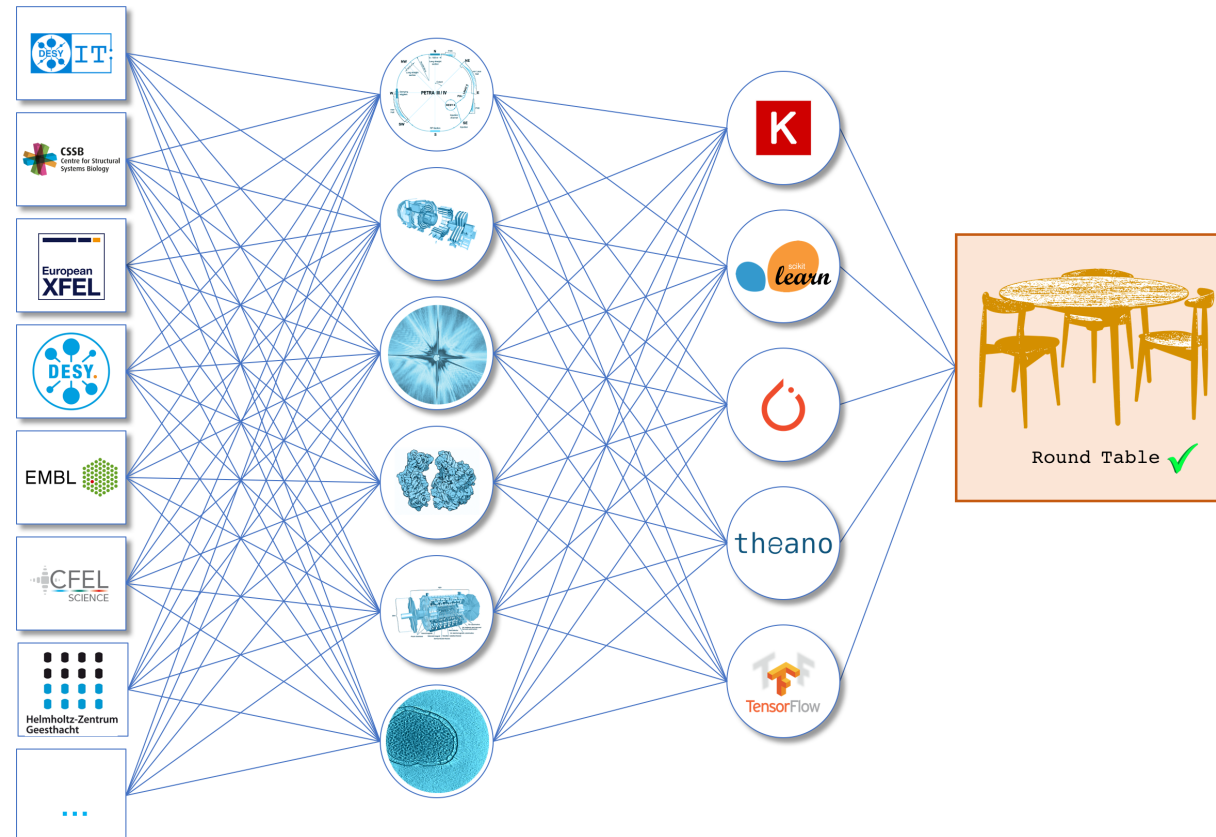


# Welcome to: 2<sup>nd</sup> Round Table on Machine and Deep Learning at the DESY Campus



## 2<sup>nd</sup> Round Table on **Machine and Deep Learning at the DESY Campus**

10:00 – 11:30

Welcome

Convolutional Neural Networks for electron microscopy tomography

Generative Models for Fast Calorimeter Simulation

ML methods for FEL scattering data analysis

Machine learning in the DESY ATLAS group

**11:30 - 11:45 Coffee Break**

11:45 – 13:00

Automation of CMS workflow recovery

Neural networks for small angle scattering data analysis

Anomaly Detection for SRF Cavities

Classification for Single Particle Imaging experiments

**13:00 - 14:00 Lunch Break**

14:00 - 15:00 Snap ML - Accelerated Machine Learning for Business

15:00 - 16:00 Discussion and Conclusions



# Convolutional Neural Networks for CryoEM-tomography

In collaboration with Militec/ Marlovits (CSSB)

Philipp Heuser, DESY-IT

29/11/2019

Round Table on ML/DL@DESY





# Object Detection for Cryo Electron Tomography

Finding Type III Secretion System (T3SS) in minicells for subtomogram averaging



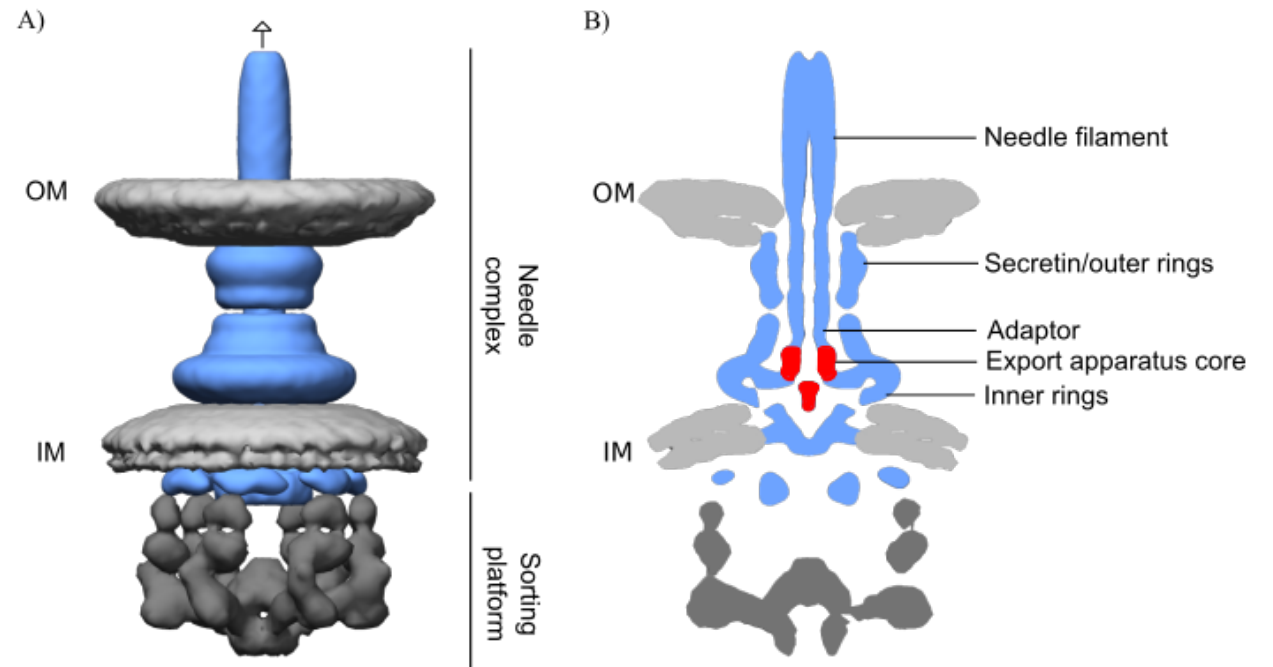
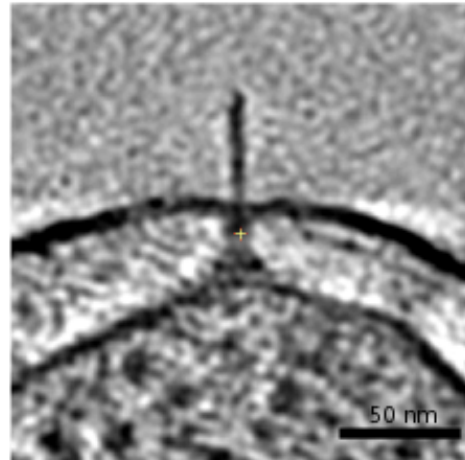
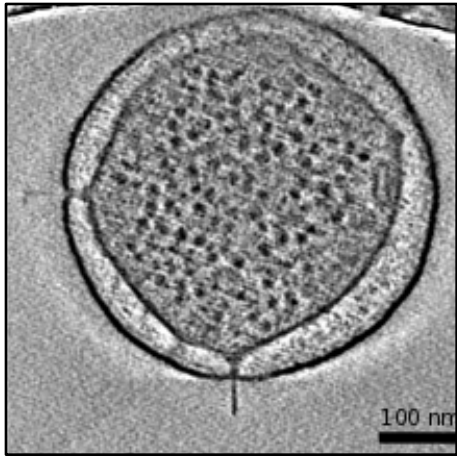
**CSSB**

Centre for Structural  
Systems Biology

With:

Sean Miletic, Thomas Marlovits

CSSB - Hamburg

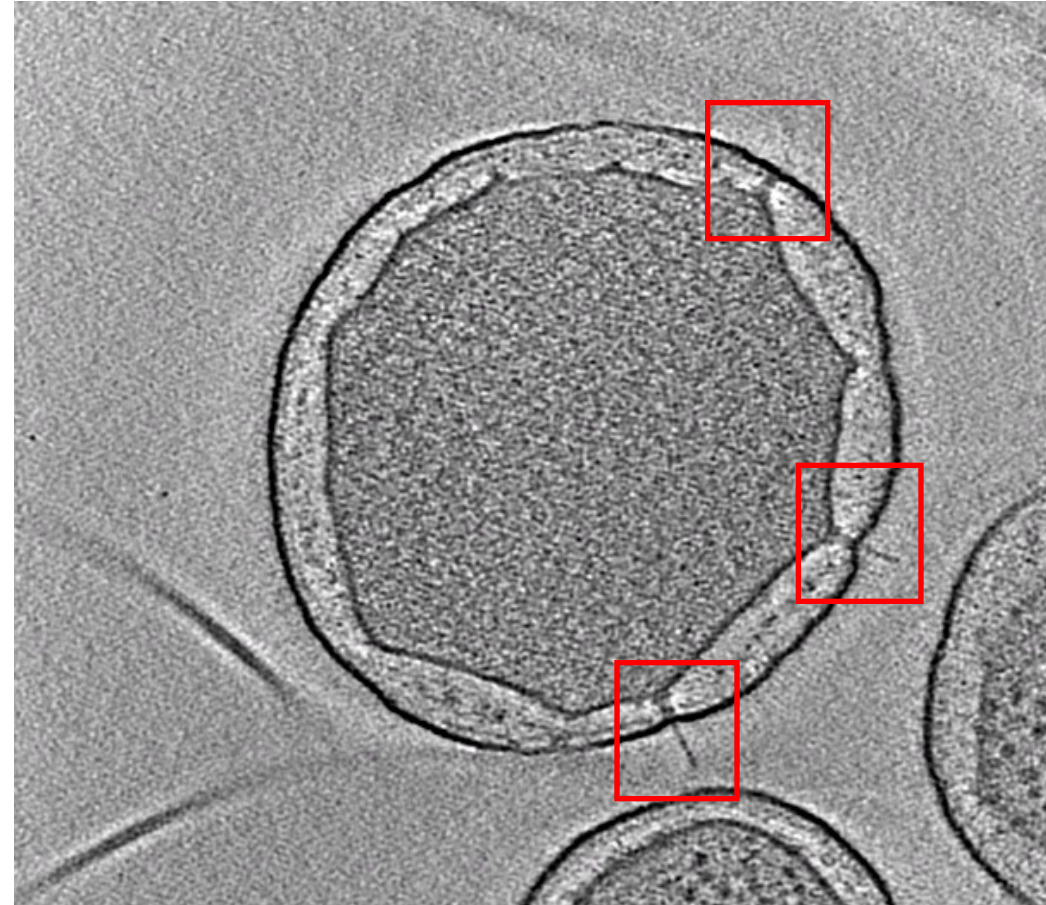
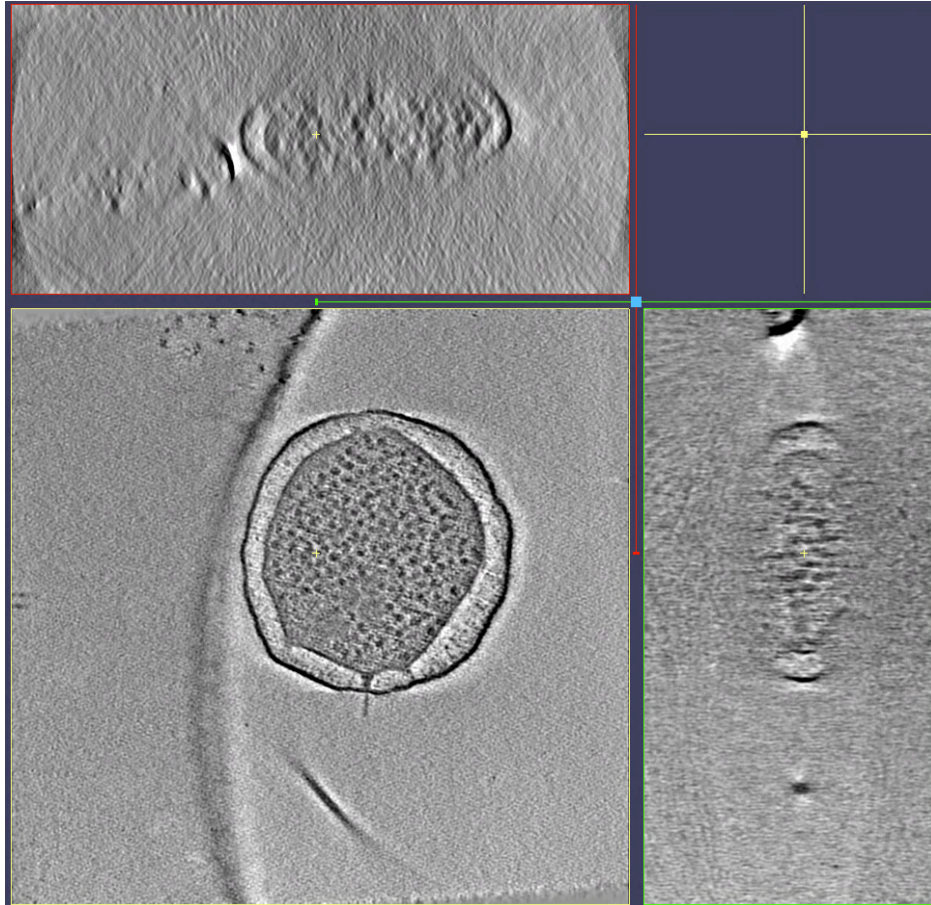


Hu et al., 2017

# Object detection

## Finding T3SS in EM tomography for subtomogram averaging

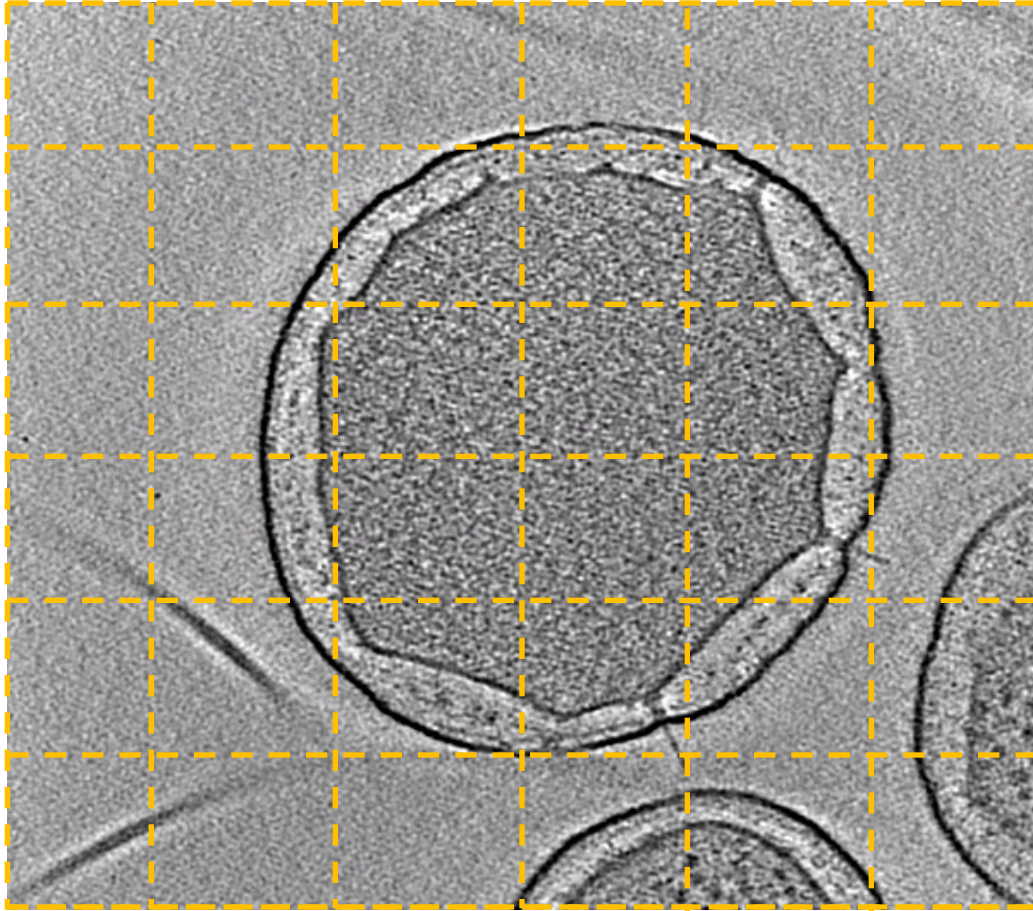
Philipp Heuser, DESY-IT, Scientific Computing  
Thomas Marlovits, Sean Miletic, CSSB



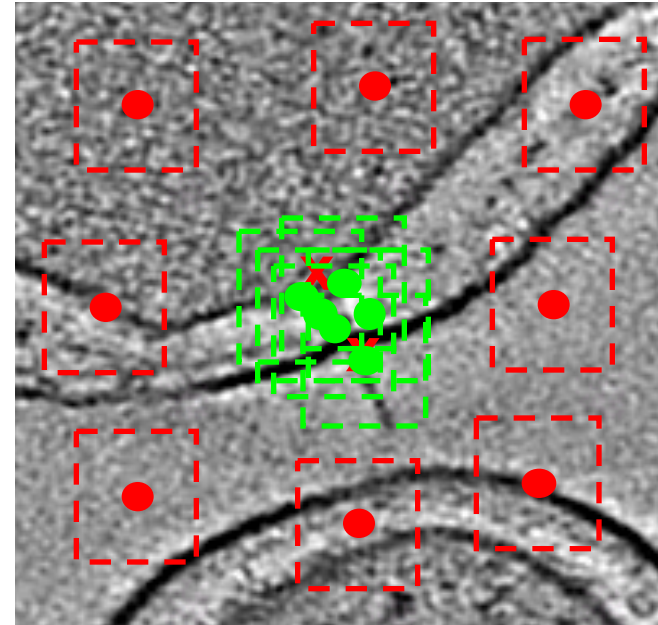


# Object detection

## How to detect a few tiny objects



- get 50x50 px subsamples from images, with stride 1
- Assign label to each patch
- → **Image Classification task**



# LeNet-5 (1998) for classification

Yann LeCun, et al.

- pioneering 7-level convolutional network by LeCun et al in 1998,
- classifies digits, was applied by several banks to recognise hand-written numbers on checks digitized in 32x32 pixel greyscale images.

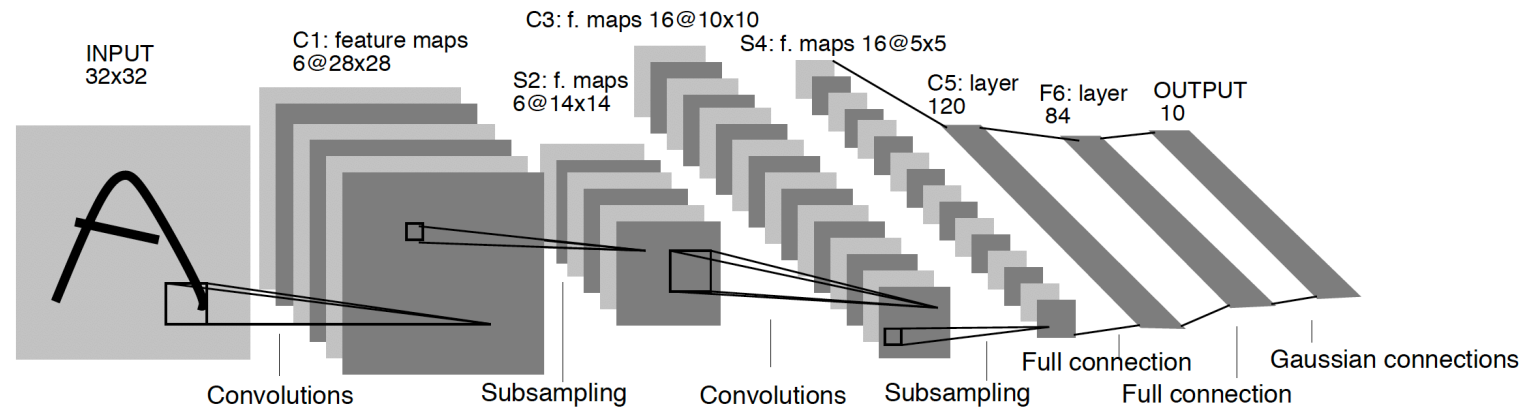
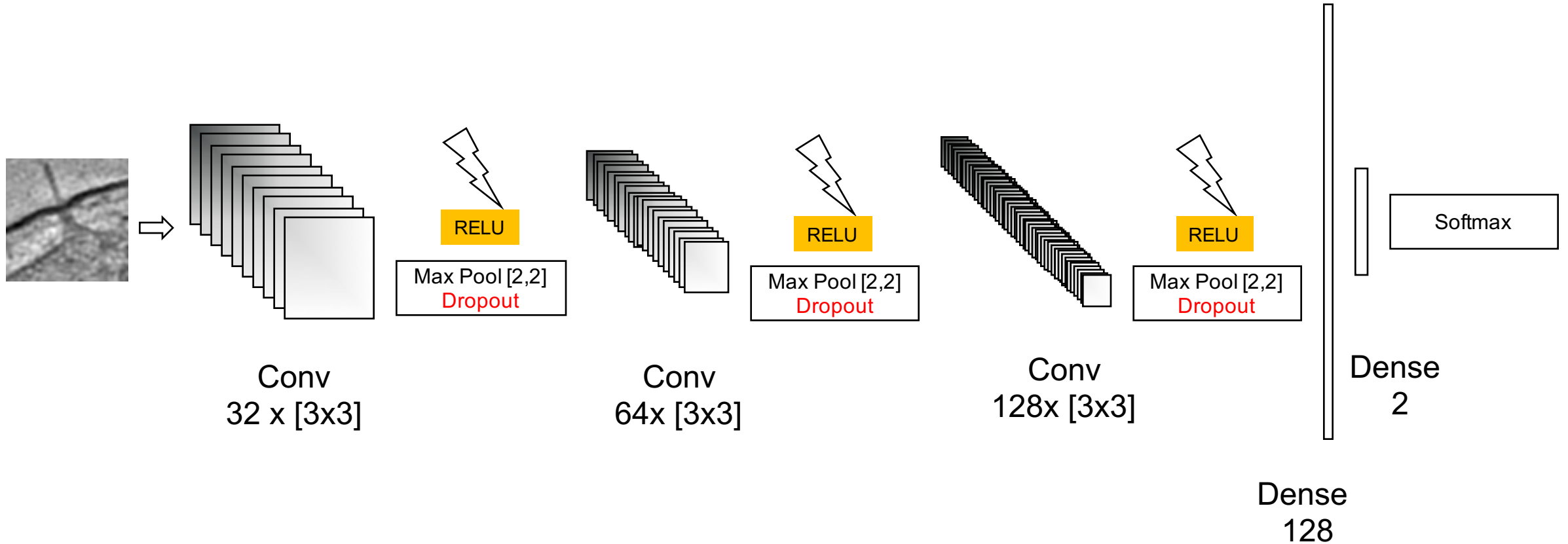


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

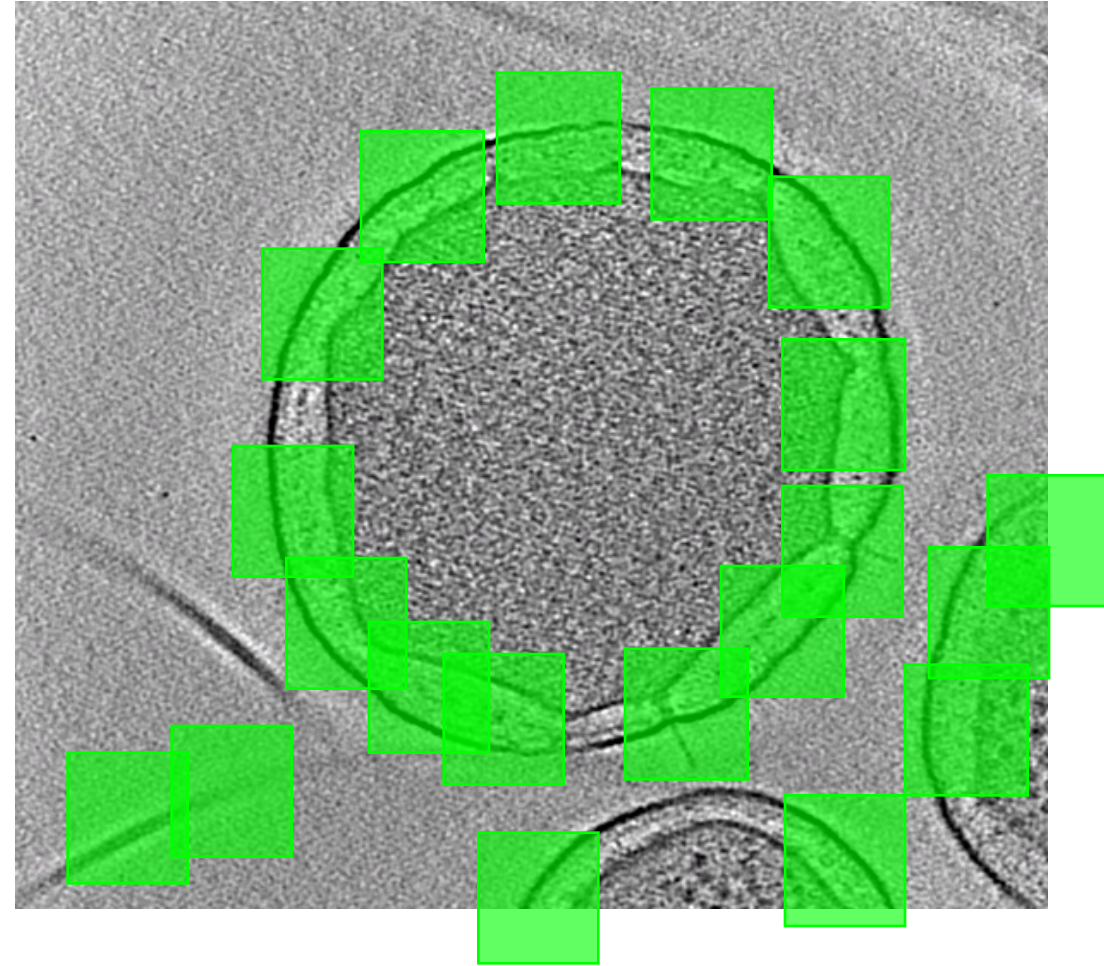
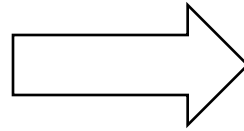
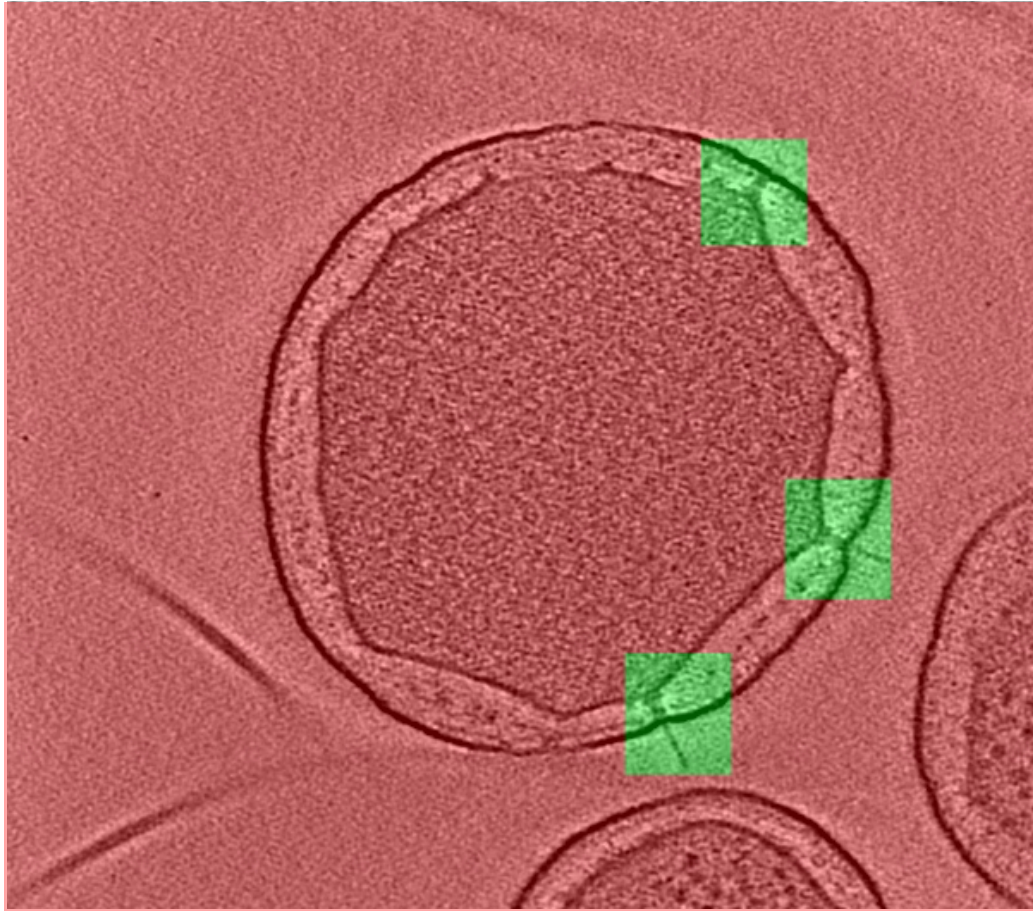
Lecun, Y., Bottou, L., Bengio, Y. & Haffner, P. Gradient-based learning applied to document recognition. *Proceedings of the IEEE* **86**, 2278–2324 (1998).

# Modified Network



# Challenge

Few true answers vs. lots of false answers





# Challenge

## Preselection of training data

### Analysis with standard features:

e.g.

Mean

Median

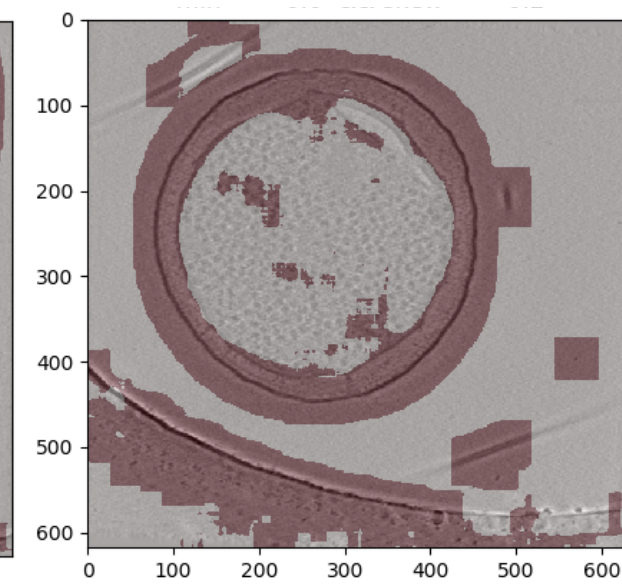
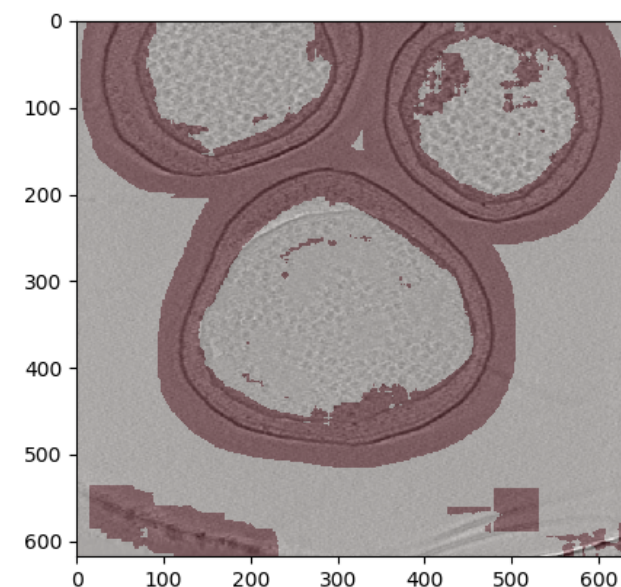
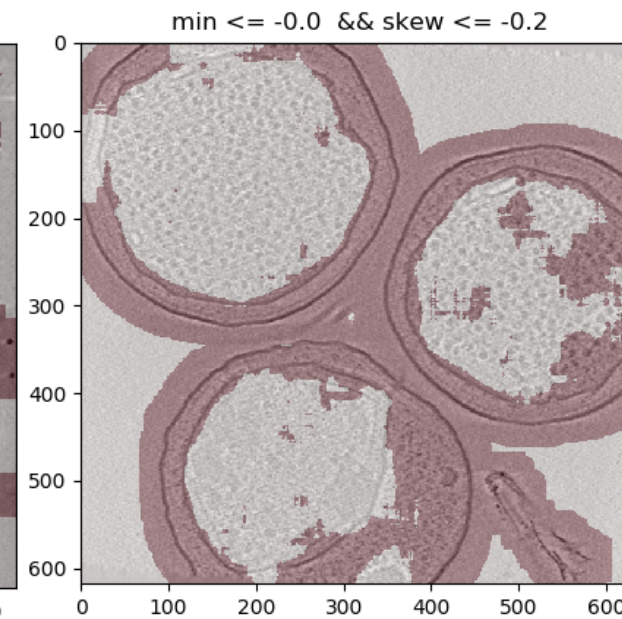
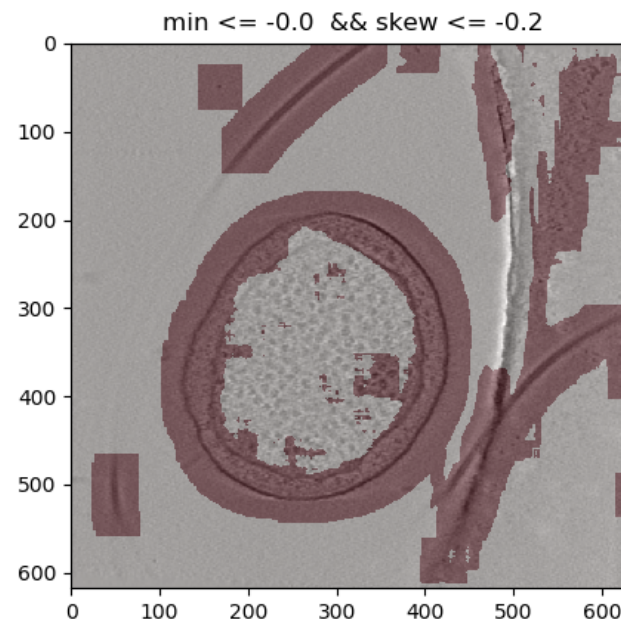
**Skewness**

**Min**

Max

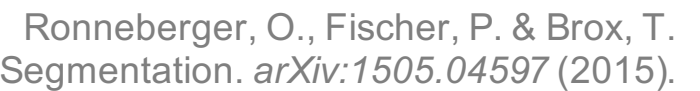
Kurtosis

Etc....





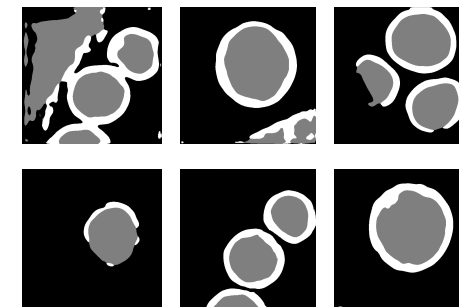
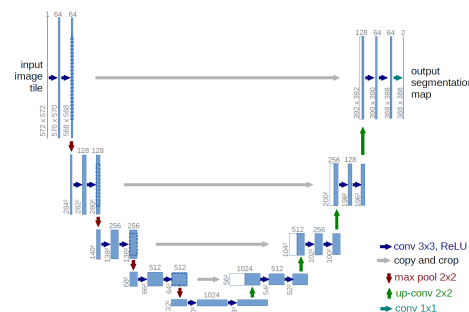
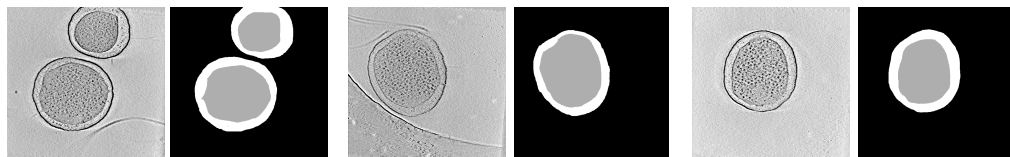
## U-Net



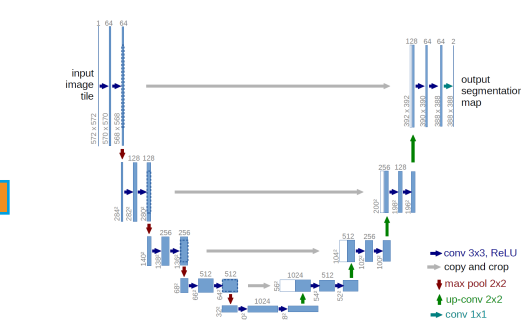
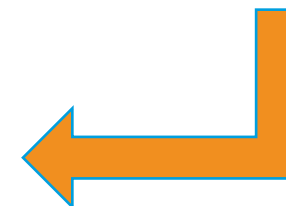
# Segmentation

## U-Net

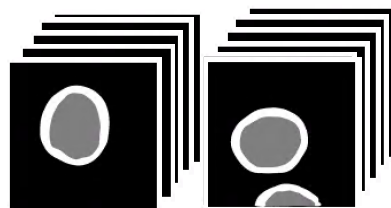
segmented 18 2D slices by hand



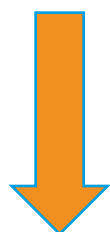
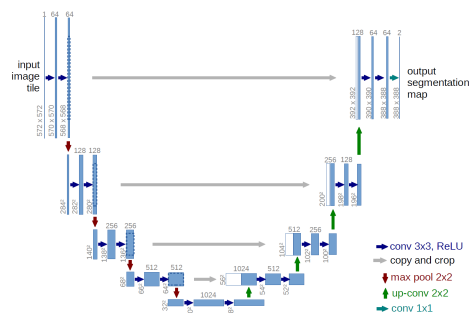
Manually corrected  
12 particularly bad  
predictions



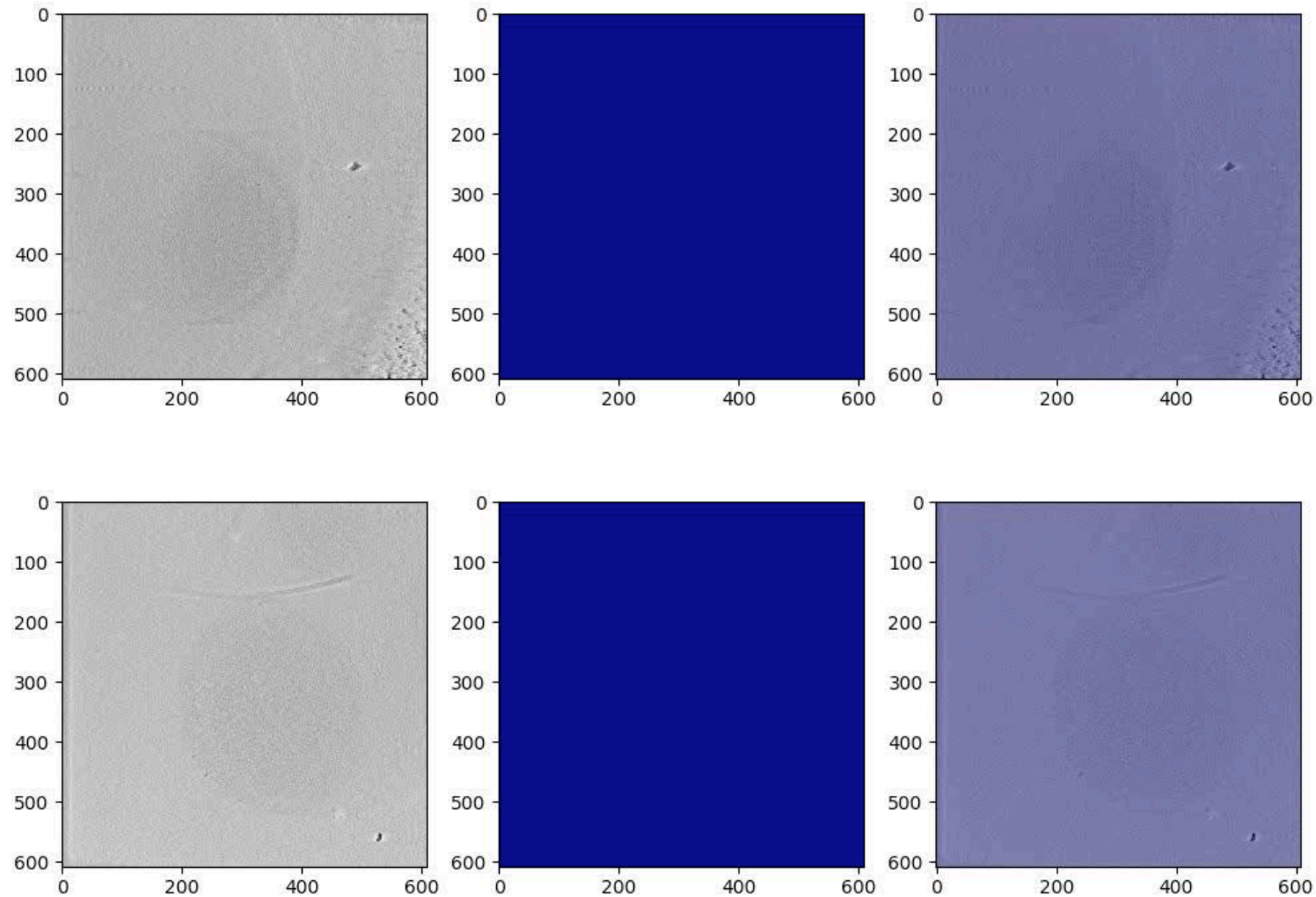
re-trained with 30 2D images



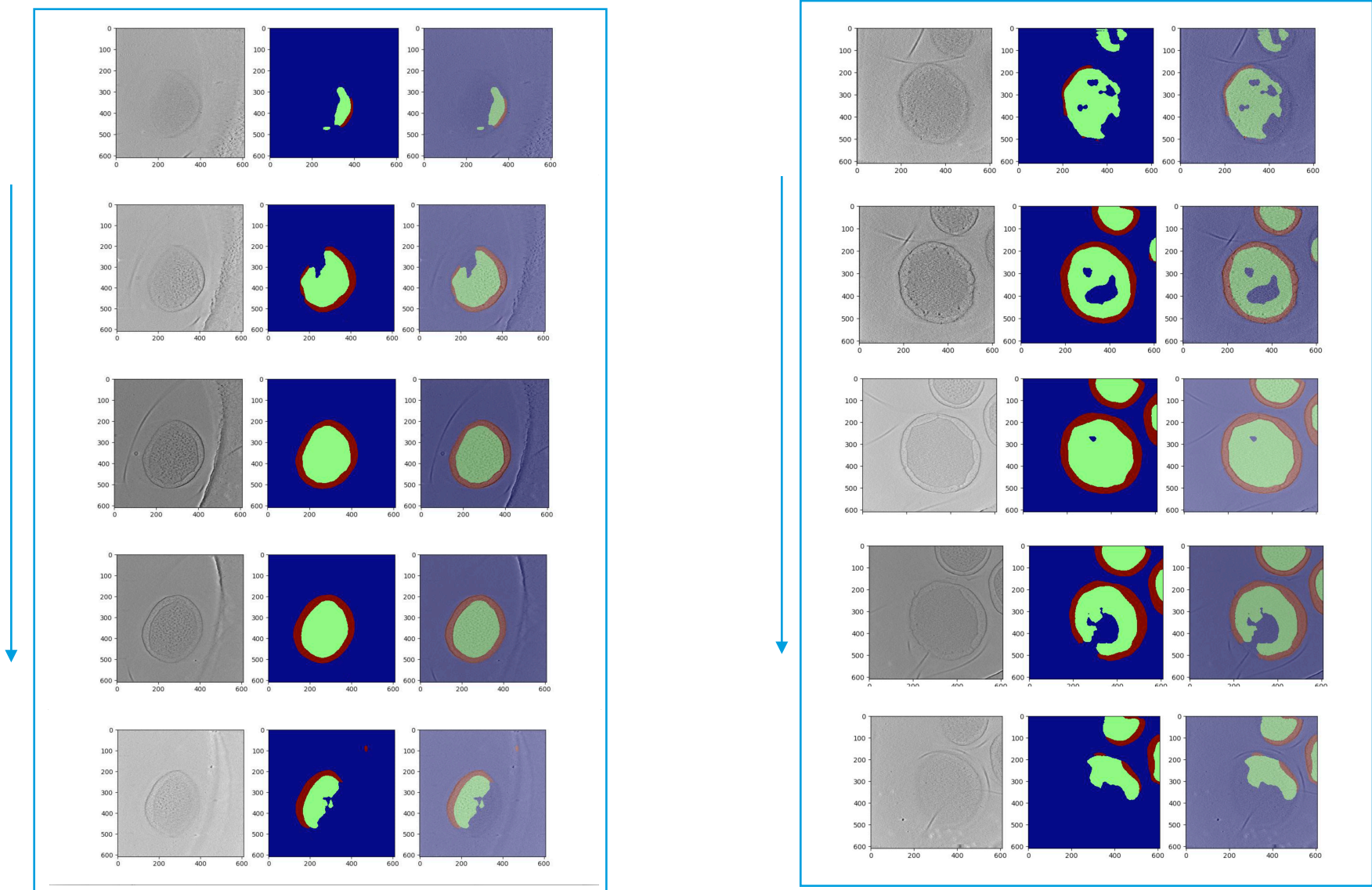
Applied to 4 3D volumes;  
corrected and added all falsely  
predicted and some randomly  
selected images to training data  
(509 2D images)



# Final trained U-Net

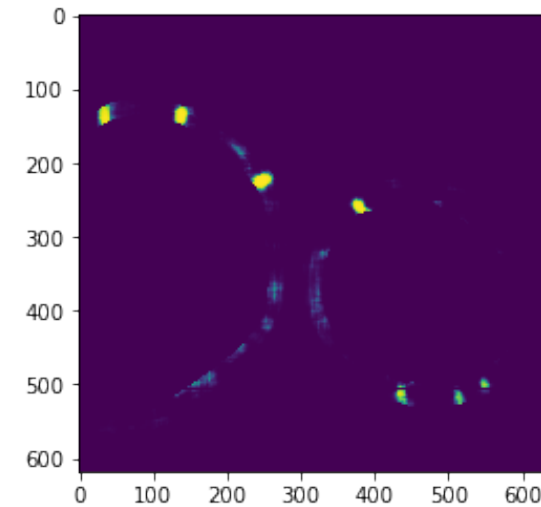
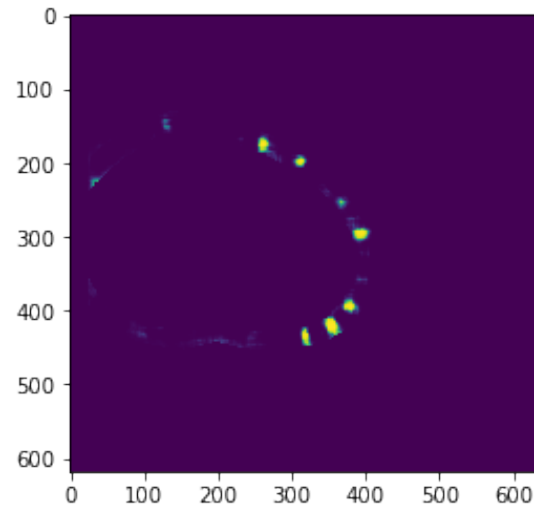
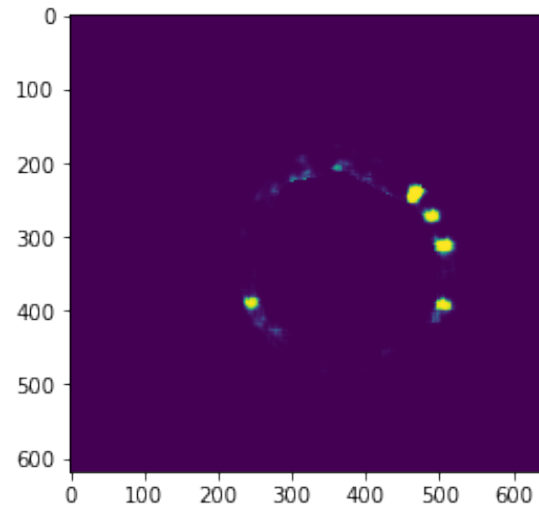
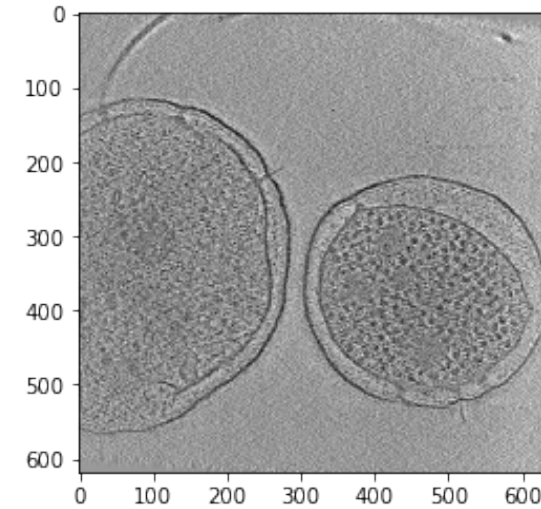
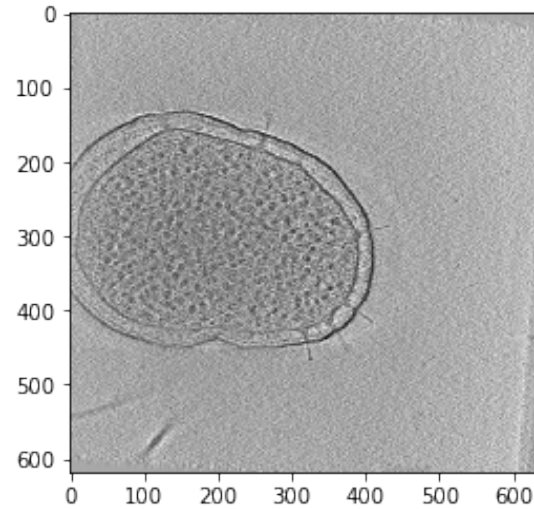
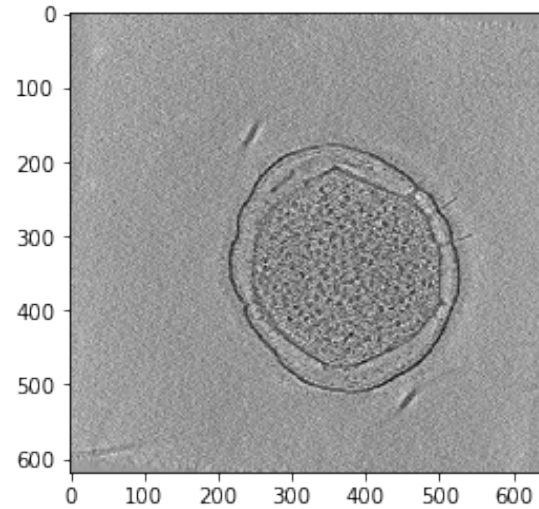


# Final trained U-Net

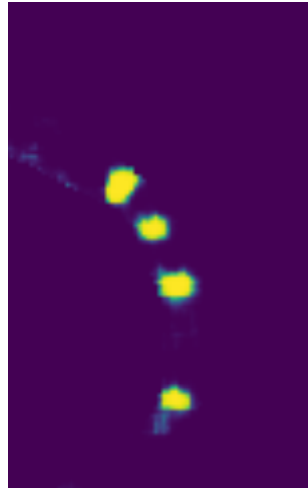


# T3SS found!

Searching only within the membrane



# T3SS candidates



clustering hits

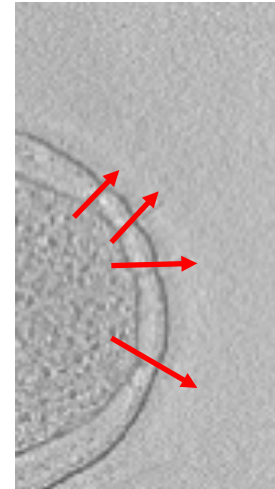
+



segmentation

=

T3SS candidates &  
direction



subtomogram  
averaging  
software

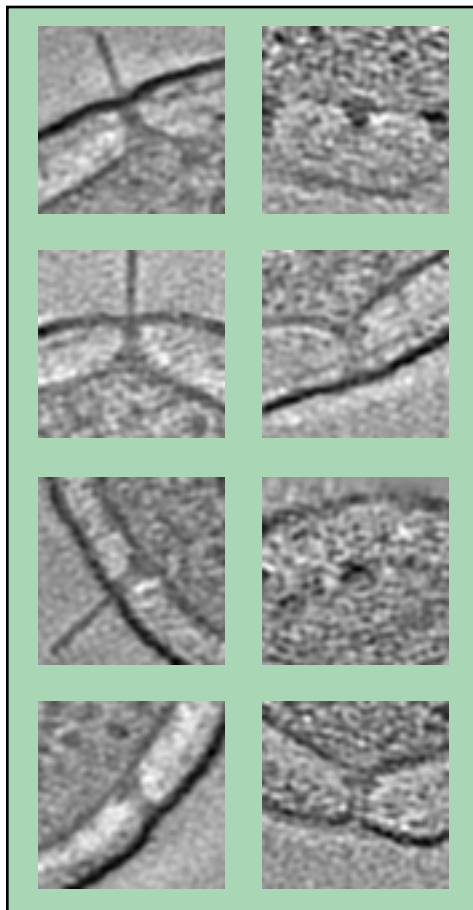


# TP/FP

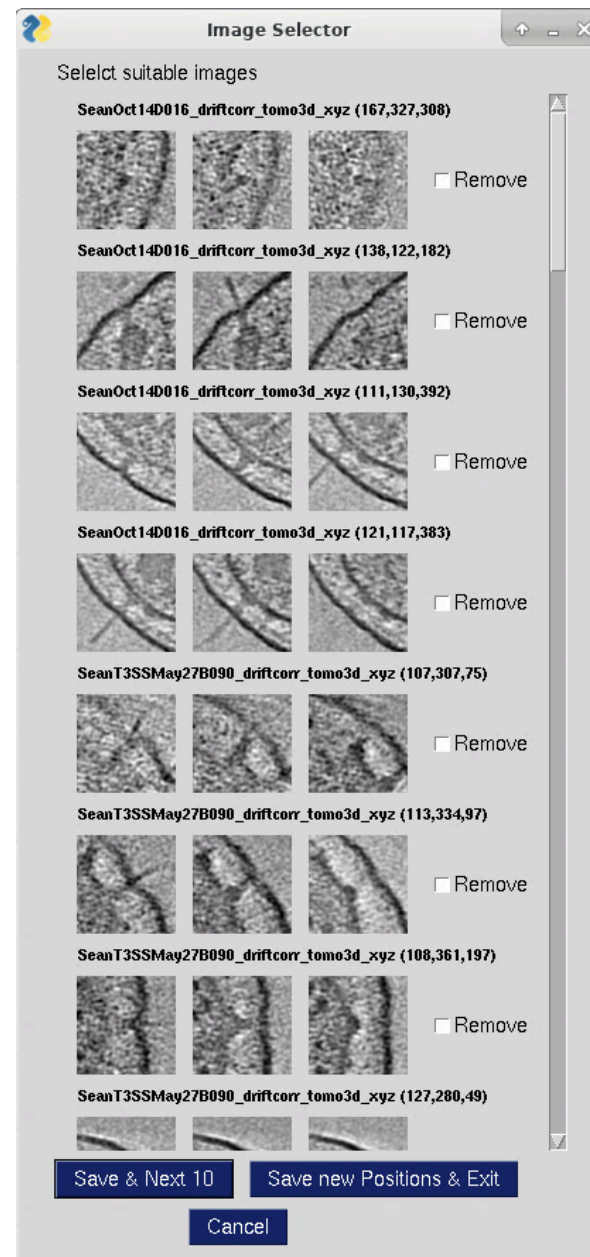
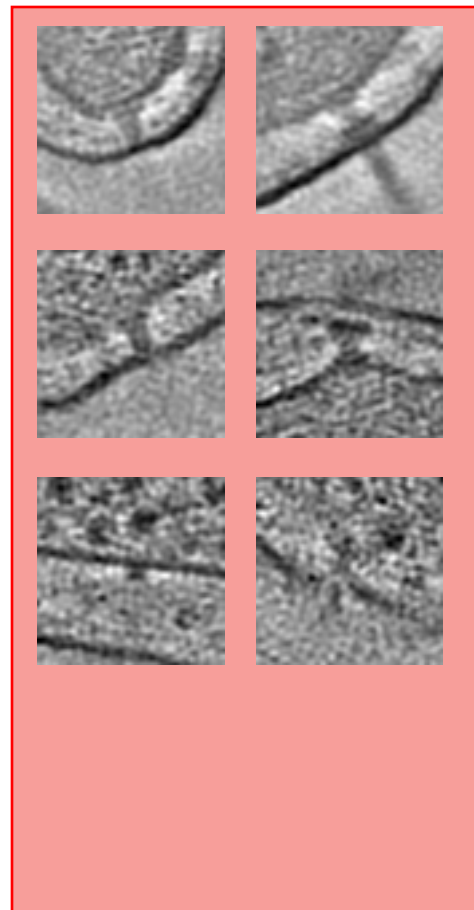
## Ground truth?

Currently we have about the same number of FP as TP.

TP

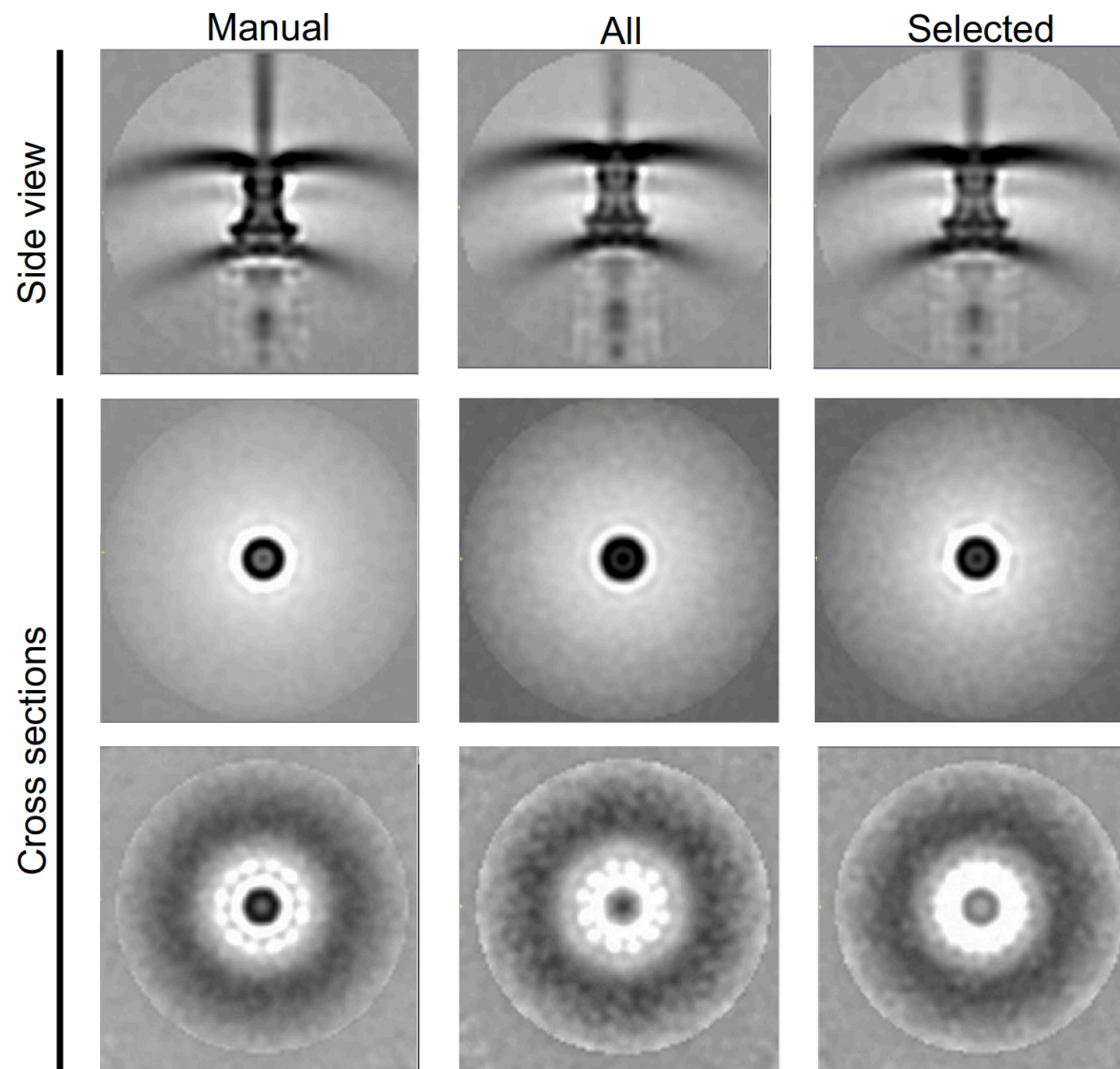


FP





# 3D reconstruction



# Acknowledgments

## Thanks to...



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