

# Convolutional Neural Networks for DESY photon science

Philipp Heuser, DESY-IT

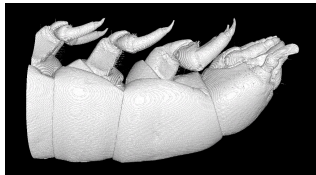
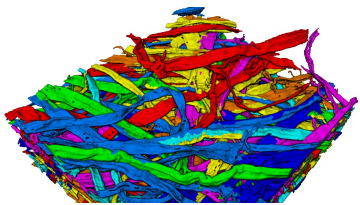
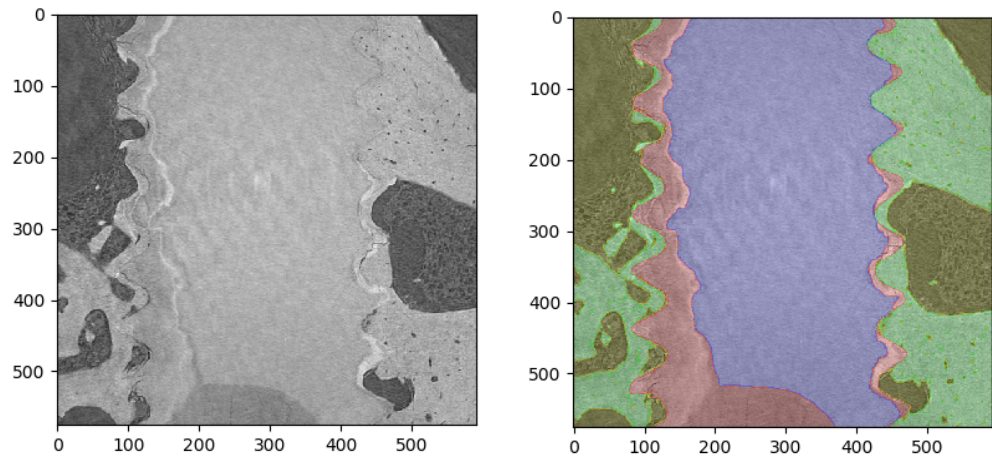
29/11/2019

Round Table on ML/DL@DESY

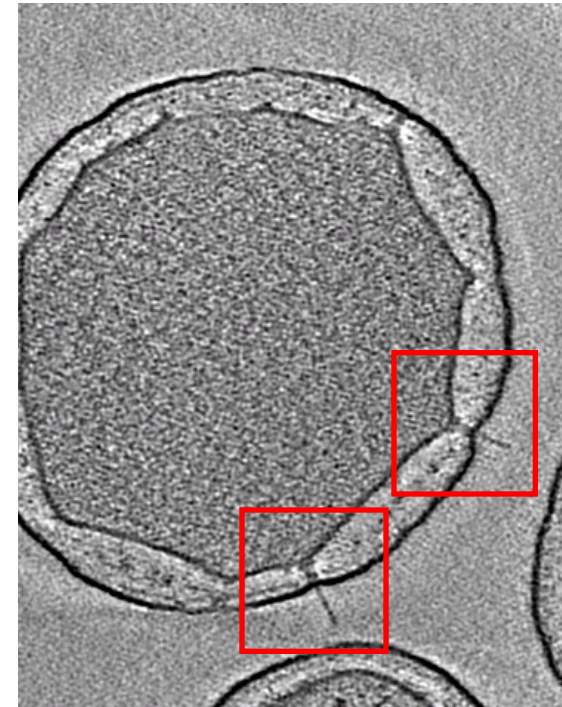


# Projects

## Helmholtz Zentrum Geesthacht (HZG) / DESY-IT Segmentation of X-ray tomography data



## CSSB / DESY-IT Object Detection for Cryo Electron Tomography



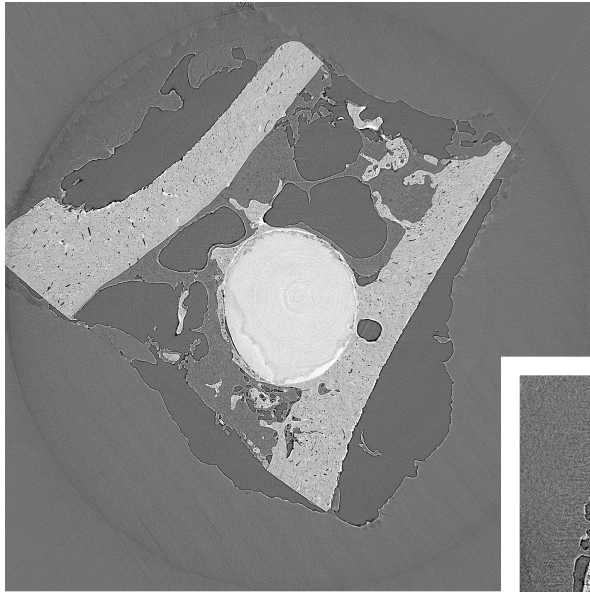


# Automated Volumetric Interpretation

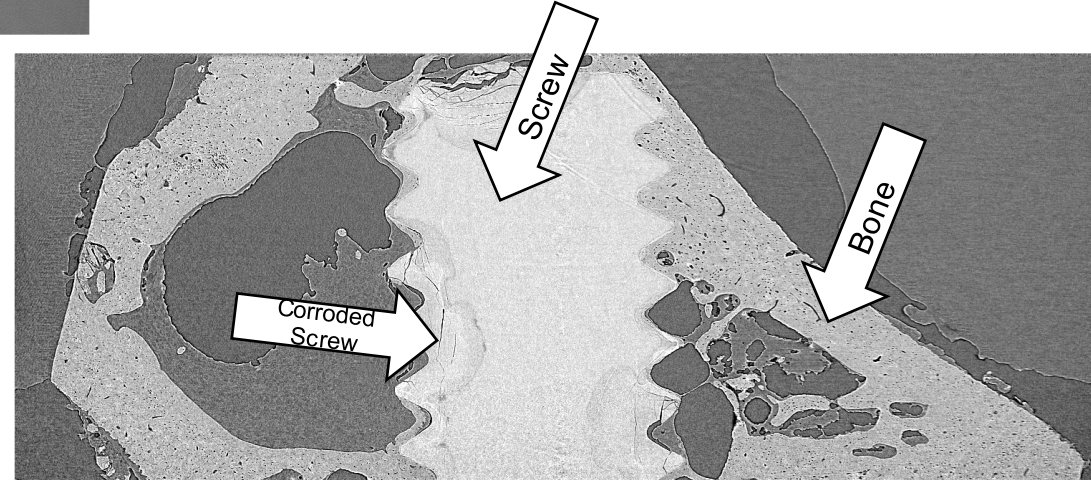
Philipp Heuser, DESY-IT, Scientific Computing  
Julian Moosmann, Helmholtz Zentrum Geesthacht, HZG



## Semantic segmentation of bone implants (HZG)



Certain bone implants will be absorbed over time. Investigating the physiological processes over time by **X-ray tomography** requires an accurate segmentation of a significant number of comparably large volumetric datasets.

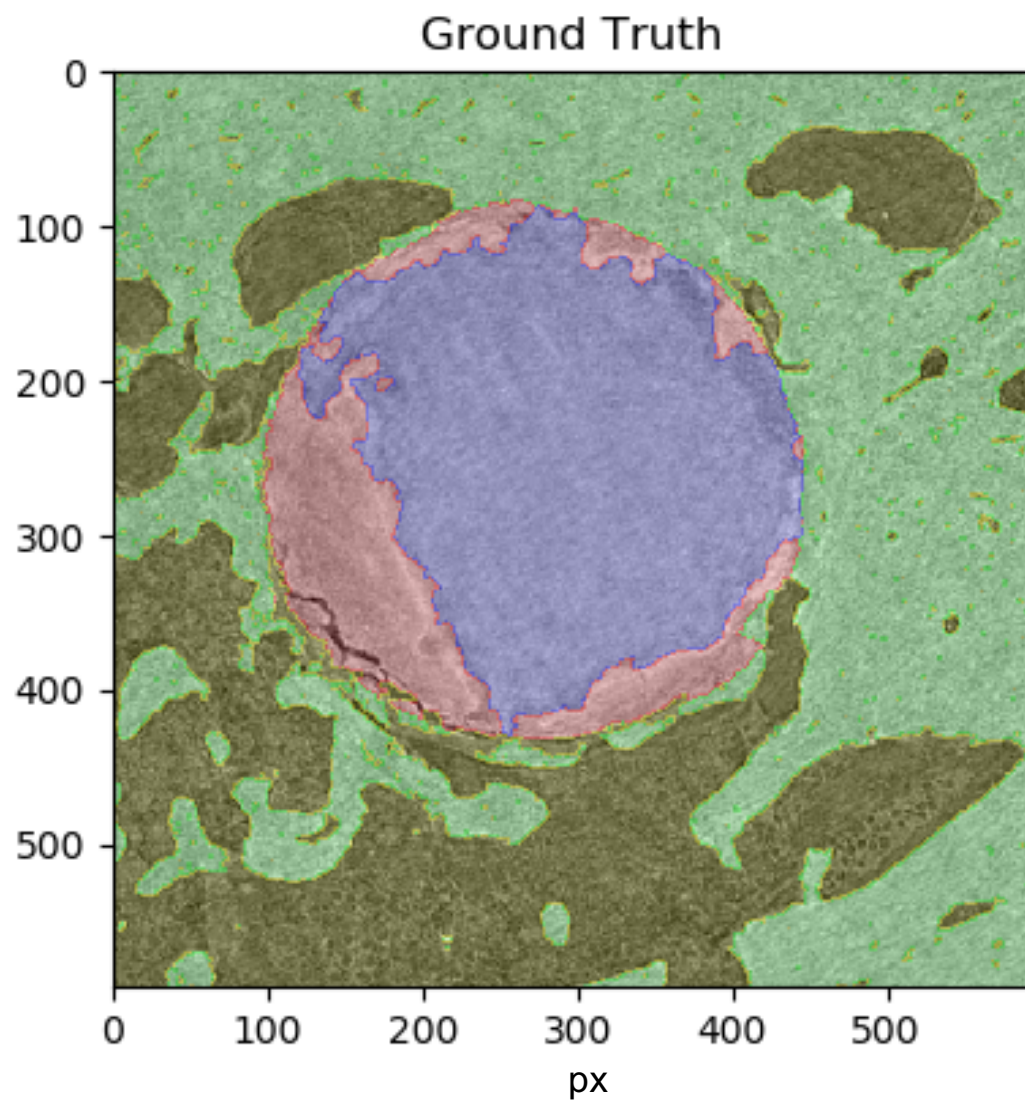
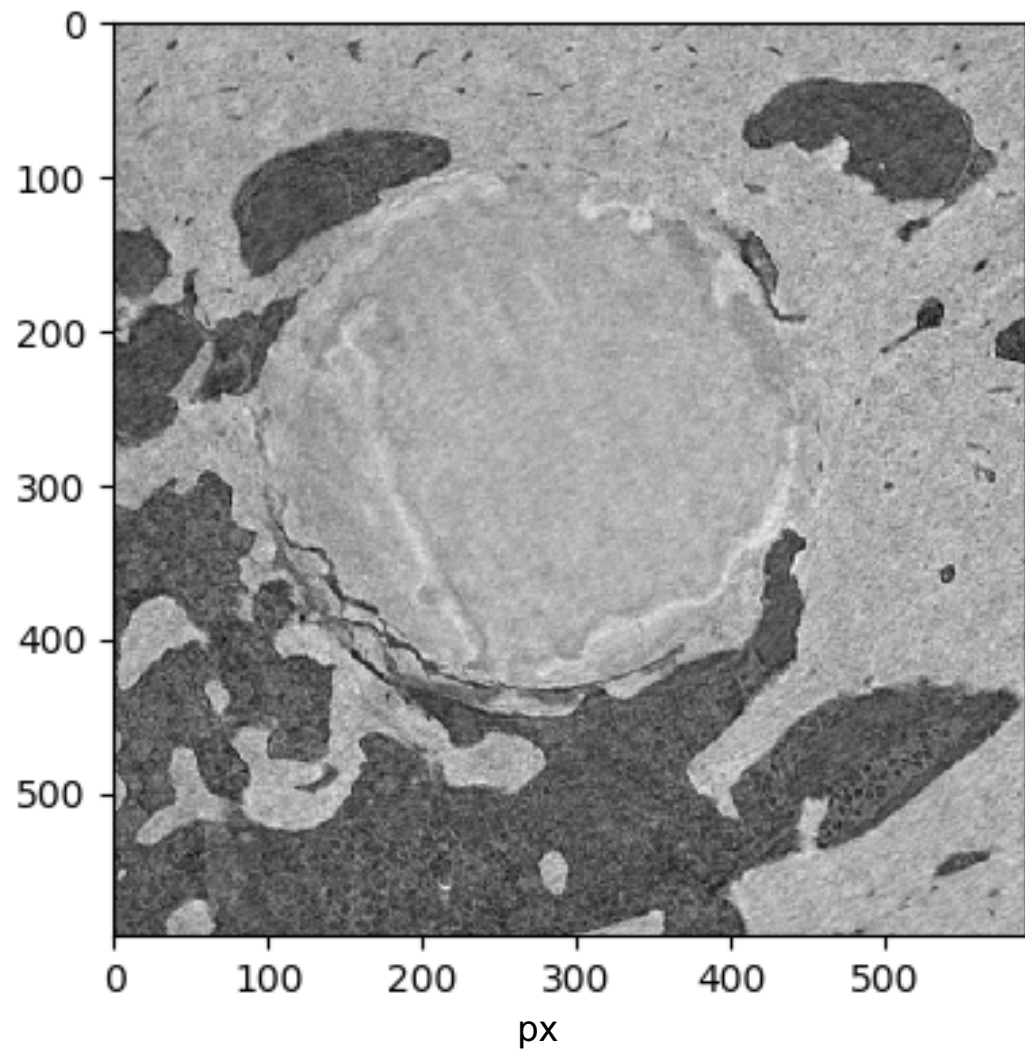


# U-Net



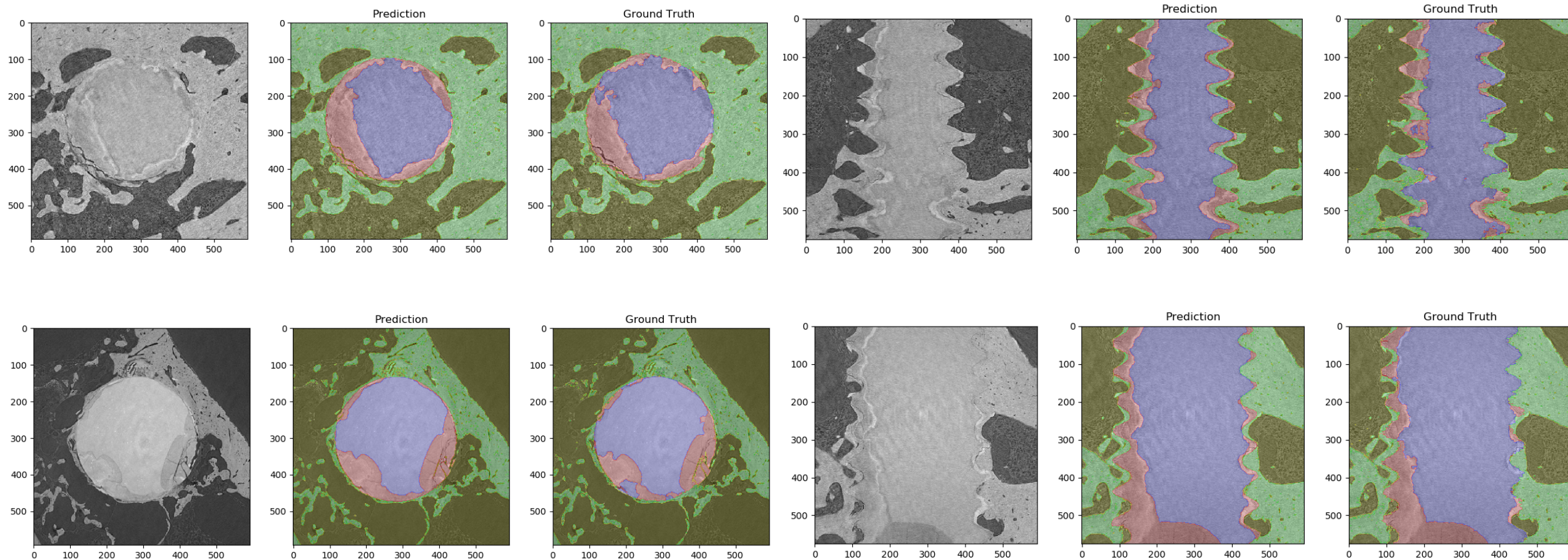


# Weak ground truth



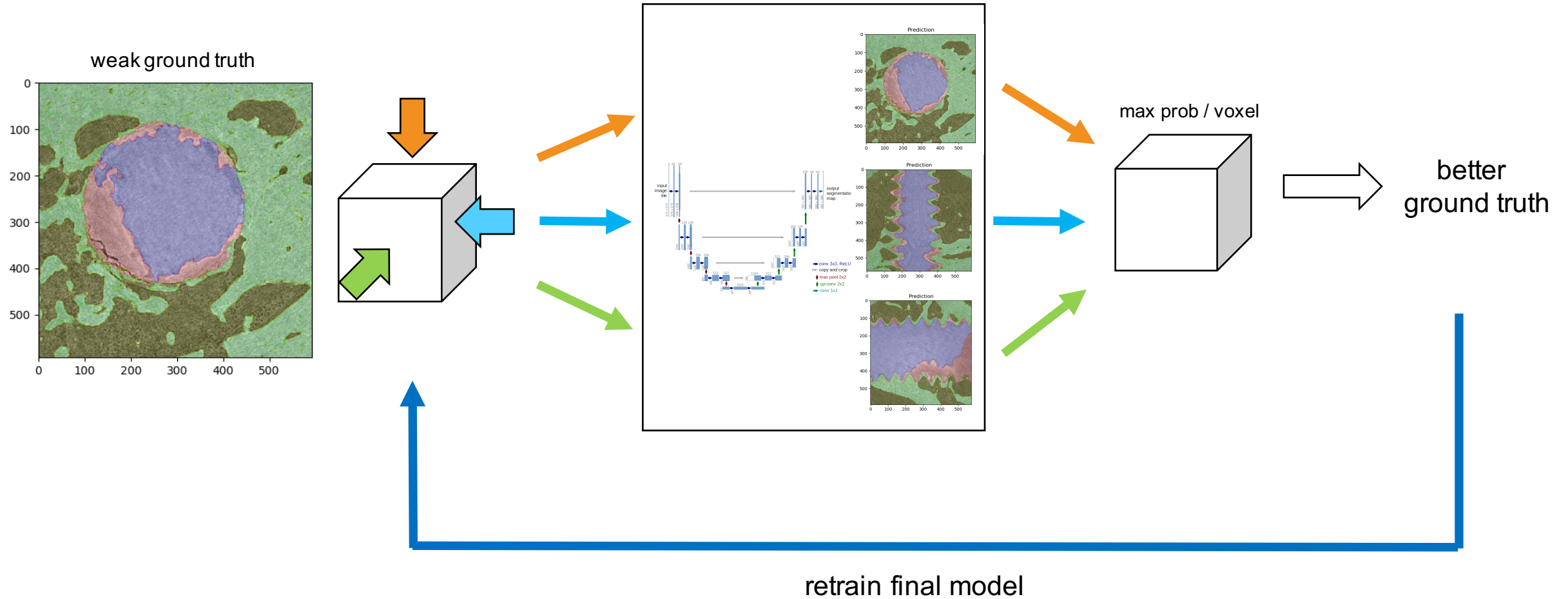
# Segmentation

Trained on ~ 100,000 images





# Training with weak ground truth





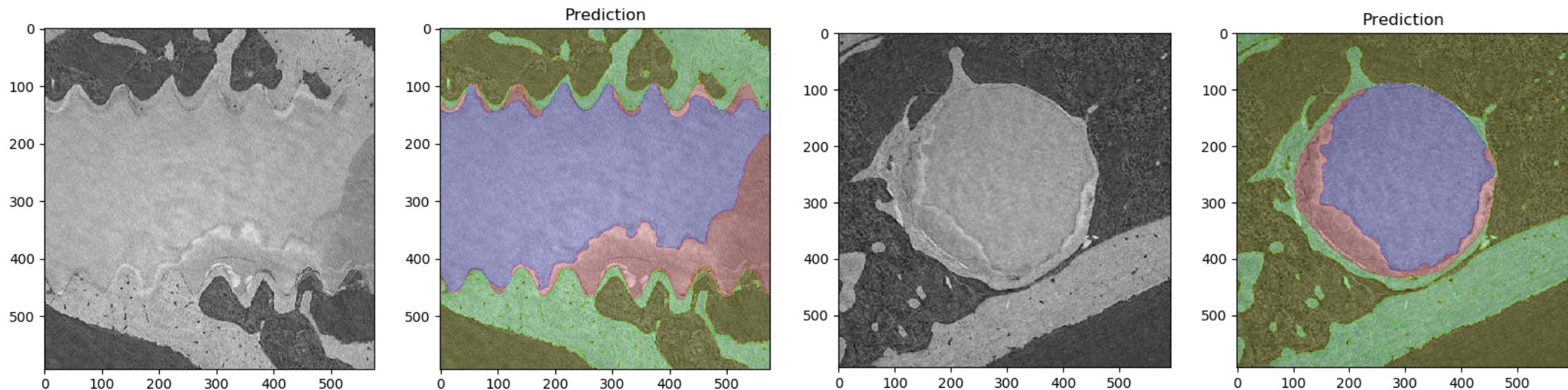
# Automated Volumetric Interpretation

Trained on **~15,942** images from **11** 3D datasets

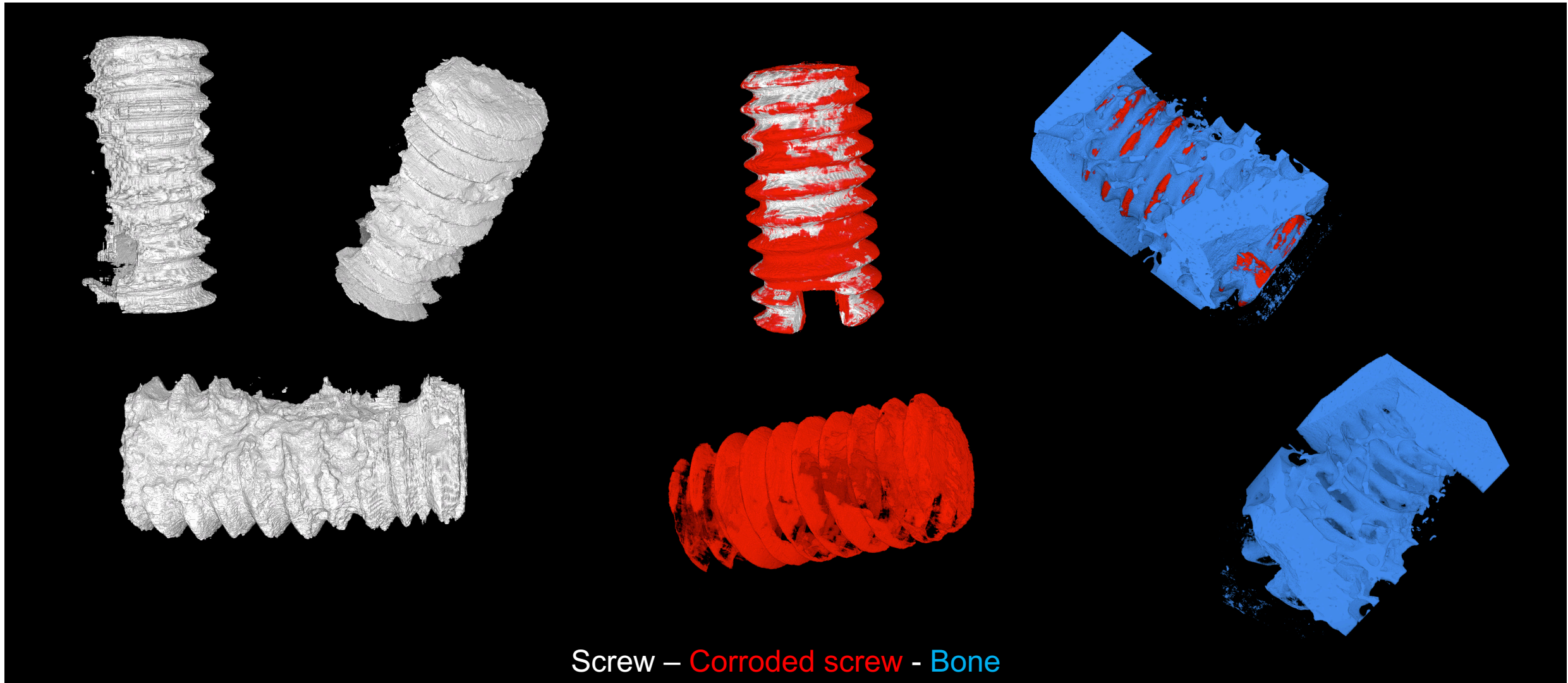
Each image 5 times **augmented**, yielding **95,652** images for training

Training for 15 epochs using central 600 pixels takes **7 days** using one V100 GPU (Keras)

**Inference on Test-Sets (not used for training), yields very high accuracy**



# Segments



# Object Detection for Cryo Electron Tomography

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



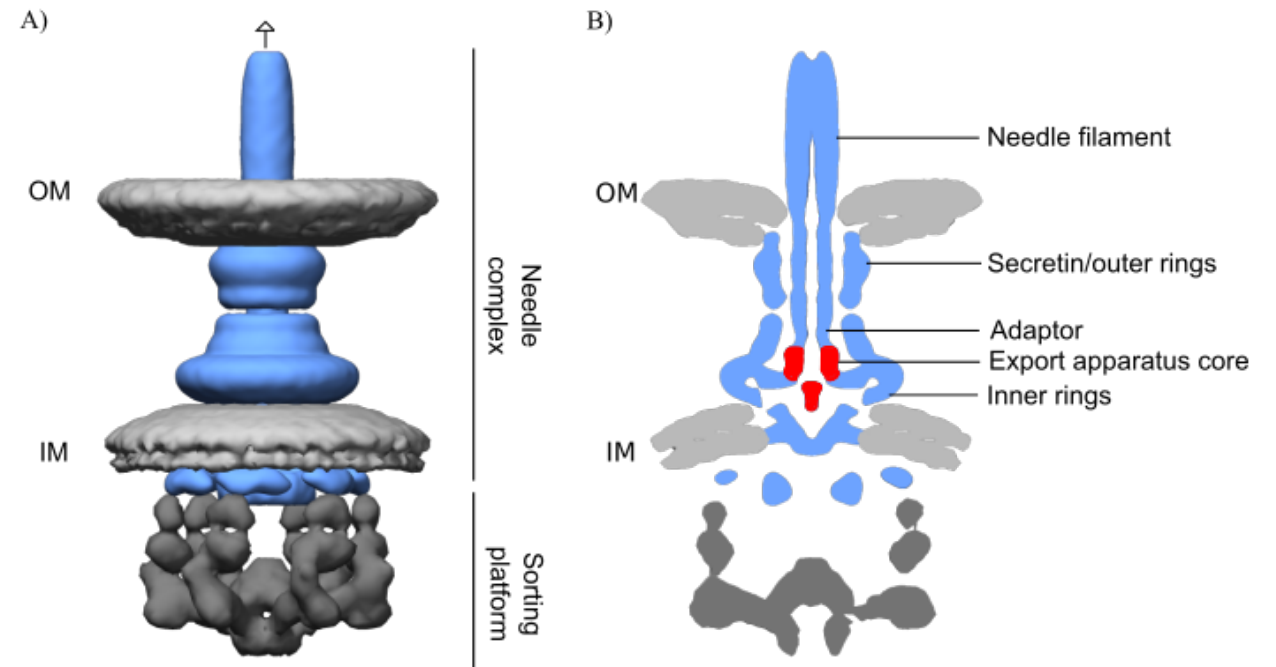
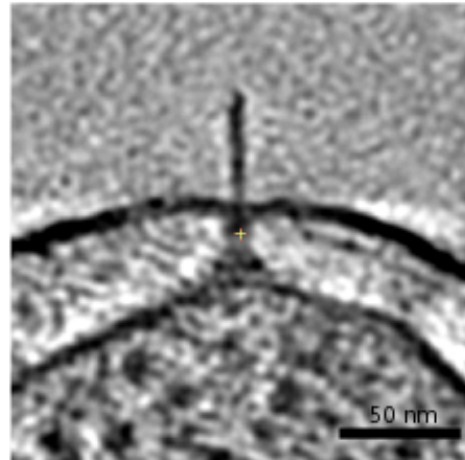
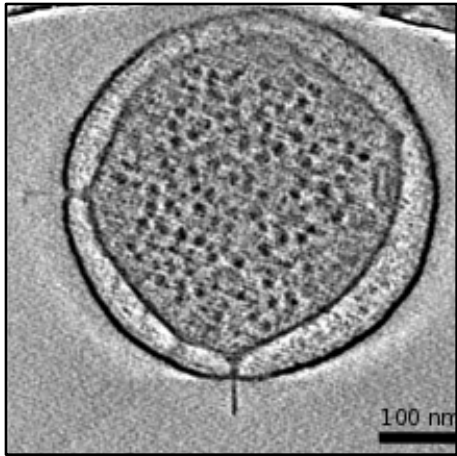
**CSSB**

Centre for Structural  
Systems Biology

With:

Sean Miletic, Thomas Marlovits

CSSB - Hamburg



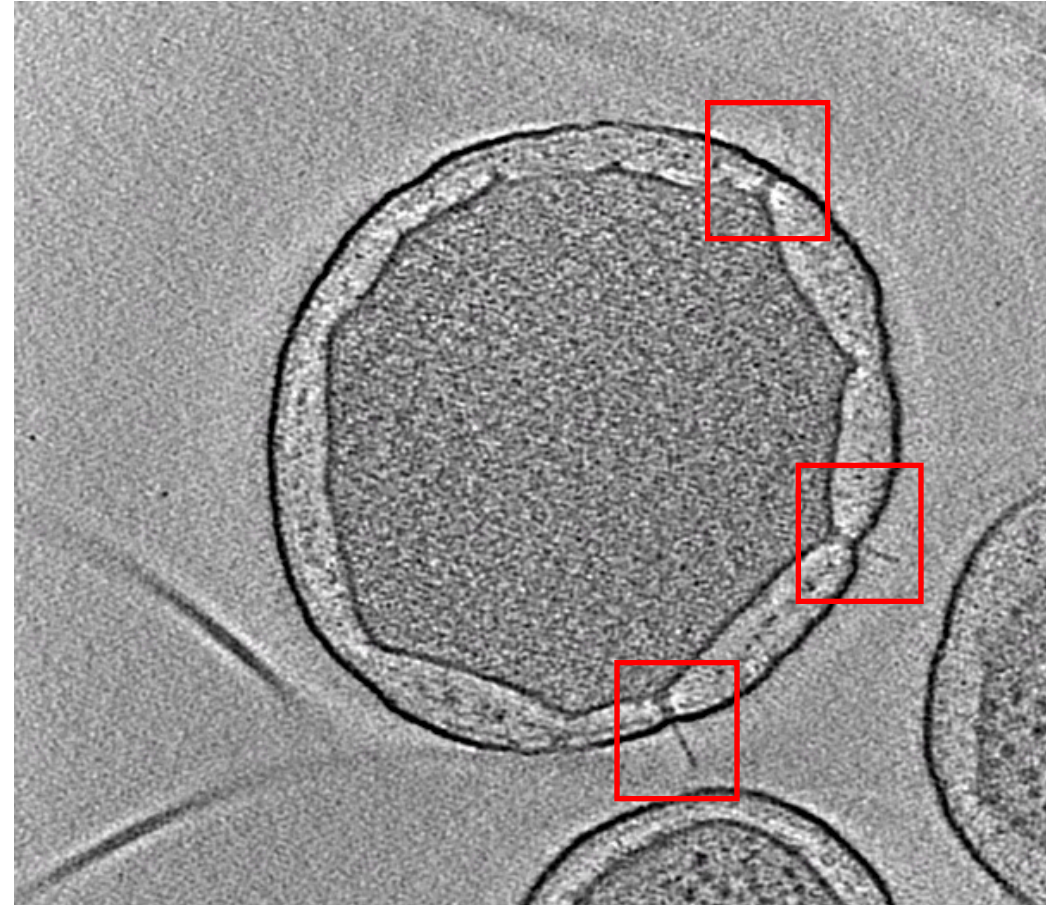
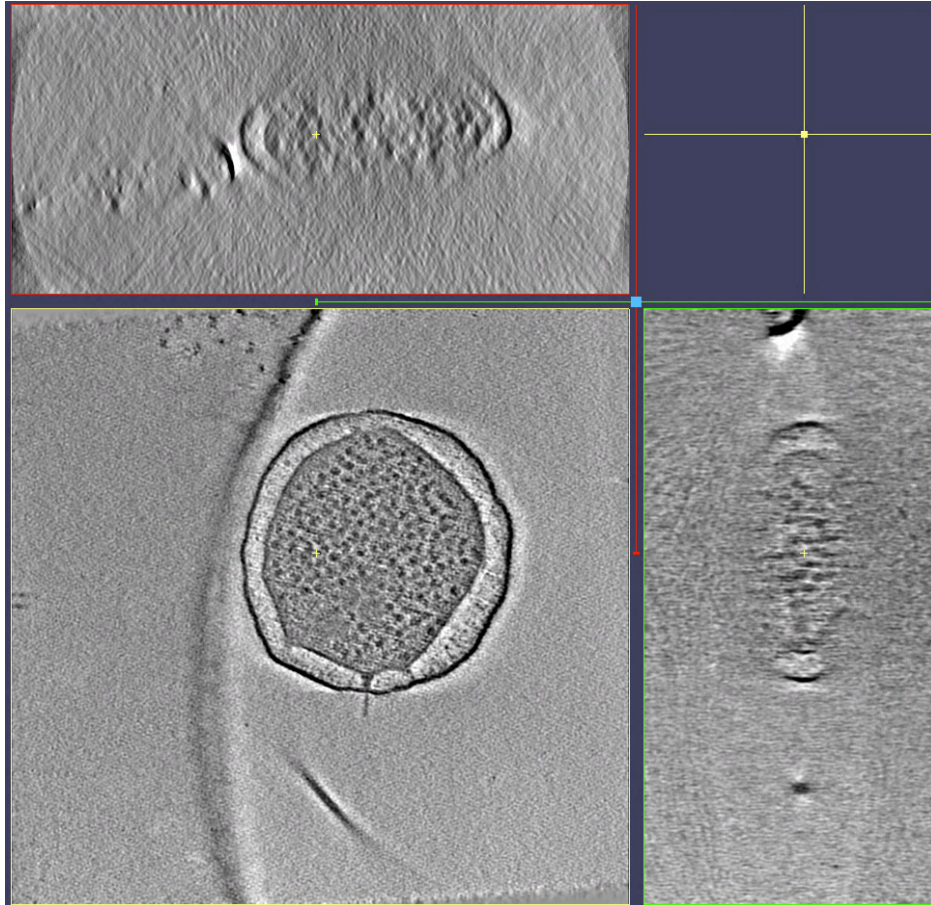
Hu et al., 2017



# Object detection

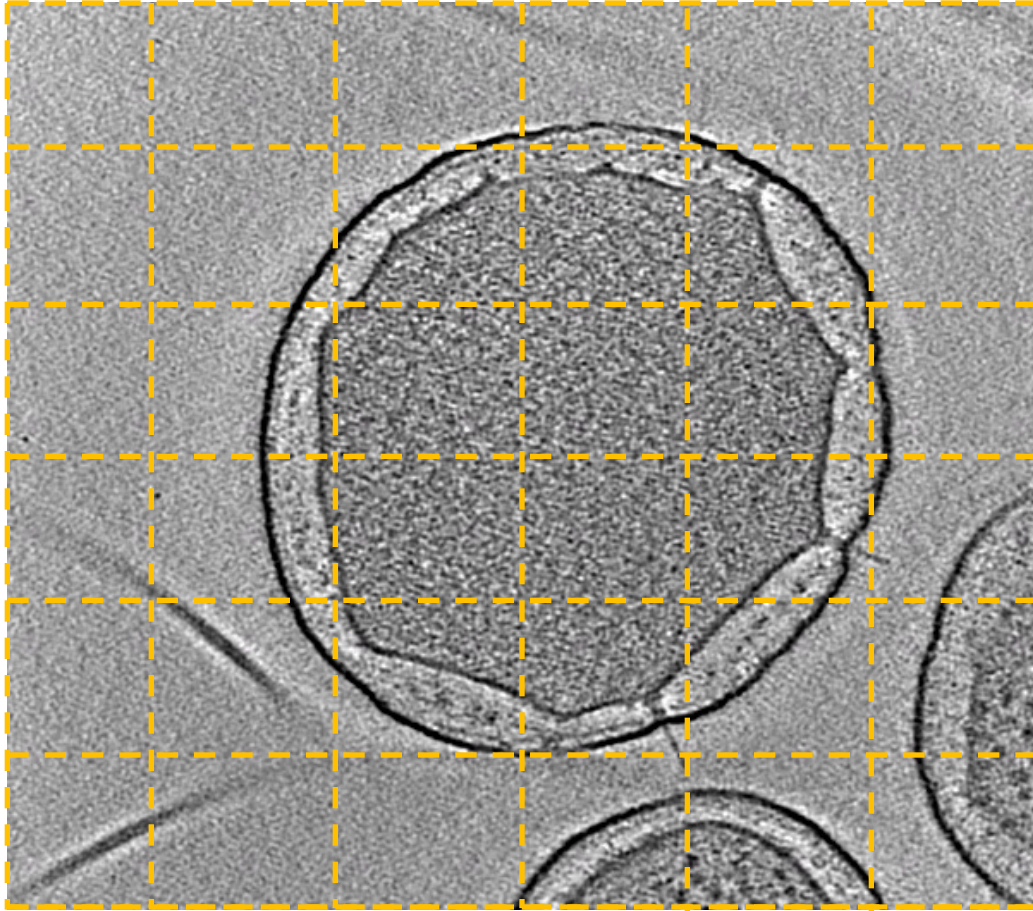
## Finding T3SS in EM tomography for subtomogram averaging

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

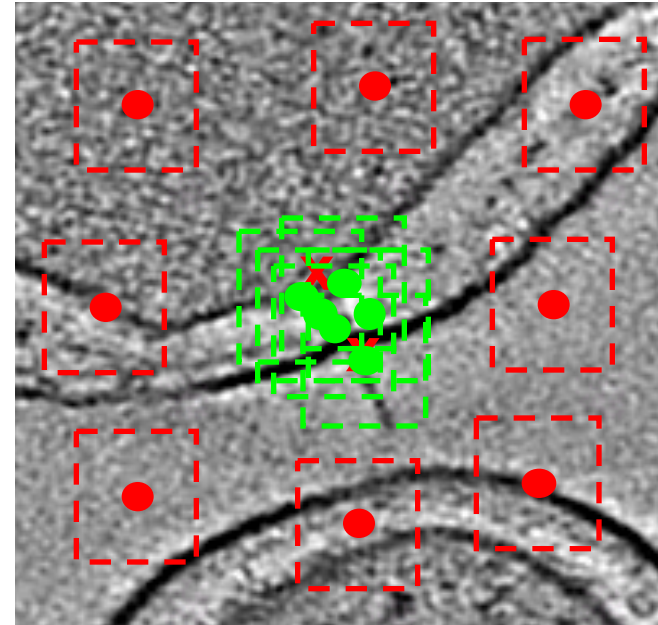


# Object detection

## 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.

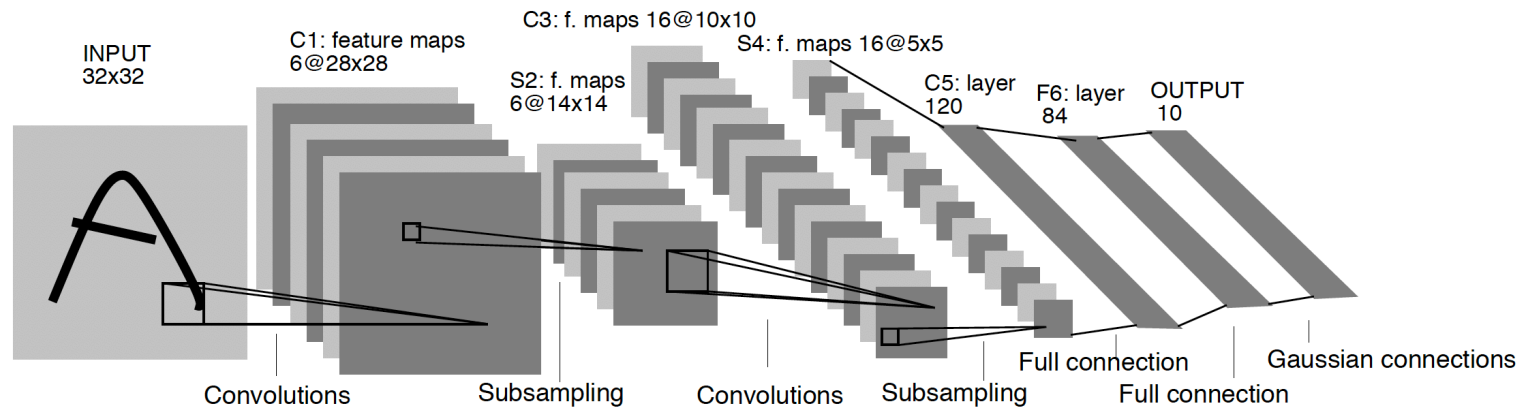
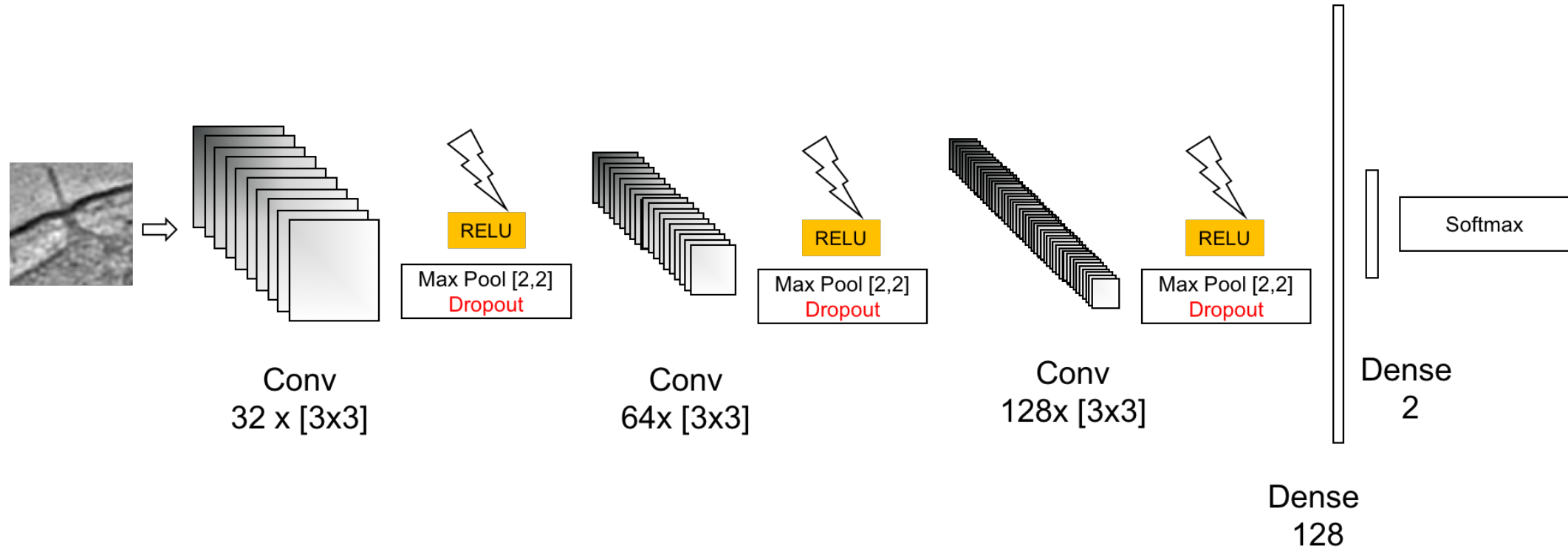


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

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

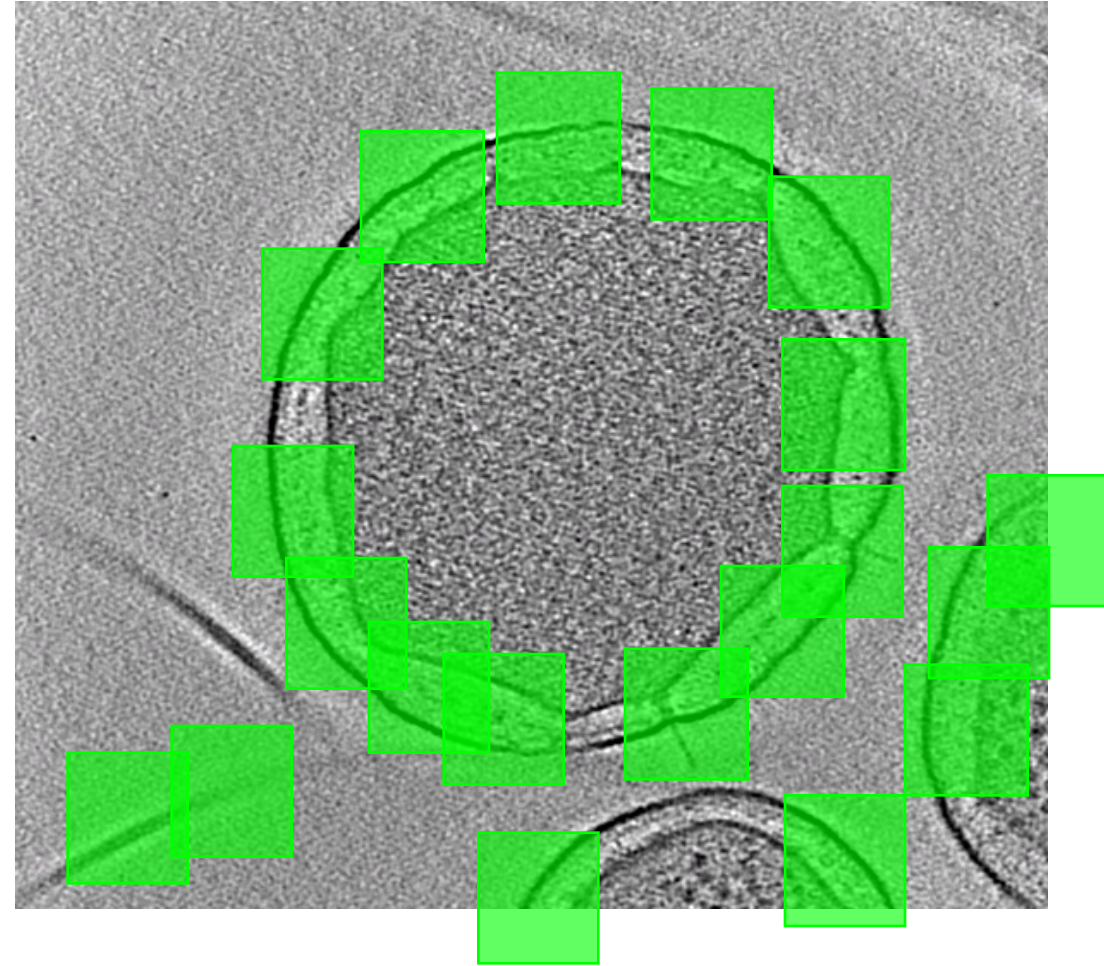
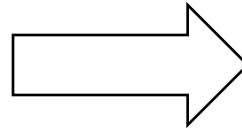
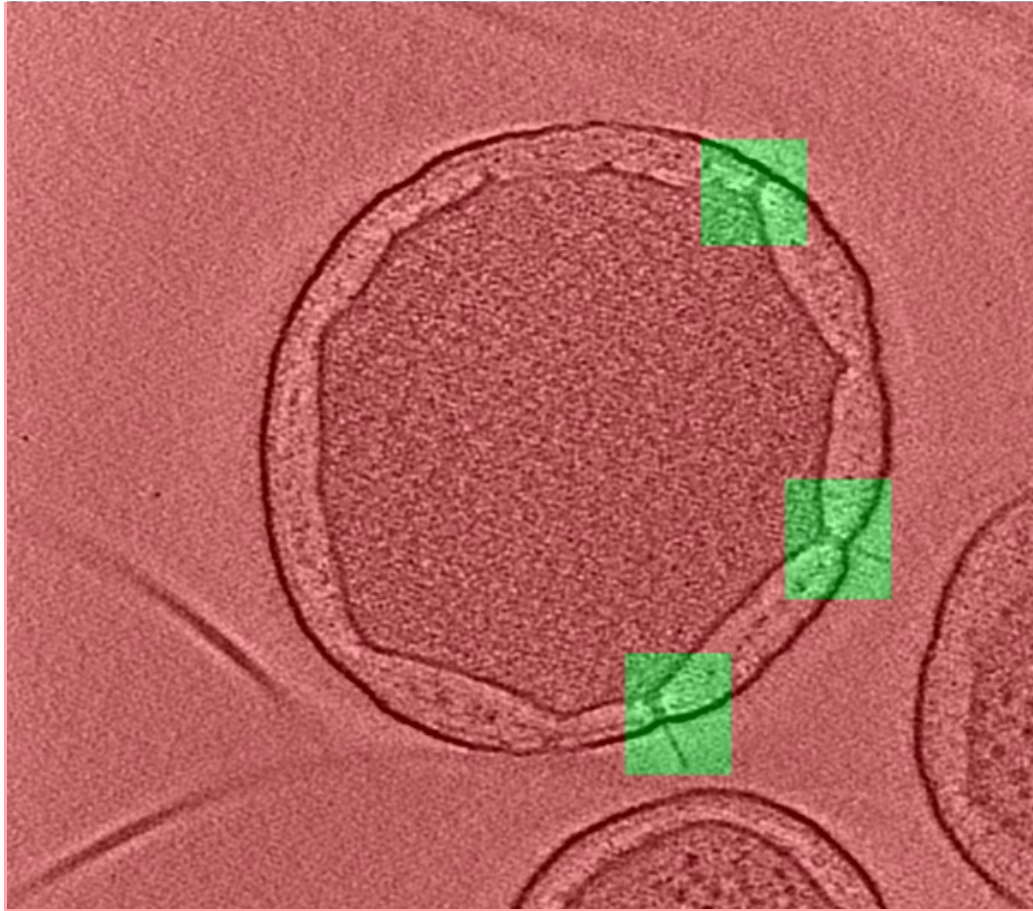


# Modified Network



# Challenge

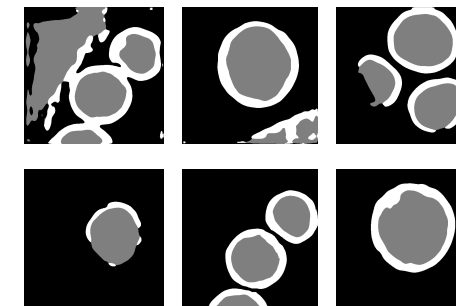
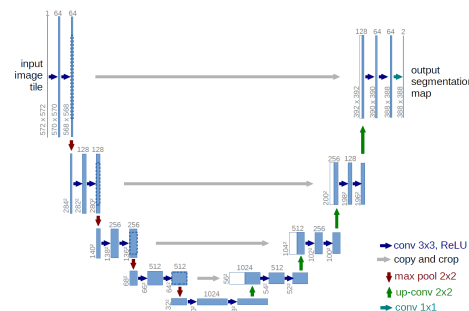
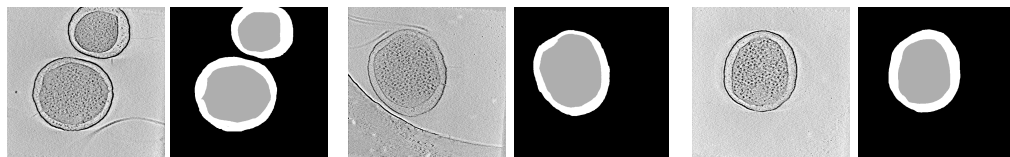
Few true answers vs. lots of false answers



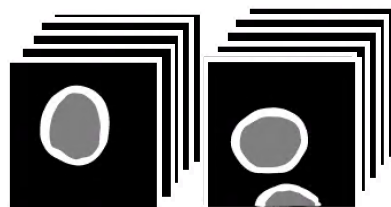
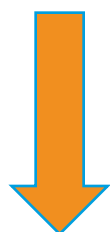
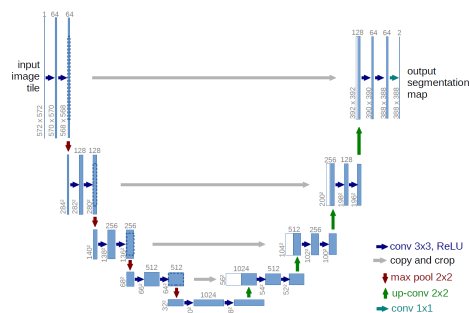
# Segmentation

## U-Net

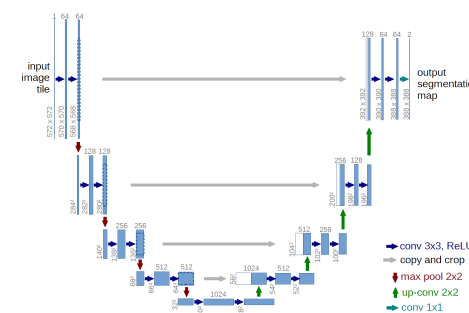
segmented 18 2D slices by hand



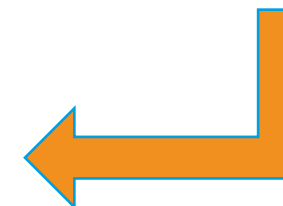
Manually corrected  
12 particularly bad  
predictions



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

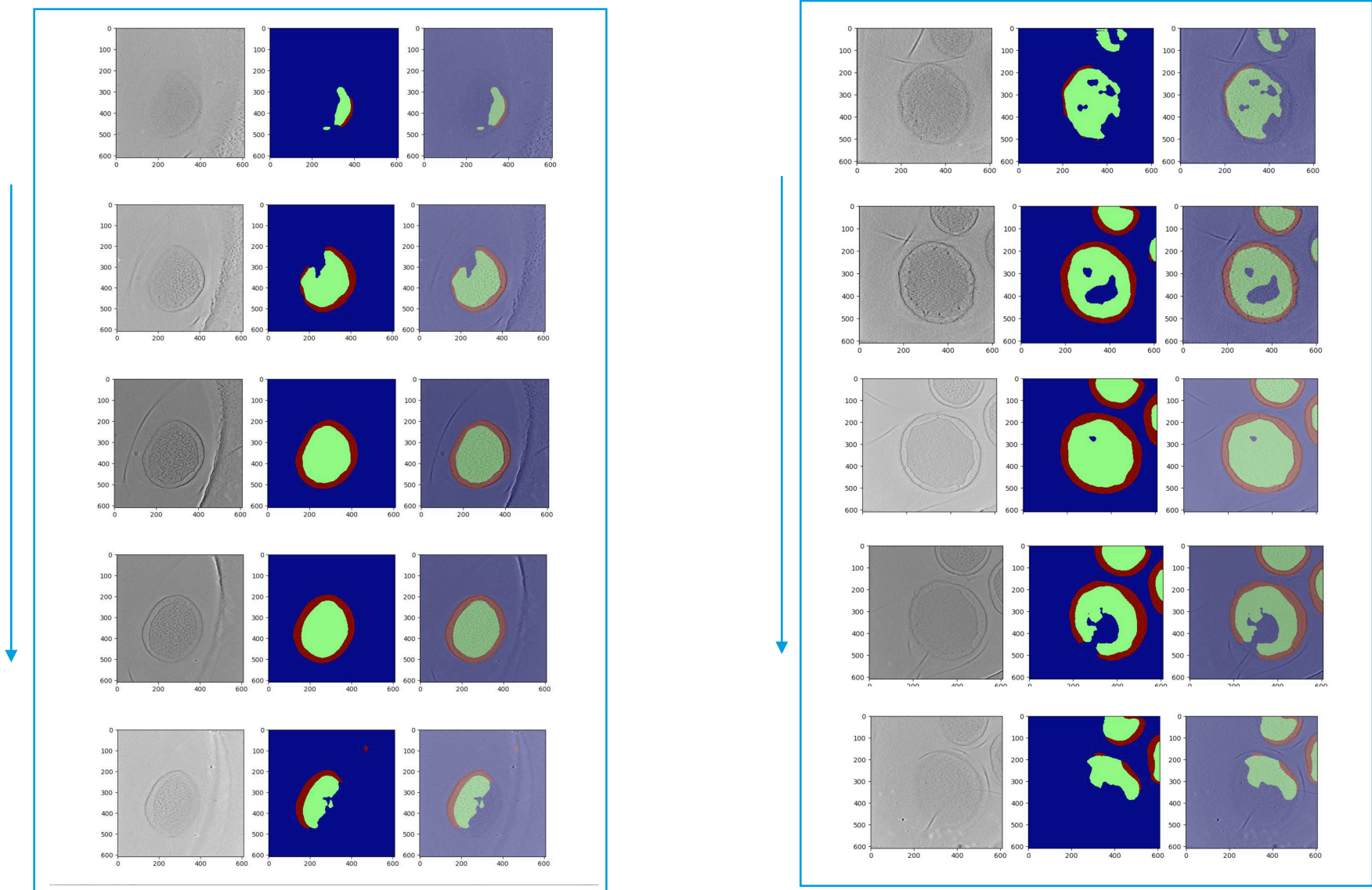


re-trained with 30 2D images



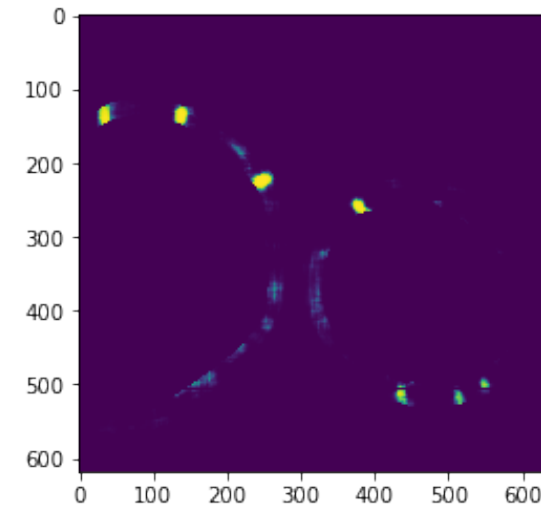
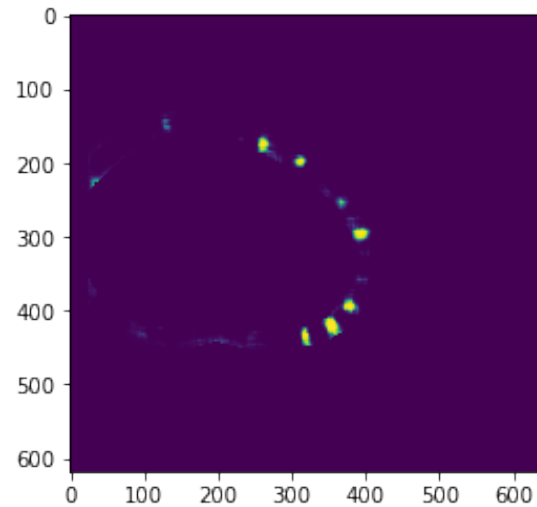
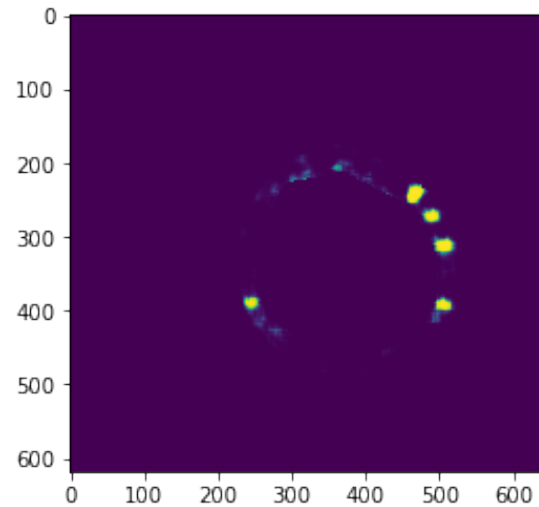
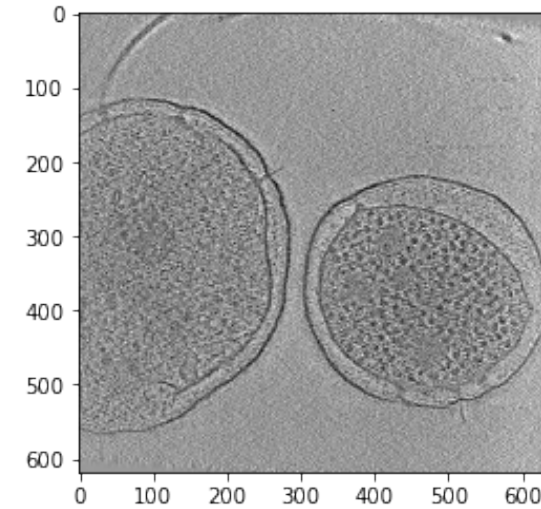
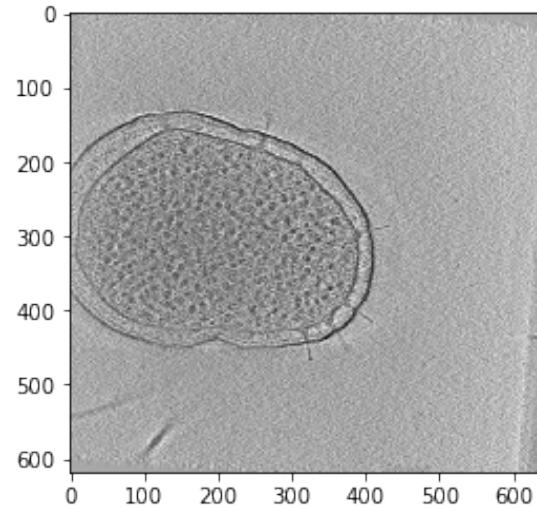
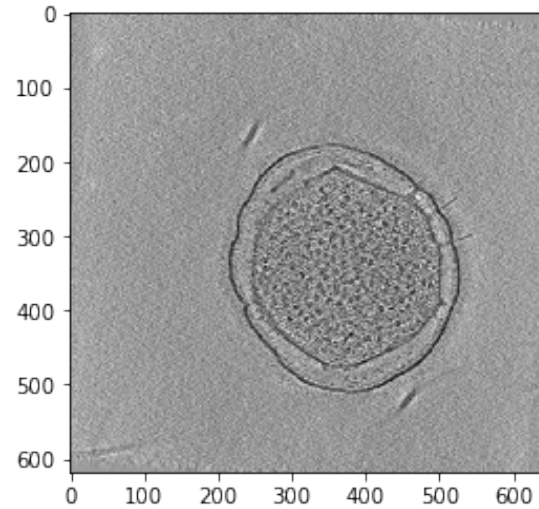


# Final trained U-Net

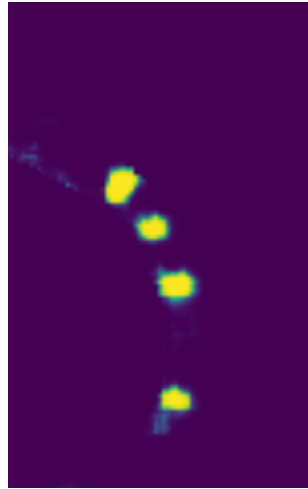


# T3SS found!

Searching only within the membrane



# T3SS candidates



clustering hits

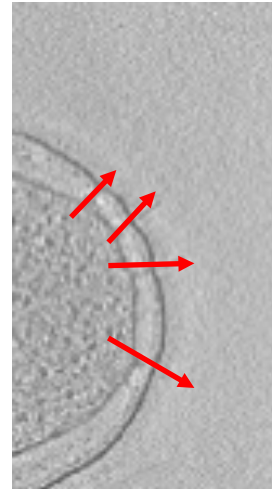
+



segmentation

=

T3SS candidates &  
direction



subtomogram  
averaging  
software

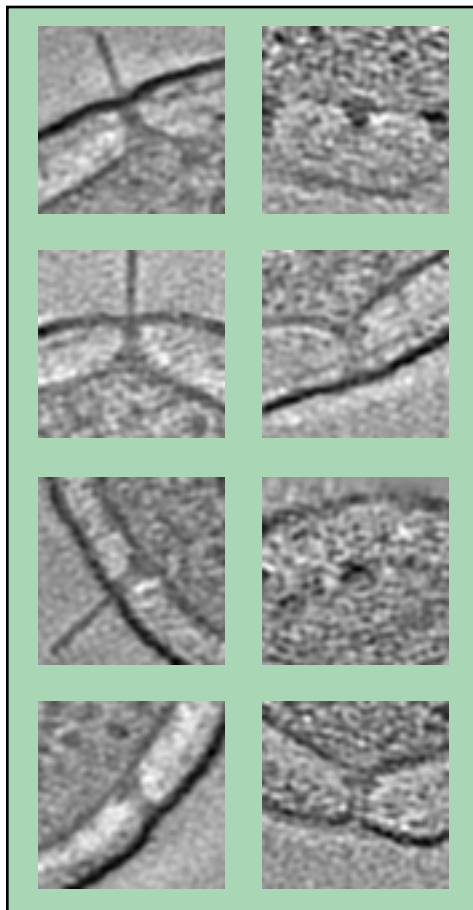


# TP/FP

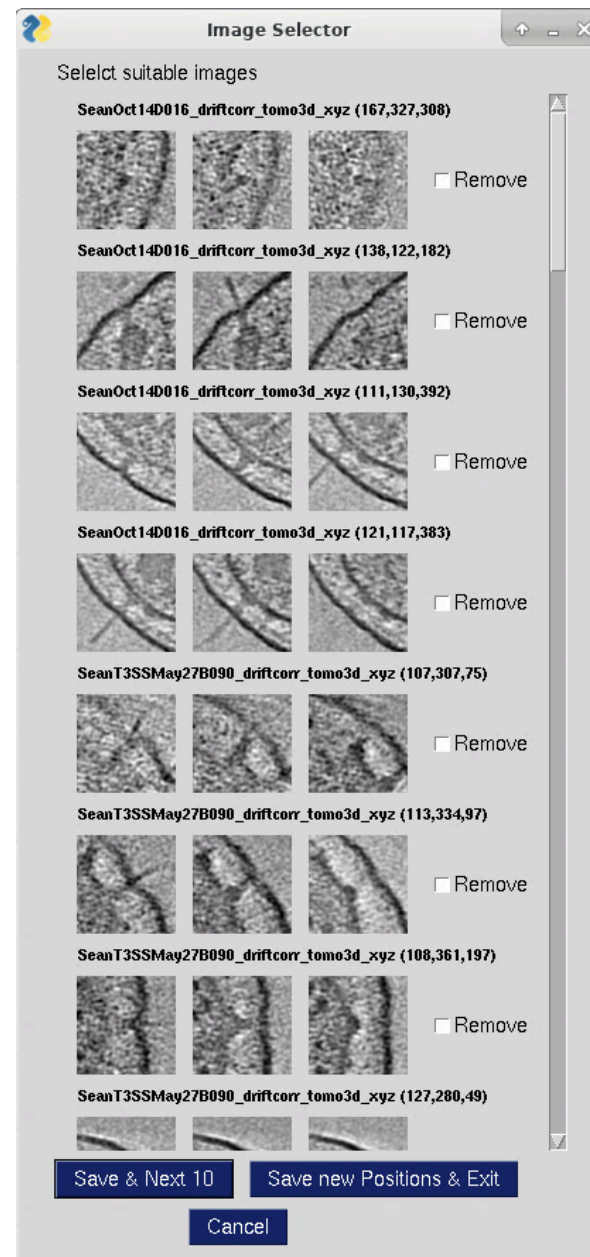
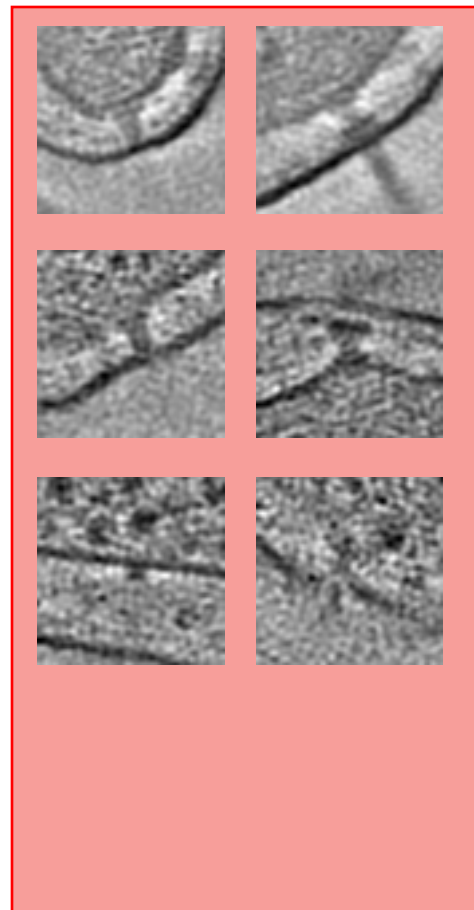
## Ground truth?

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

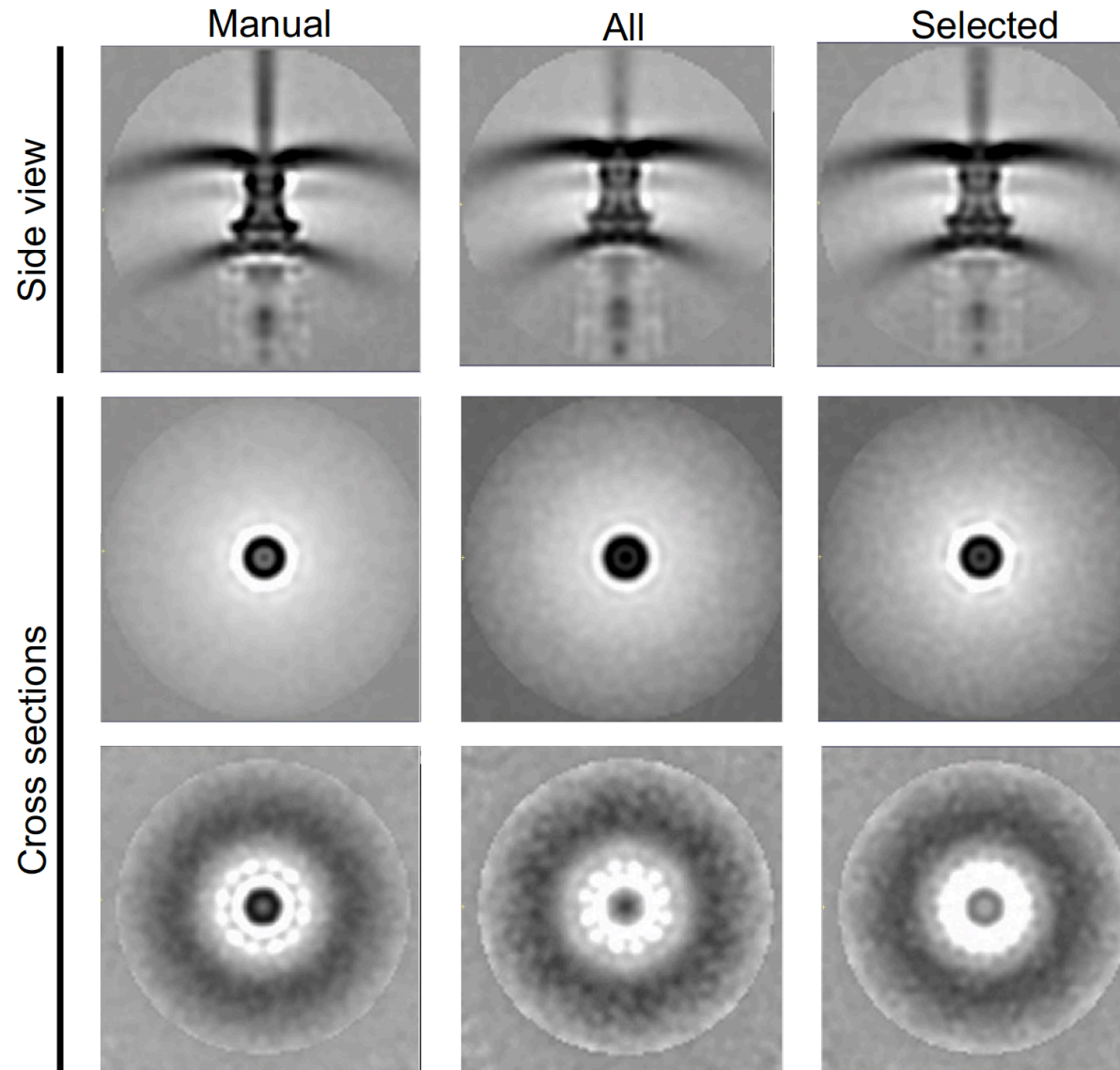
TP



FP



# 3D reconstruction



# Outlook

- Experiments with the network
- Using 3D convolutional network
- Using a better ground truth
- Retrain on novel data with full cells and with new camera
- Train on different transmembrane complexes



# Acknowledgments

## Thanks to...



DESY-IT  
Frank Schlünzen



Julian Moosmann  
Diana Krüger



Funding:  
Helmholtz Association  
Initiative and Networking Fund  
project number ZT-I-0003



Thomas Marlovits  
Sean Miletic  
Wolfgang Lugmayr