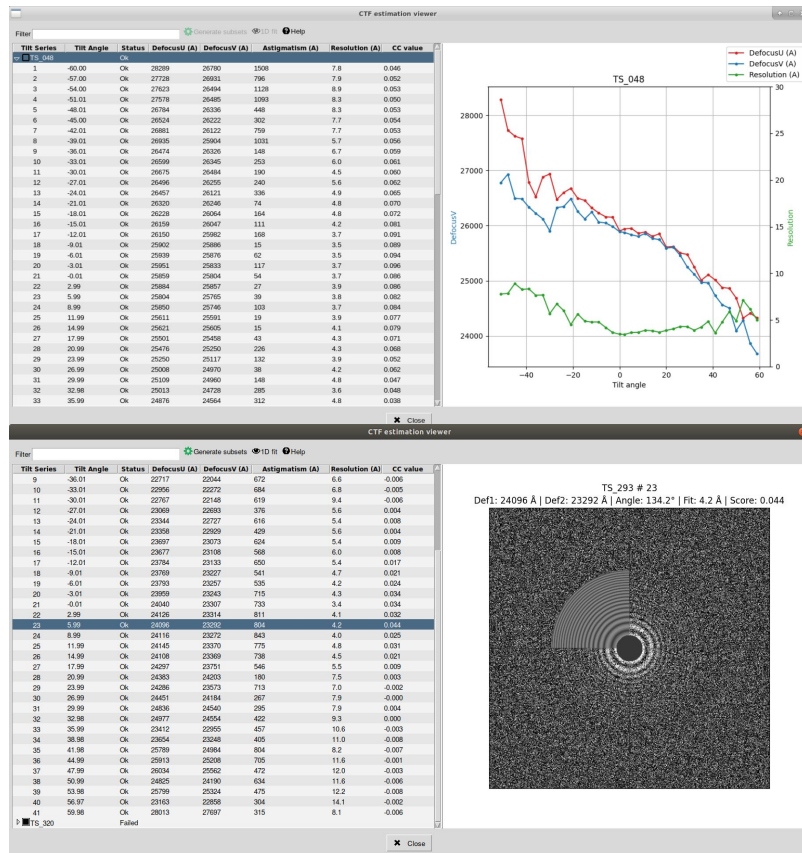
CHIMERA

Visualization tools

3DMOD

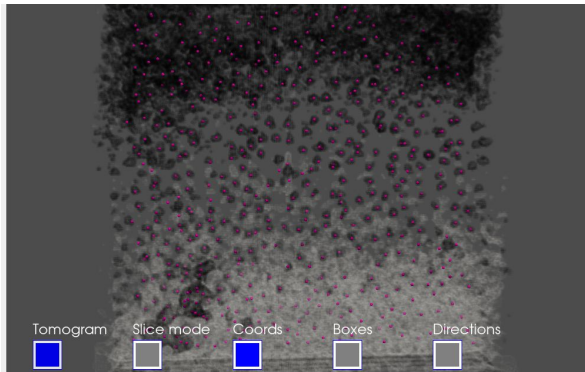
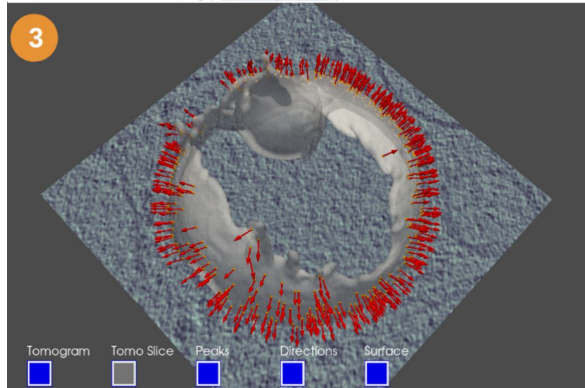


CTF VIEWER

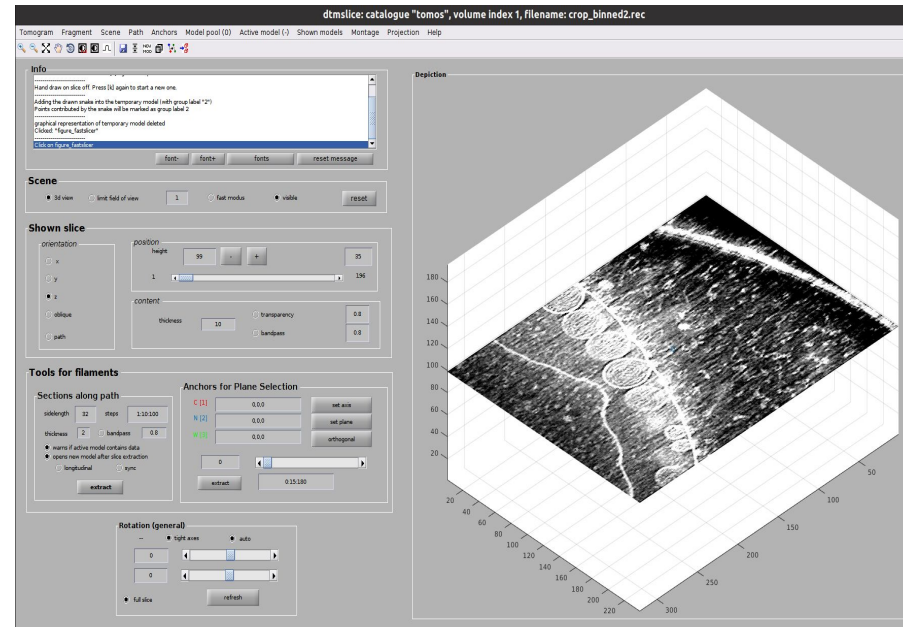


Visualization tools

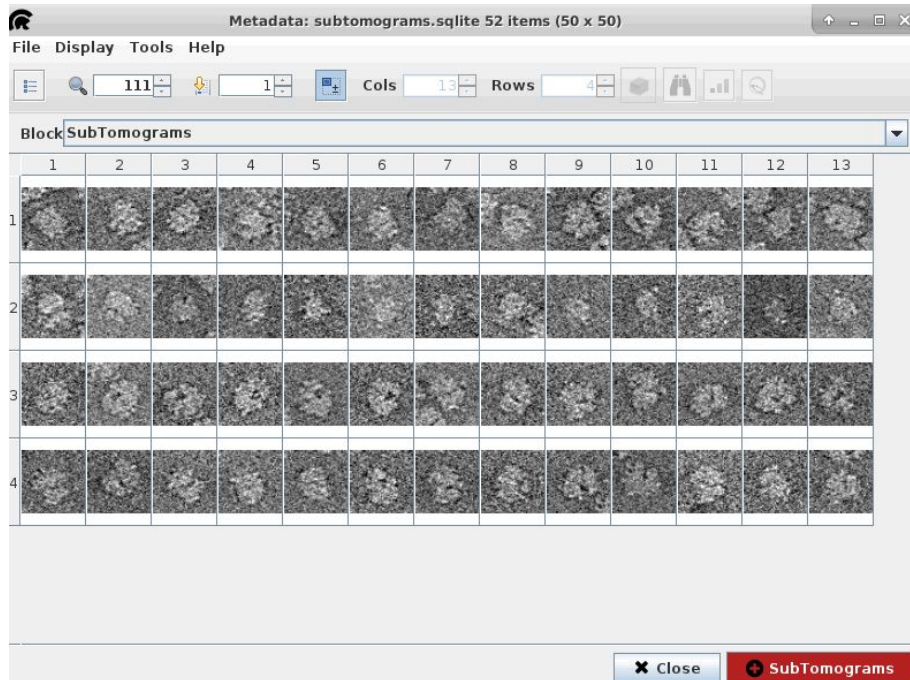
TOMOVIZ



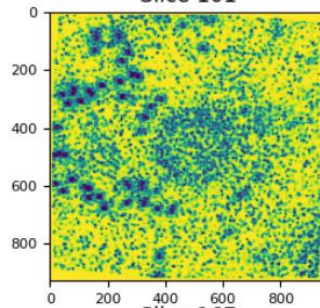
DYNAMO



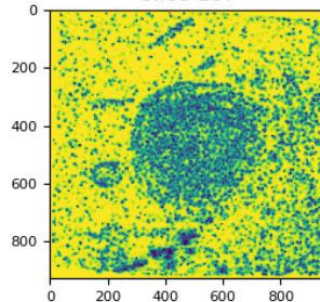
Visualization tools



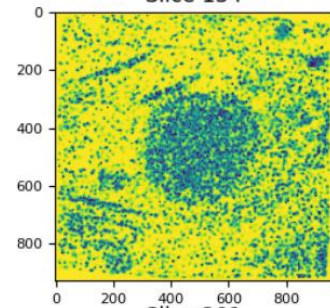
Slice 101



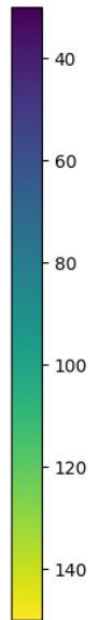
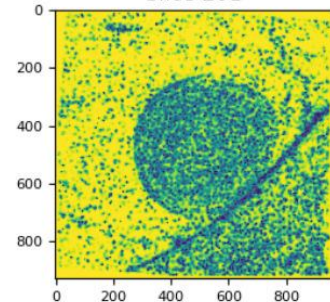
Slice 167



Slice 134



Slice 201



Example I: Importing Tilt series, visualization with Imod

The screenshot displays the Imod software interface. On the left, a table lists the tilt series data. On the right, a 3D visualization window shows a grayscale image of a sample with several dark spots. A control panel for the 3D window is overlaid on the image, showing various settings.

Tilt series	Order	Tilt angle	Included	Accum. dose	Path
TS_54	TiltSeries (41 items)				
1	40	-60.00	True	120.0	1@Runs/000485_Protl
2	39	-57.00	True	117.0	2@Runs/000485_Protl
3	36	-54.00	True	108.0	3@Runs/000485_Protl
4	35	-51.00	True	105.0	4@Runs/000485_Protl
5	32	-48.00	True	96.0	5@Runs/000485_Protl
6	31	-45.00	True	93.0	6@Runs/000485_Protl
7	28	-42.00	True	84.0	7@Runs/000485_Protl
8	27	-39.00	True	81.0	8@Runs/000485_Protl
9	24	-36.00	True	72.0	9@Runs/000485_Protl
10	23	-33.00	True	69.0	10@Runs/000485_Protl
11	20	-30.00	True	60.0	11@Runs/000485_Protl
12	19	-27.00	True	57.0	12@Runs/000485_Protl
13	16	-24.00	True	48.0	13@Runs/000485_Protl
14	15	-21.00	True	45.0	14@Runs/000485_Protl
15	12	-18.00	True	36.0	15@Runs/000485_Protl
16	11	-15.00	True	33.0	16@Runs/000485_Protl
17	8	-12.00	True	24.0	17@Runs/000485_Protl
18	7	-9.00	True	21.0	18@Runs/000485_Protl
19	4	-6.00	True	12.0	19@Runs/000485_Protl
20	3	-3.00	True	9.0	20@Runs/000485_Protl
21	1	0.00	True	3.0	21@Runs/000485_Protl
22	2	3.00	True	6.0	22@Runs/000485_Protl
23	5	6.00	True	15.0	23@Runs/000485_Protl
24	6	9.00	True	18.0	24@Runs/000485_Protl

3dmod: 54.mrc

File Edit Image Special Help

Object 1 / 1

Contour --x-- / 0

Point

X 1 / 3710

Y 1 / 3838

Z 19 / 41

Black 61

White 87

Mode

Movie

Model

Image size 3710 x 3838, 41 sections.

3dmod 4.11.20 Copyright 1994-2021
Regents of the Univ. of Colo.

Zero terminal commands. 100% windows clicks and typing.

Example II: Aretomo, visualization with ScipionTomo viewer

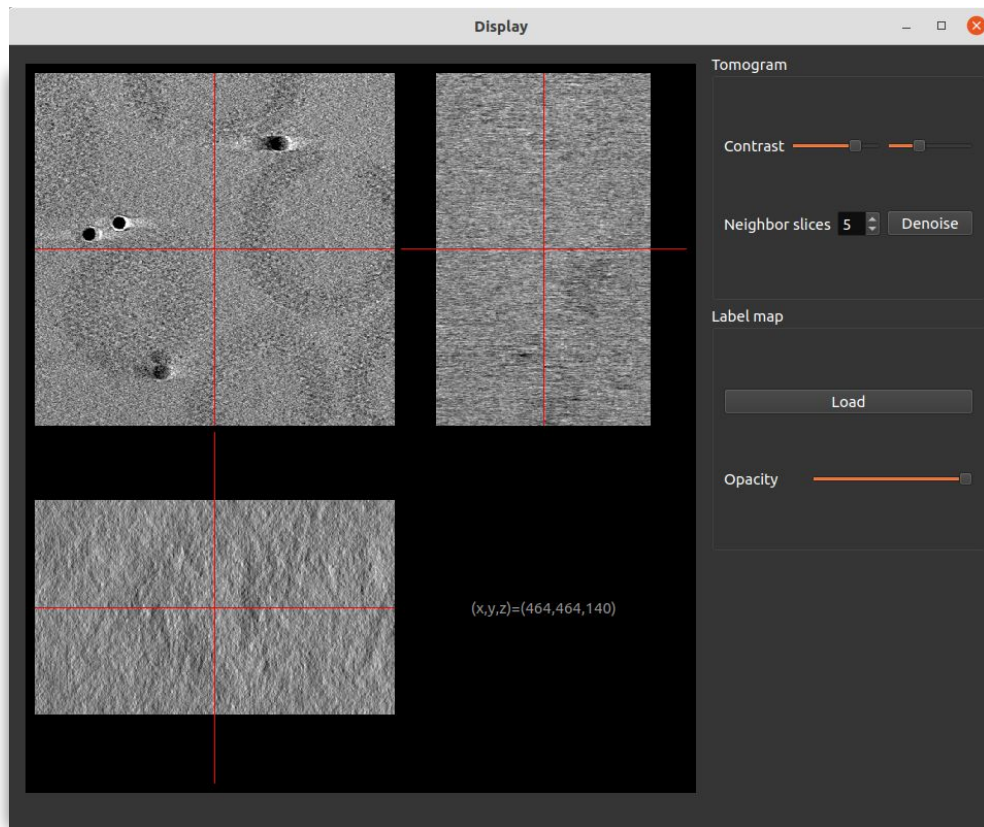
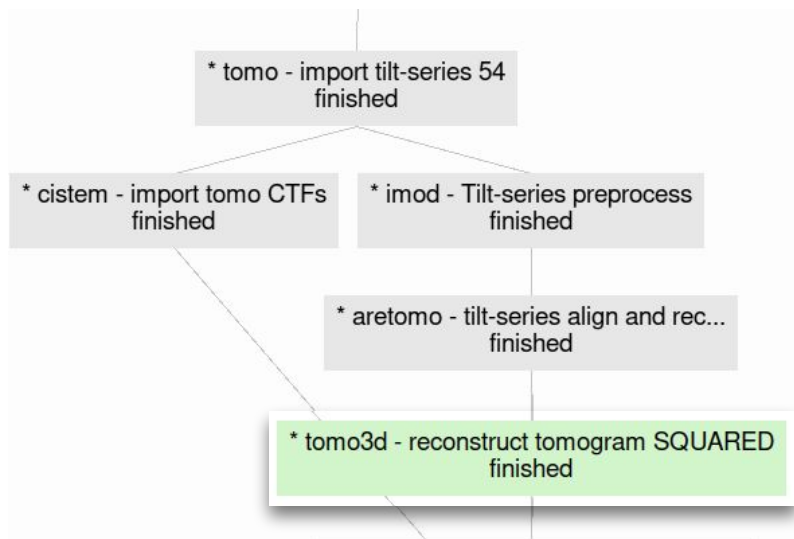
The screenshot displays the ScipionTomo viewer interface. At the top, the title bar reads "Tilt series viewer". Below it, a menu bar includes "Imod", "Xmipp", "Scipion", "Save", and "Help". A "Filter" input field is present above a table of tilt series data.

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

Navigation icons (back, forward, home, etc.) are located above the micrograph. The micrograph shows a grayscale image of a biological specimen with a curved boundary. Below the micrograph, the text "Tilt image at 14.99°" is displayed. A "Close" button is at the bottom center.

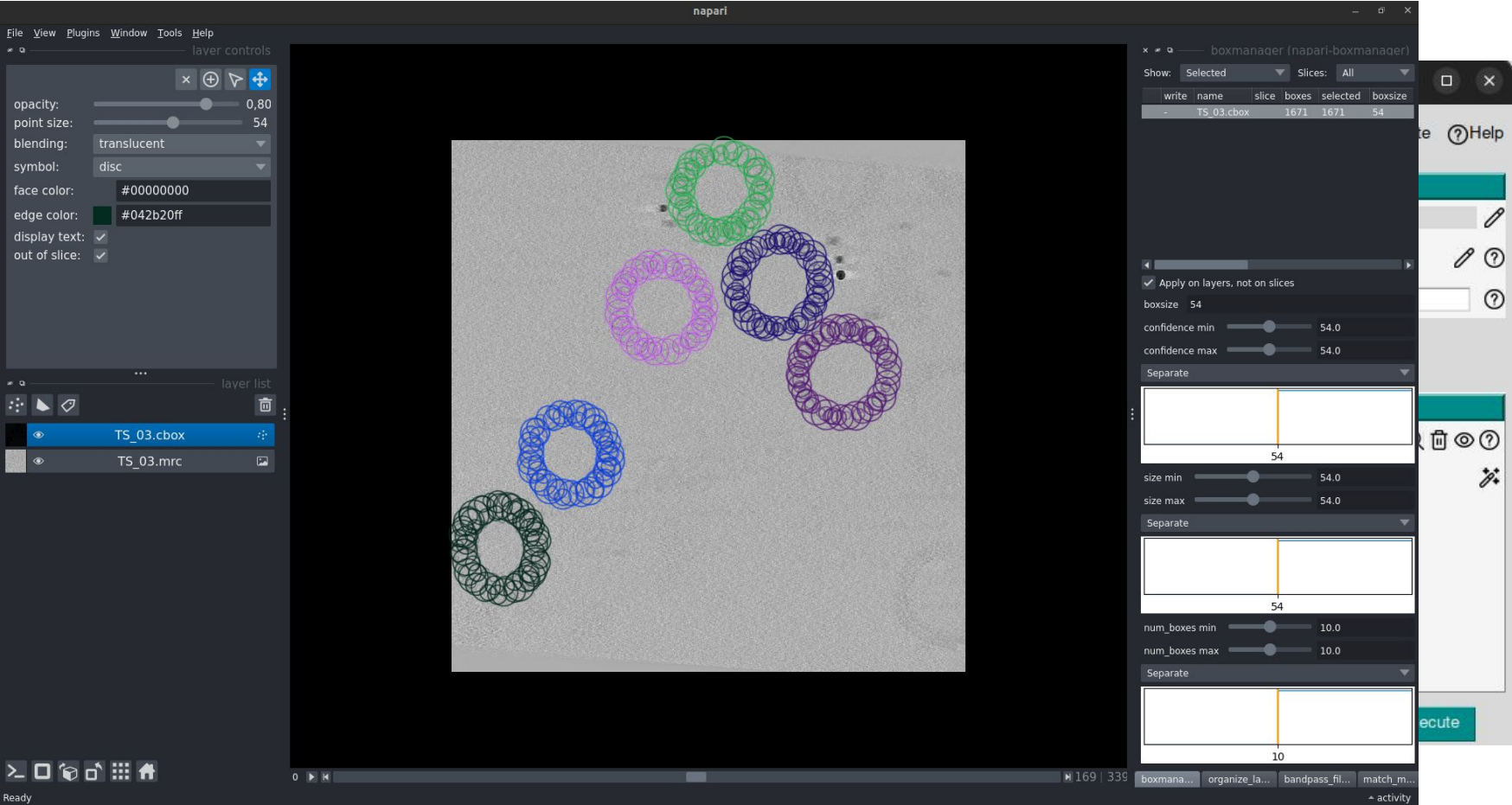
Zero terminal commands. 100% windows clicks and typing.

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

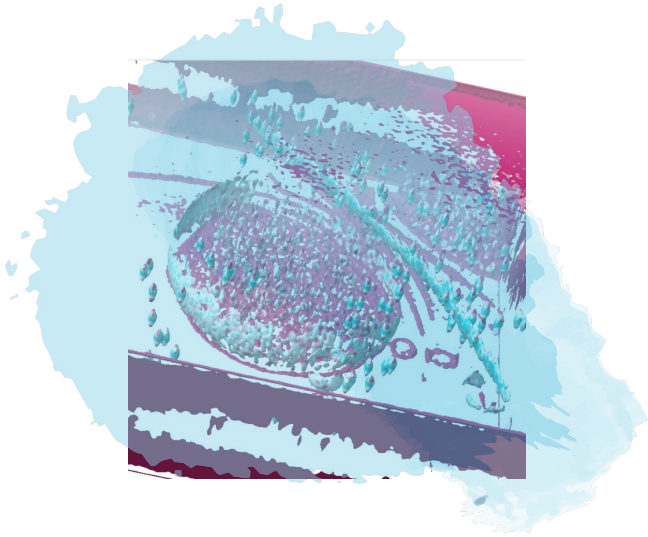


Zero terminal commands. **100% windows clicks and typing.**

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>