

# What Science can do with AI and Machine Learning

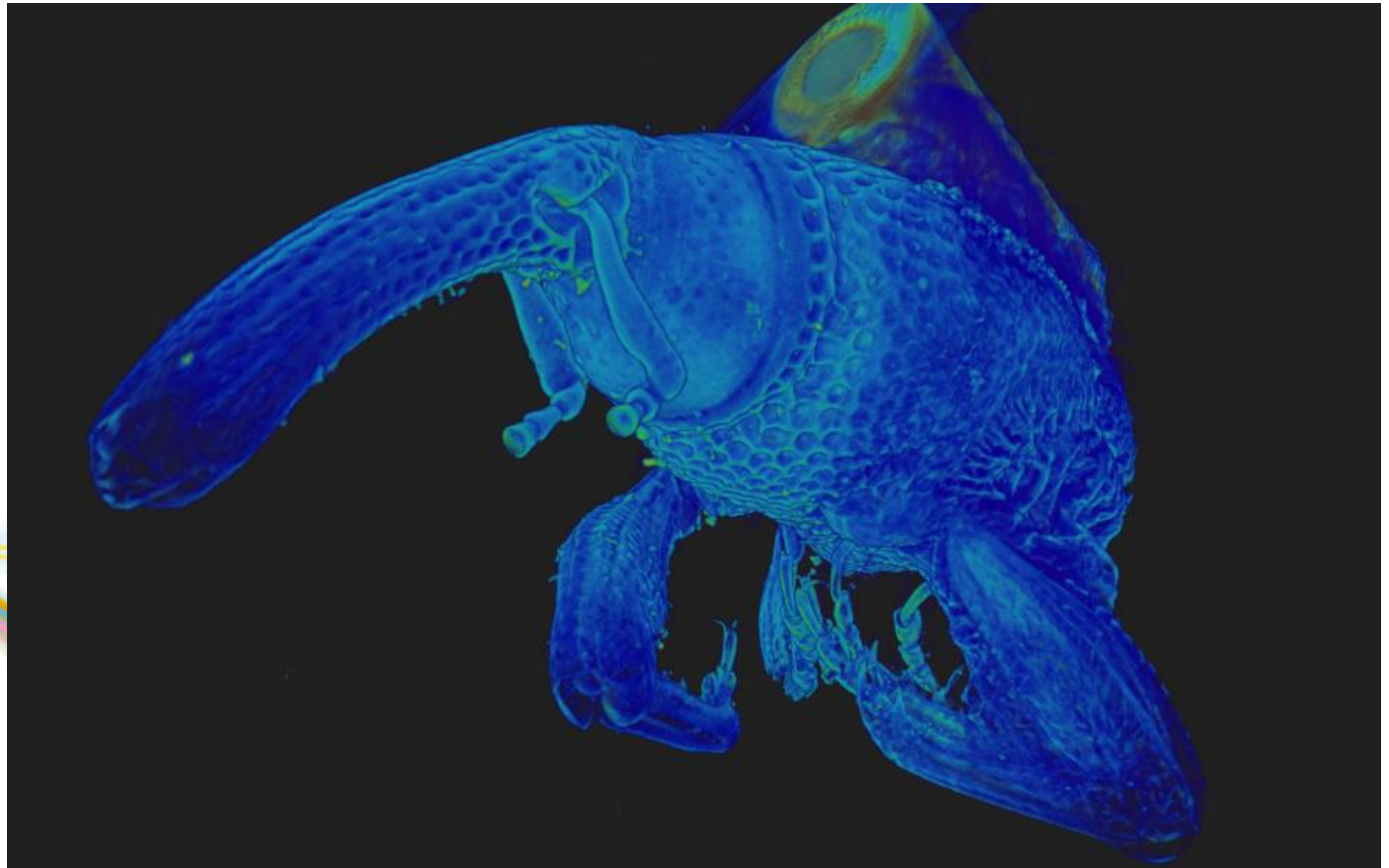
Dr Mark Basham

Data Analysis Group  
Diamond Light Source

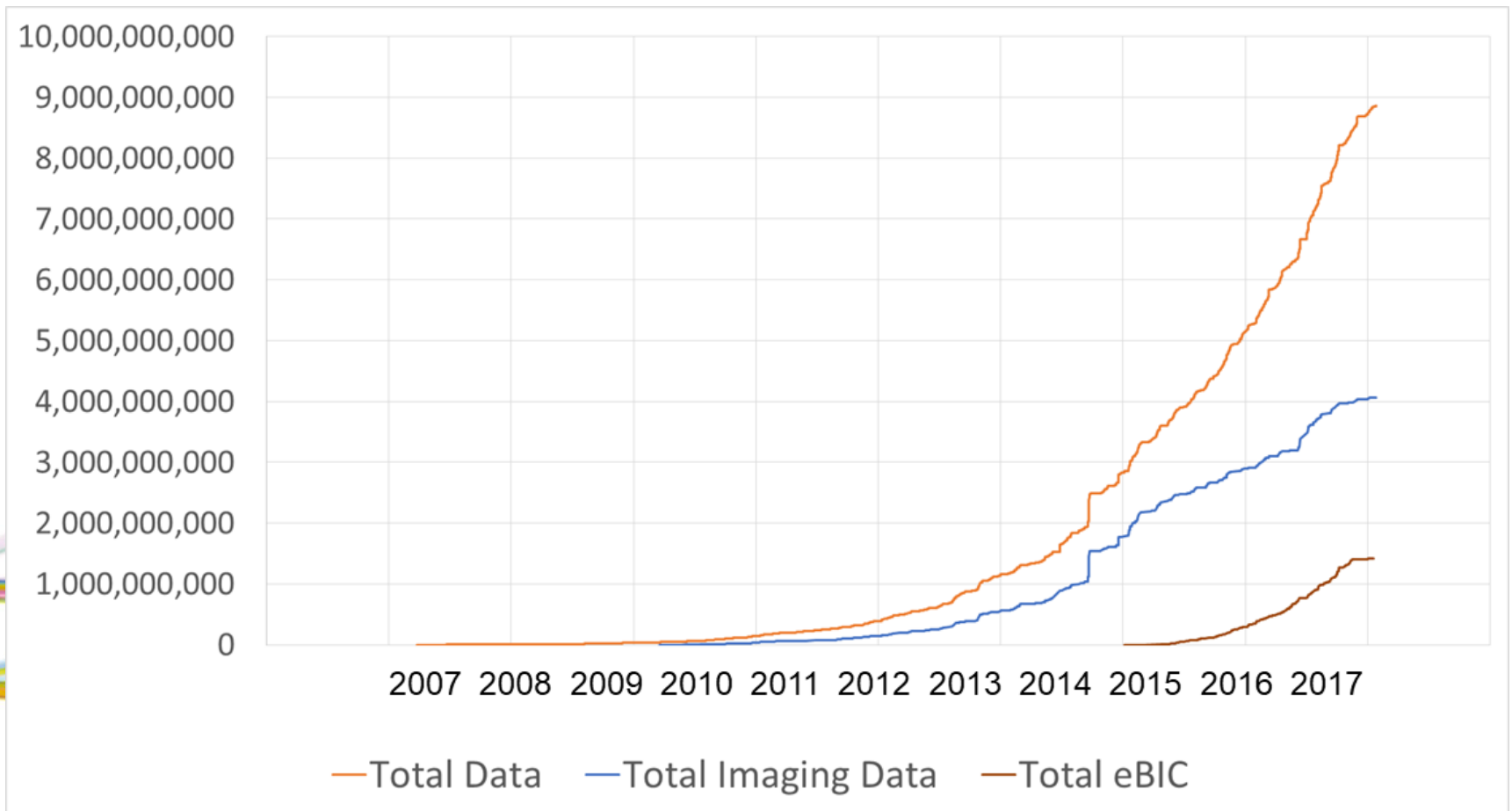


# Focus: Imaging

- Of interest to the ALC as it is cross disciplinary (3D+ imaging)
  - DLS
  - ISIS
  - CLF
  - ...



# The complexity – this is now a big data problem for DLS++



# The emerging challenge.



>3TB



30MB

PCCP  
PAPER

View Article Online  
DOI: 10.1039/C9CP00000A

**Chemical imaging of single catalyst particles with scanning  $\mu$ -XANES-CT and  $\mu$ -XRF-CT†**

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† The physicochemical state of a catalyst is a key factor in determining both activity and selectivity. However, these materials are often not structurally or compositionally homogeneous. Here we report on the 3-dimensional imaging of an industrial catalyst. Micro-focused electron X-ray absorption on carbon. The distribution of both the active Pt species and the promoter here have been mapped over a single particle of catalyst using micro-focused X-ray fluorescence computed tomography. X-ray absorption near edge spectroscopy (XANES) provided X-ray absorption fine structure revealed a mixed local coordination environment, including the presence of both metallic Pt clusters and Pt chloride species, but also no

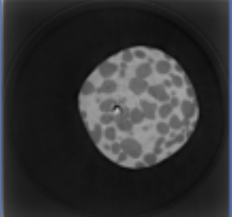
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A tomography pipeline called Savu.



savu

# Full-field tomography processing with Savu at DLS



Transmission Tomography  
(NeXus)  
30GB

Nxtomo loader

Dark/flat field correction

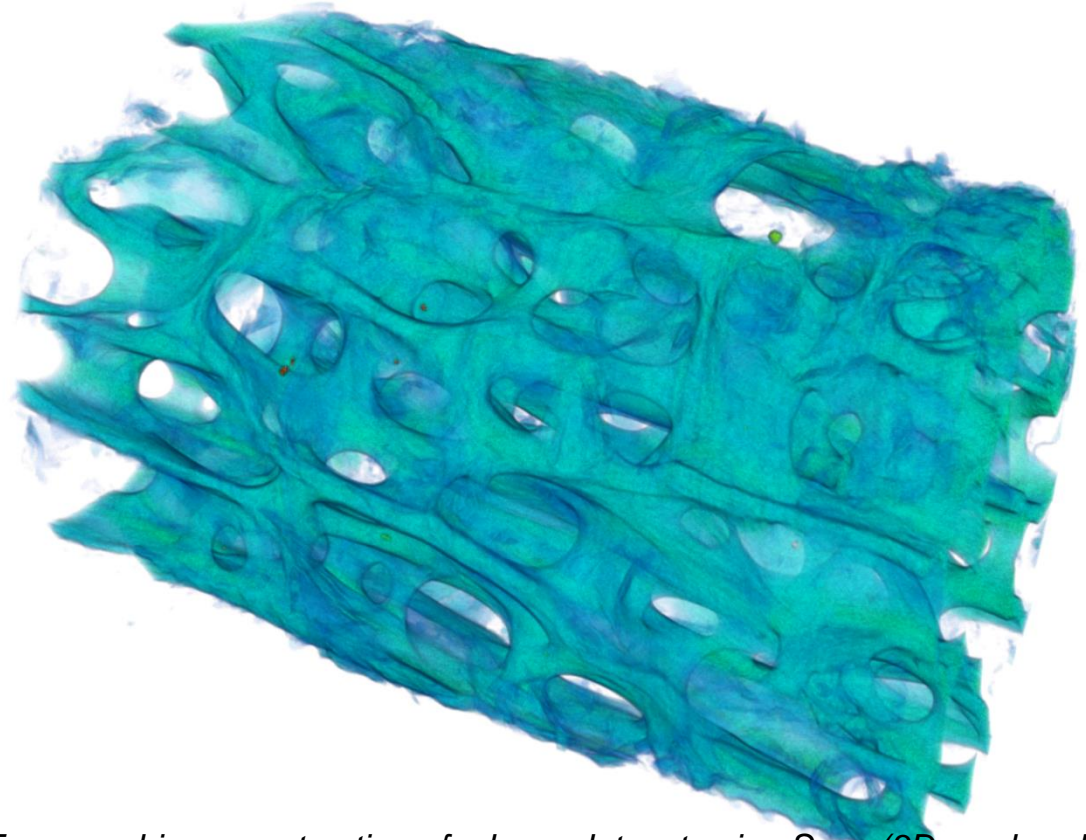
Ring artefact removal

Contrast enhancement

Auto-centering

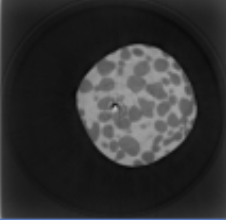
FBP/CGLS reconstruction

A typical process list for reconstructing full-field tomography data.



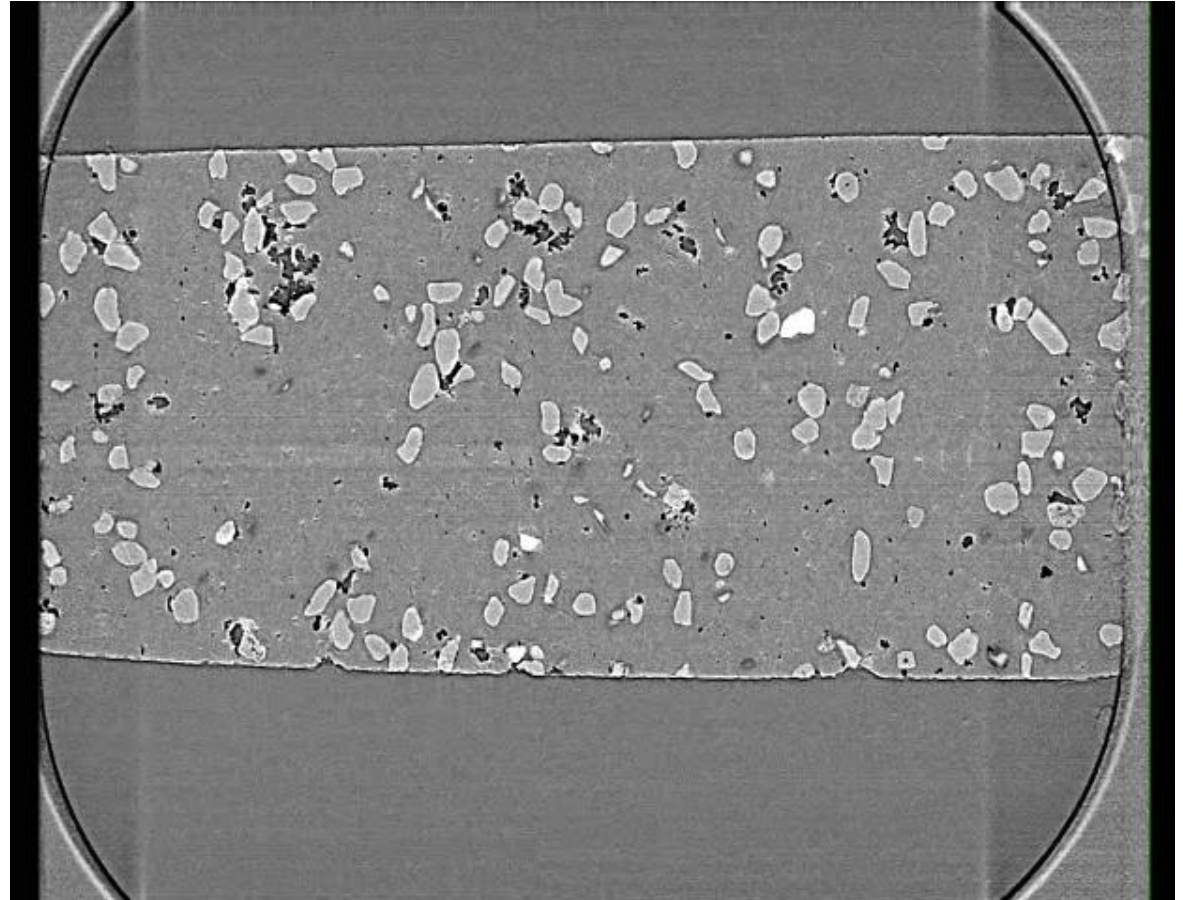
*Tomographic reconstruction of a bone dataset using Savu (3D-rendered using VisIt). Courtesy of Gianluca Tozzi, Marta Pena-Fernandez, Rachna Parwani, and Asa H. Barber (2016) from Portsmouth University. Data collected on the Diamond Manchester Imaging Branchline (I13-2) with support from Andrew J. Bodey.*

# Full-field tomography processing of 4D data with Savu at DLS



Time Resolved Tomography  
(cine)  
1500GB

- Nxtomo loader
- Dark/flat field correction
- Ring artefact removal
- Contrast enhancement
- Auto-centering
- FBP/CGLS reconstruction



A typical process list for reconstructing full-field tomography data.

# Current processing and resource requirements

- During the experiment possible
- Post processing complex



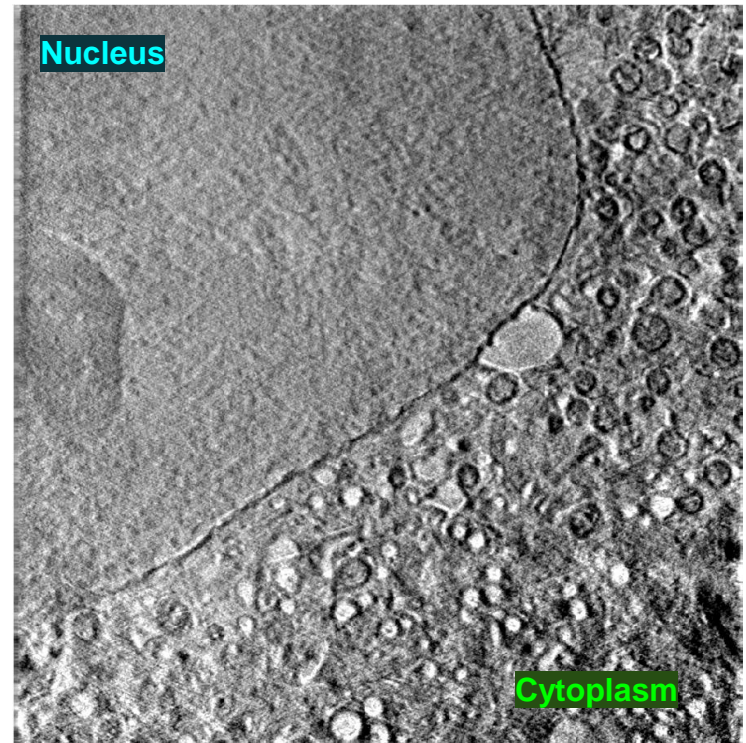




# Now What? – Segmentation...

## Challenges posed by data:

- Noisy data, missing wedge artifacts, missing boundaries
- Large amounts of data; many organelles/complexes per dataset – complex
- Tedious to manually annotate – so few training annotations available
- Each cell type/condition can look different – not generalizable
- Automated techniques usually fail

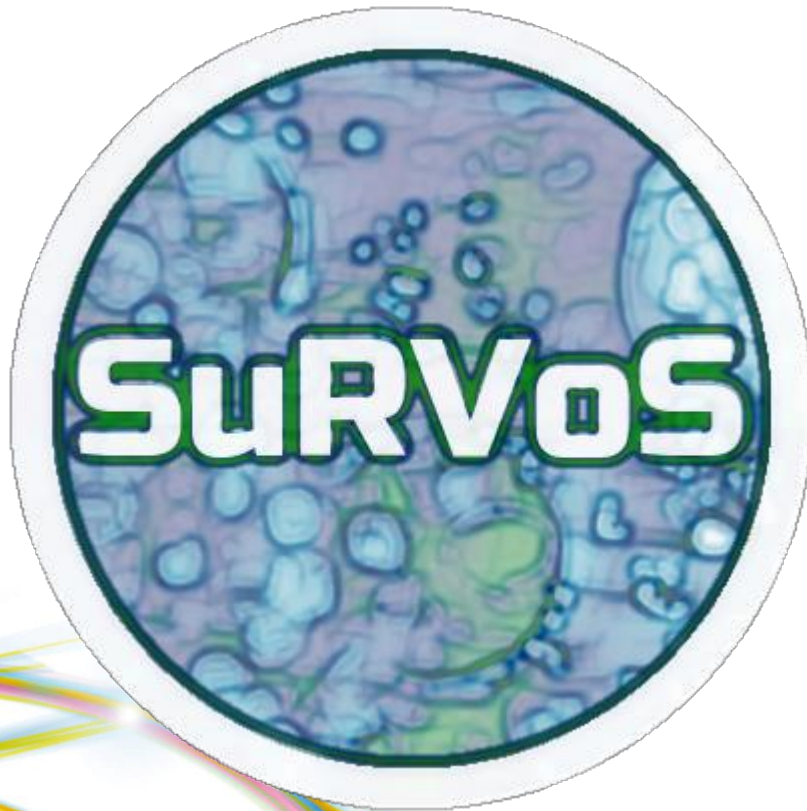


CryoSXT of neuron-like mammalian cell line; single slice

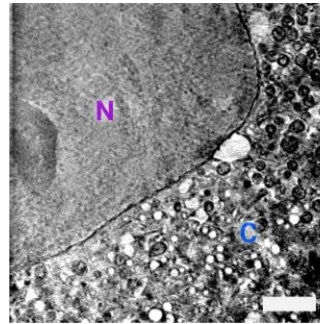
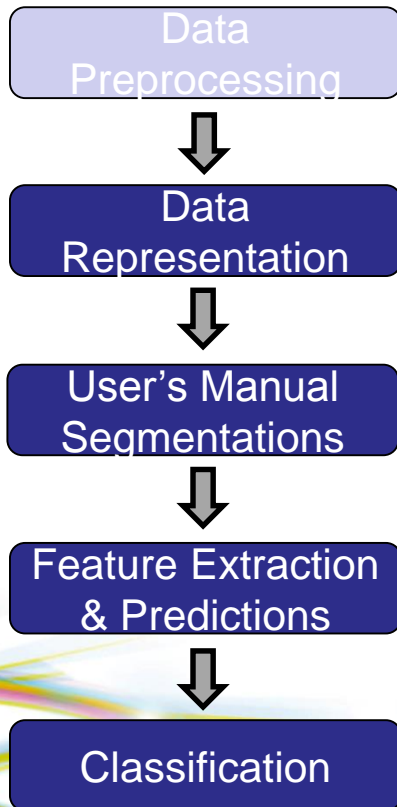
# Can we apply modern machine vision methods?

- Collaborate with a Machine Vision Group
  - Nottingham university
  - 1 PhD Post to investigate the methods 2014-2017
- Conclusions
  - Yes, but not fully automatic, semi automatic
  - SuRVoS

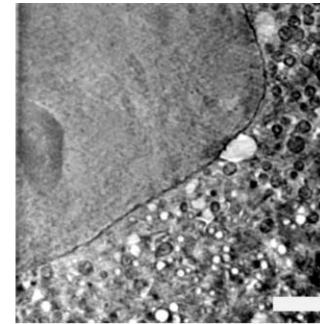
# Super-Region Volume Segmentation (SuRVoS) Workbench for Segmentation



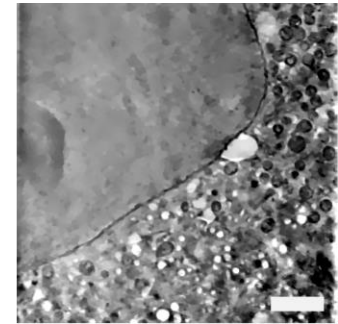
# SuRVoS – Super Region Volume Segmentation Workbench



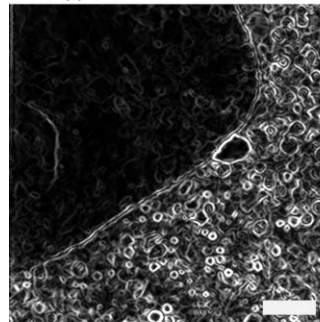
(a) Raw SIRT reconstruction



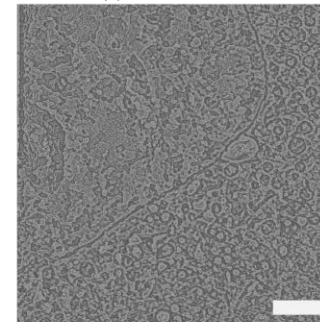
(b) Gaussian Smooth



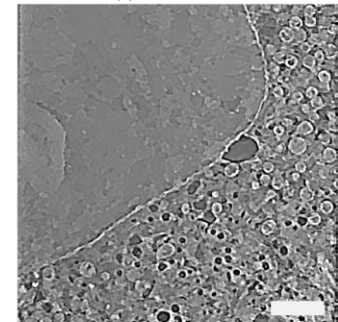
(c) Total Variation



(d) Gradient Magnitude

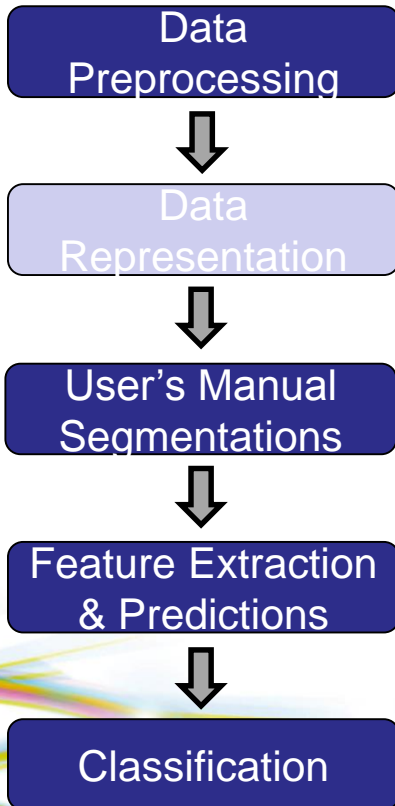


(e) Gaussian Local Normalization

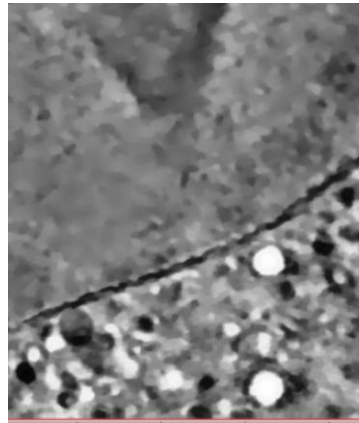


(f) Laplacian of Gaussian

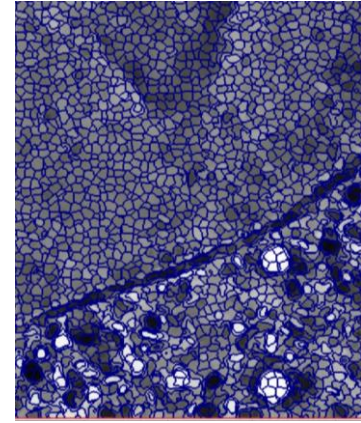
# SuRVoS – Super Region Volume Segmentation Workbench



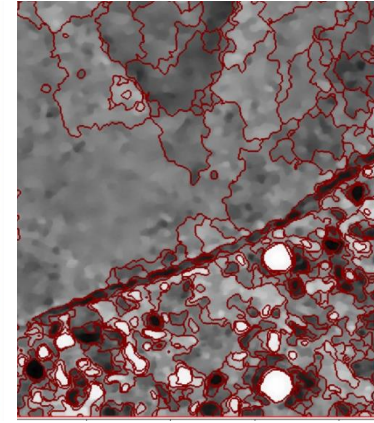
Denoised Subvolume



Super Voxels



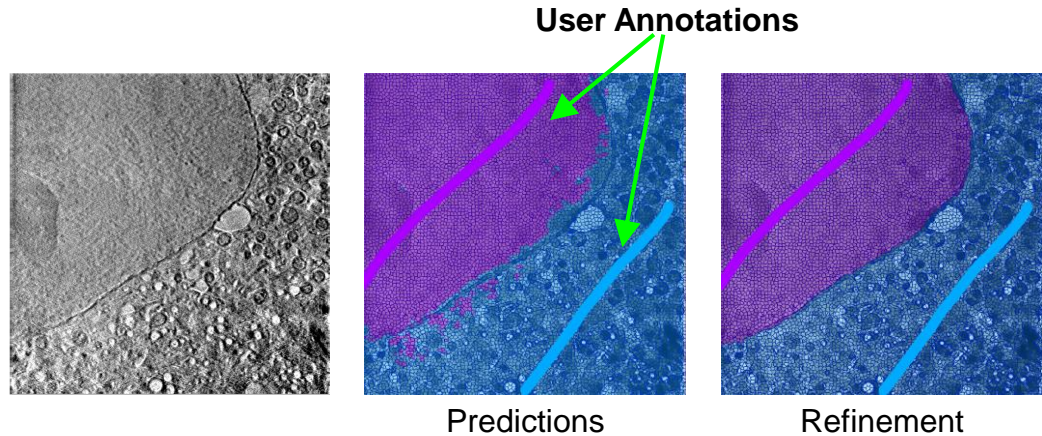
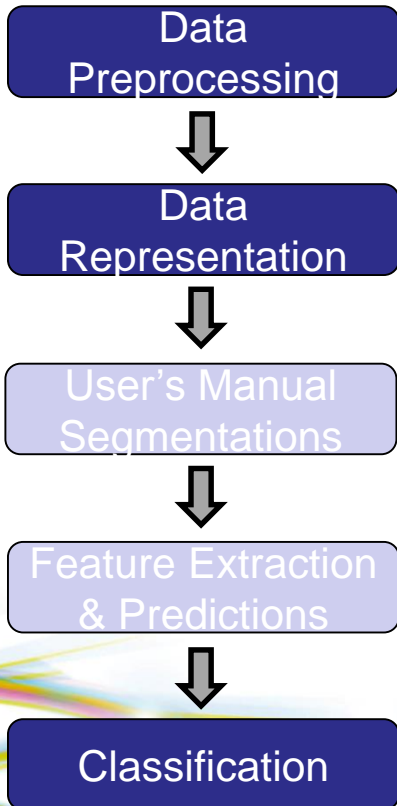
Mega Voxels



Supervoxels and megavoxels are...

- groups of similar, adjacent voxels in 3D.
- **edge preserving**, and **three-dimensional**.
- **reduce problem complexity** by several orders of magnitude.

# SuRVoS – Super Region Volume Segmentation Workbench

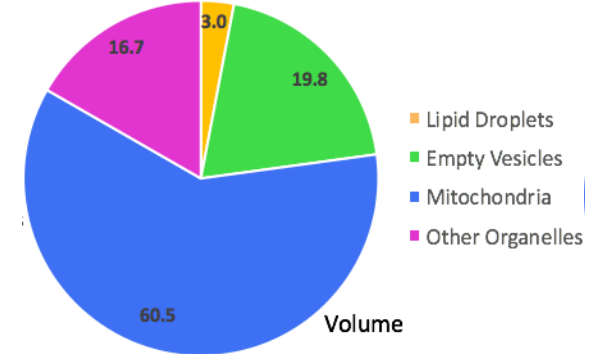
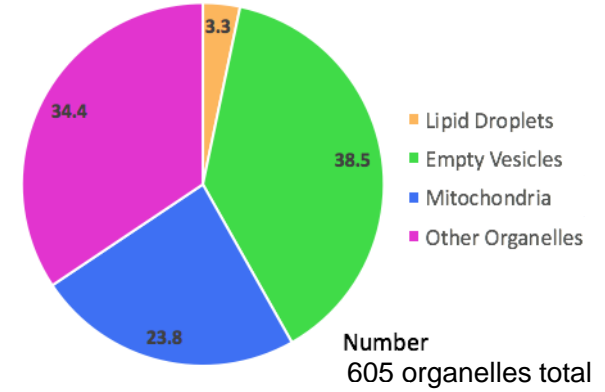
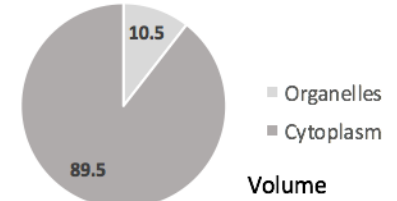
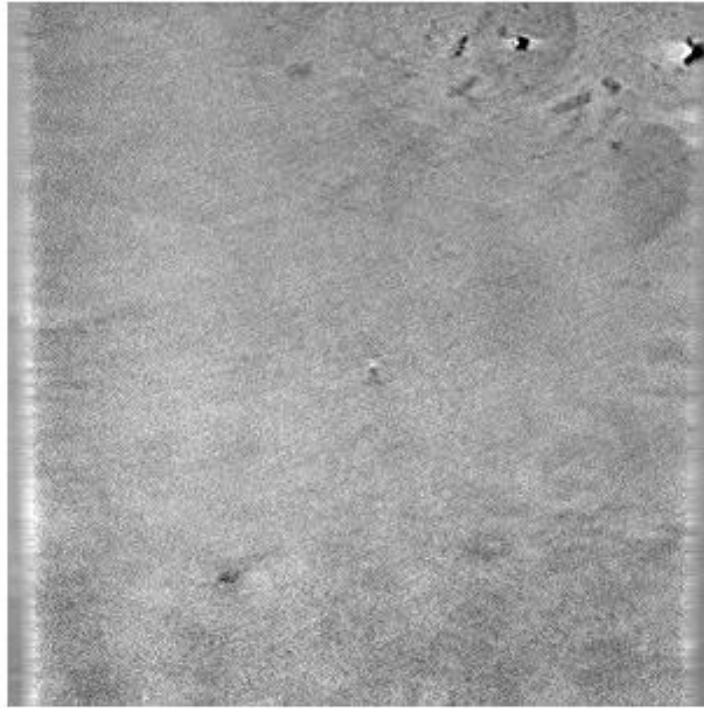


Features are extracted from voxels to represent their appearance:

- Intensity and textural features/filters
- A machine learning classifier is trained to discriminate between different classes and predict the class of each supervoxel in the volume.
- A Markov Random Field (MRF) is then used to refine the predictions.

# Segmented PC-12 mHTT-Ex1 (97Q)

- Nucleus
- Nucleolus
- Lipid Droplets
- Mitochondria
- Empty Vesicles
- Other Organelles





# My Vision of ALC

- A place to bring together the facilities data analysis communities to make use of common software and expertise.
- A common pool of HPC which is capable of dealing with this data and processing requirements. Which is available to all our facility users for post processing and analysis.

# Thank You

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