What Science can do with AI and Machine Learning

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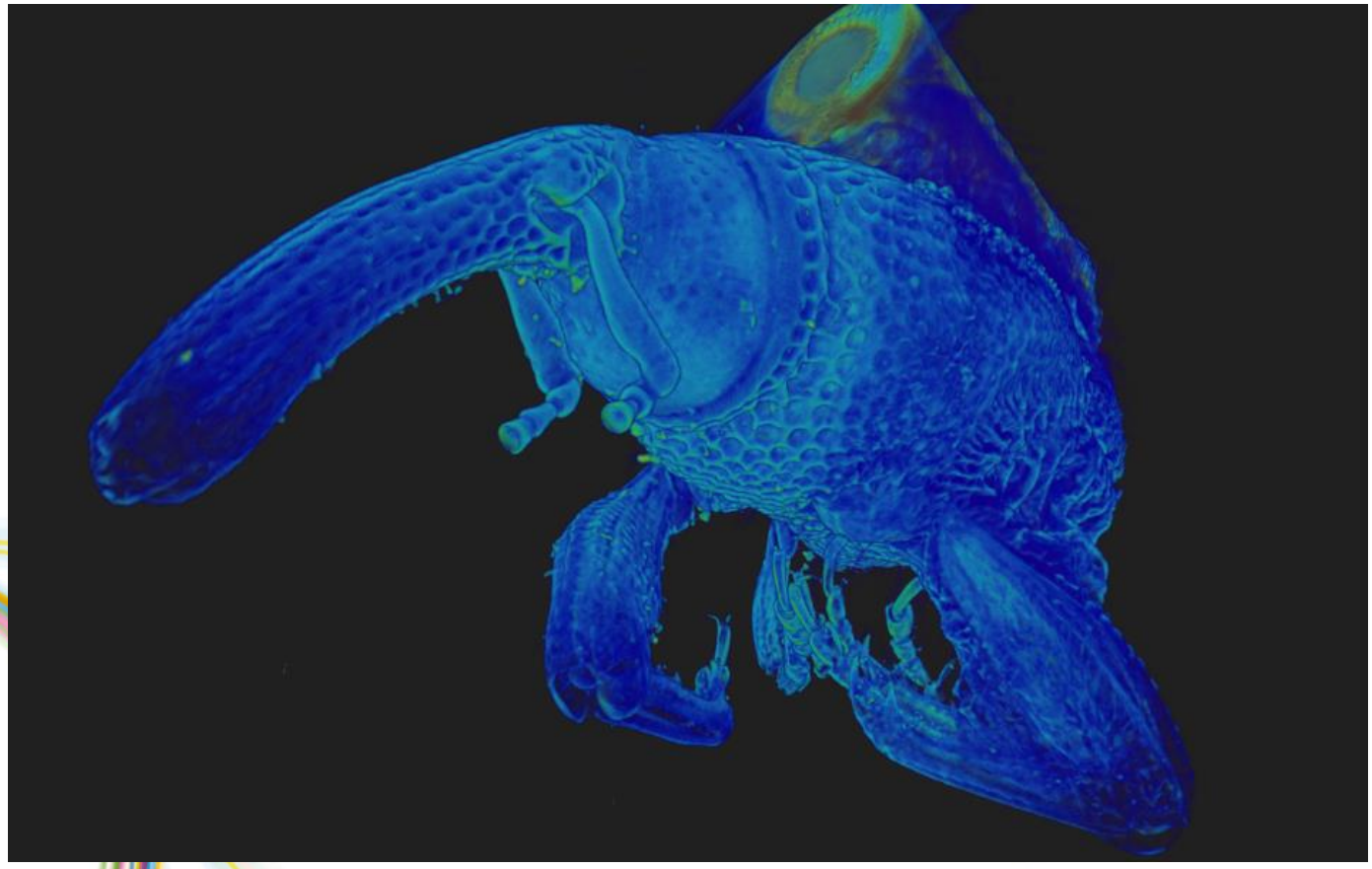
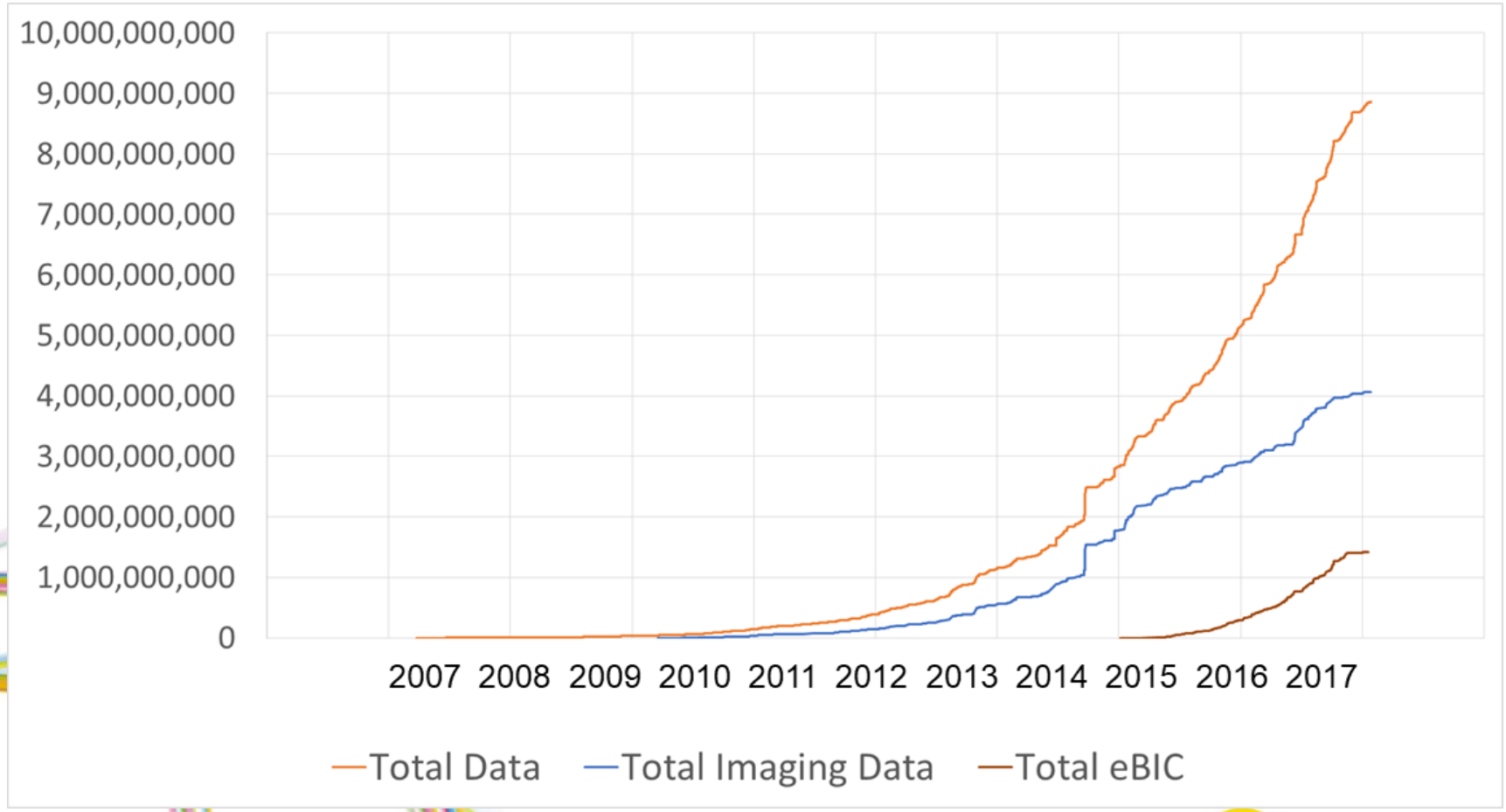
Data Analysis Group
Diamond Light Source

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

Chemical imaging of single catalyst particles with scanning μ-XANES-CT and μ-XRF-CT†

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A tomography pipeline called Savu.

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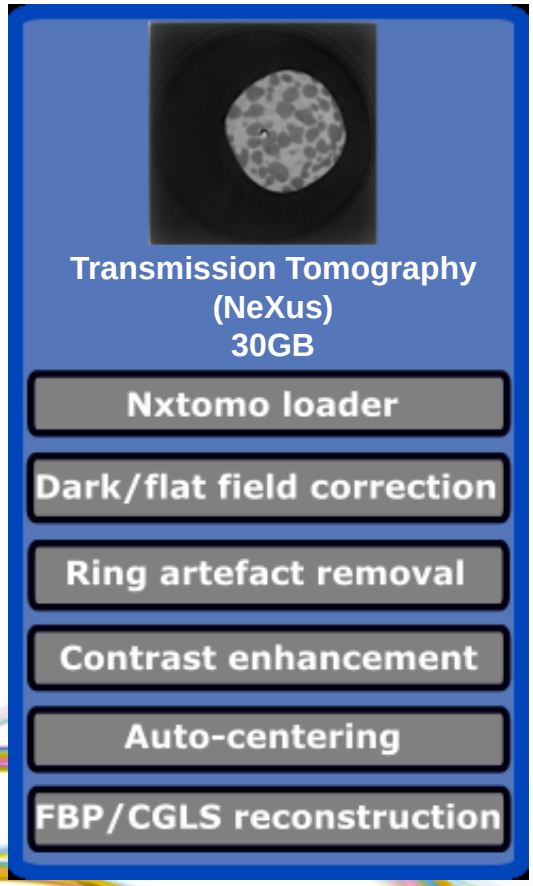
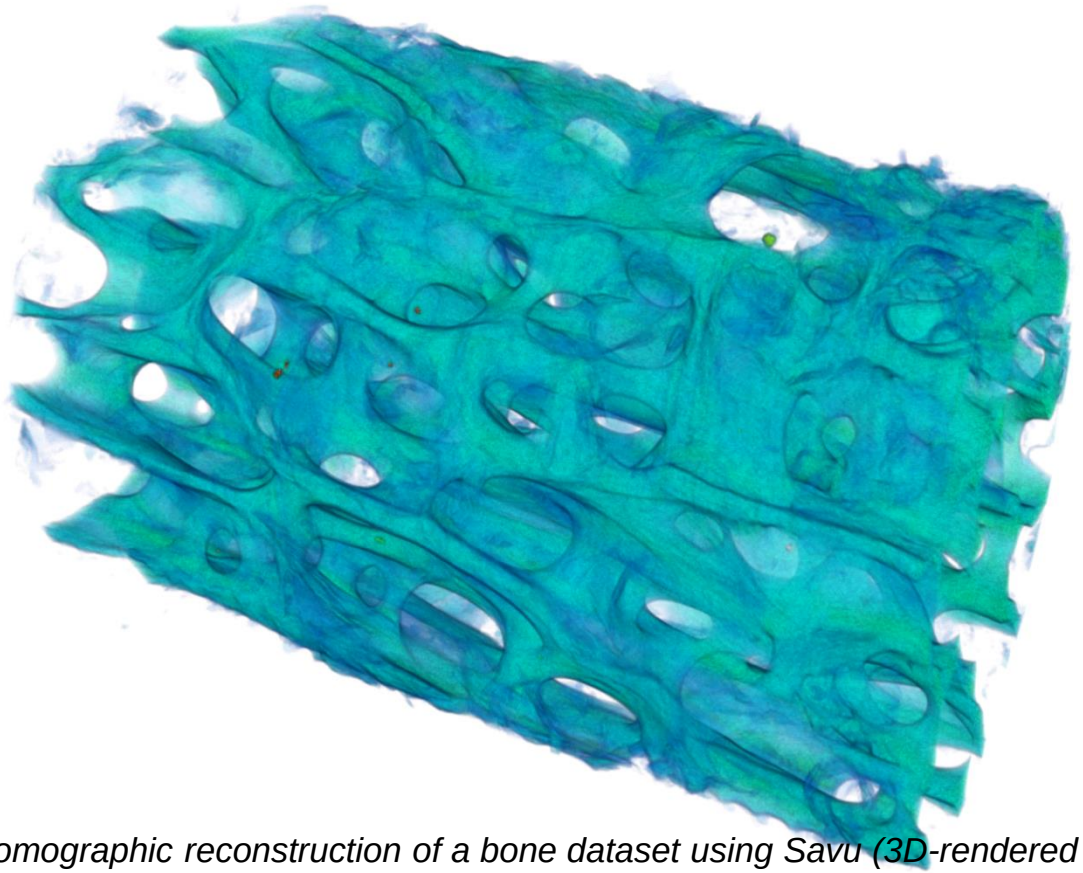
Full-field tomography processing with Savu at DLS



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.

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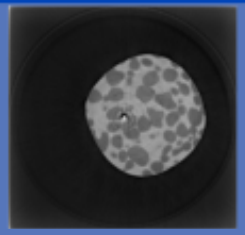
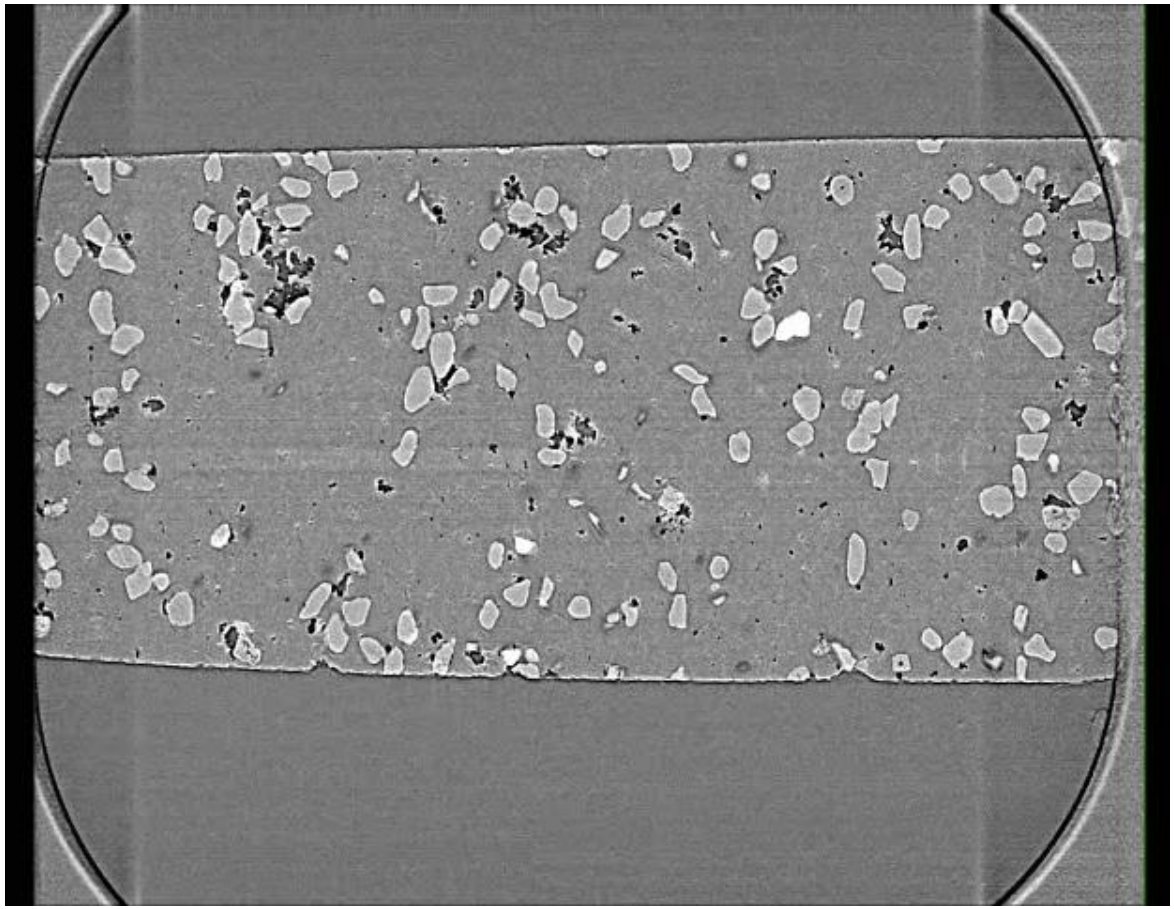
Full-field tomography processing of 4D data with Savu at DLS



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.



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Current processing and resource requirements

- During the experiment possible
- Post processing complex

The imaging challenge.

>3TB

>>3TB

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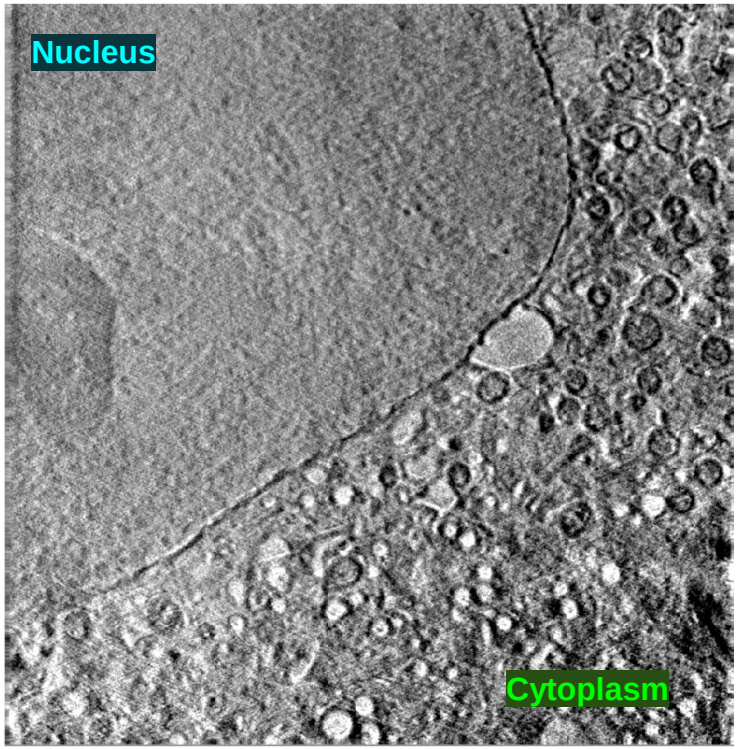
Now What? – Segmentation…

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

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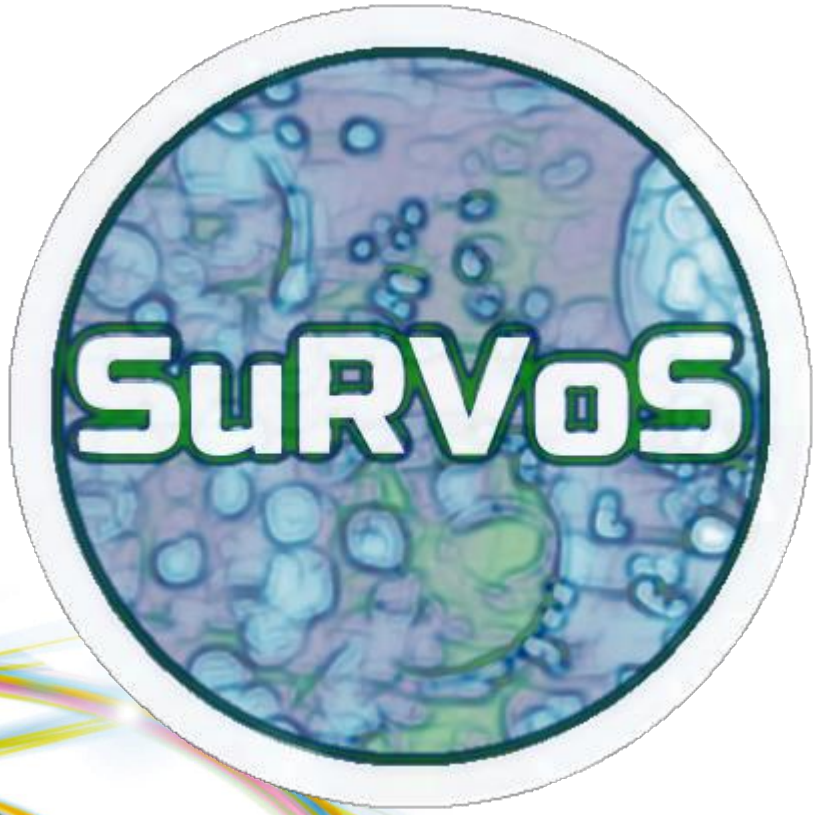
Can we apply modern machine vision methods?

- 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



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B24 beamline

The University of Nottingham
Computer Vision Laboratory

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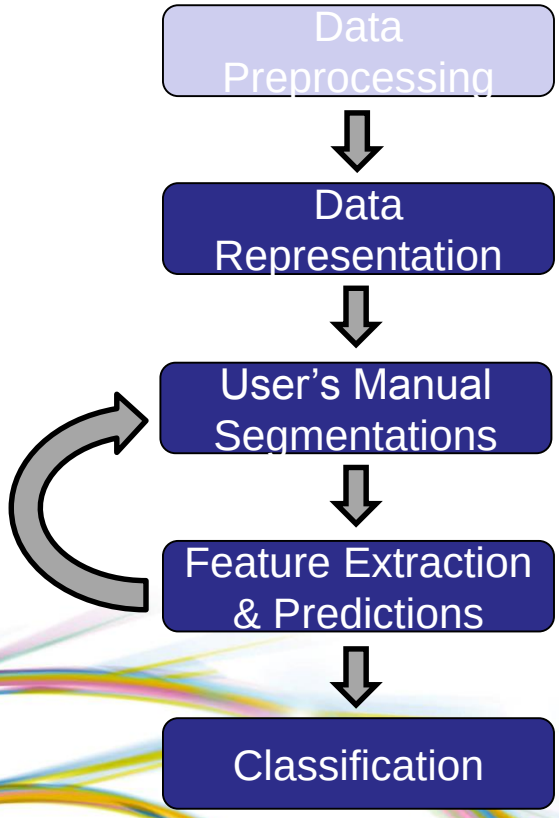
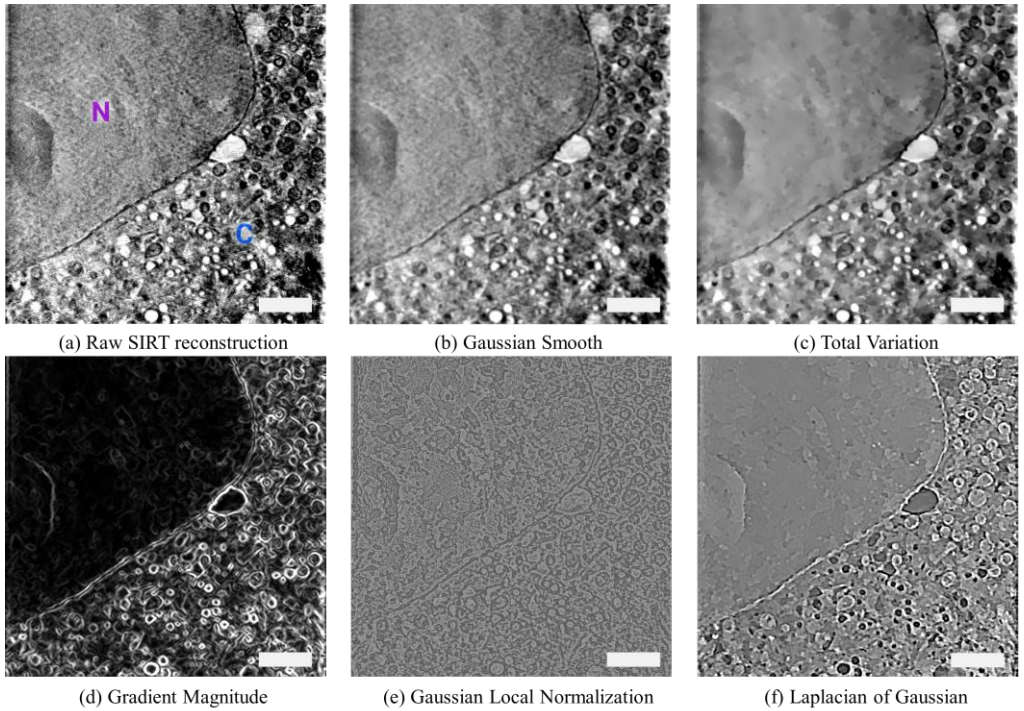
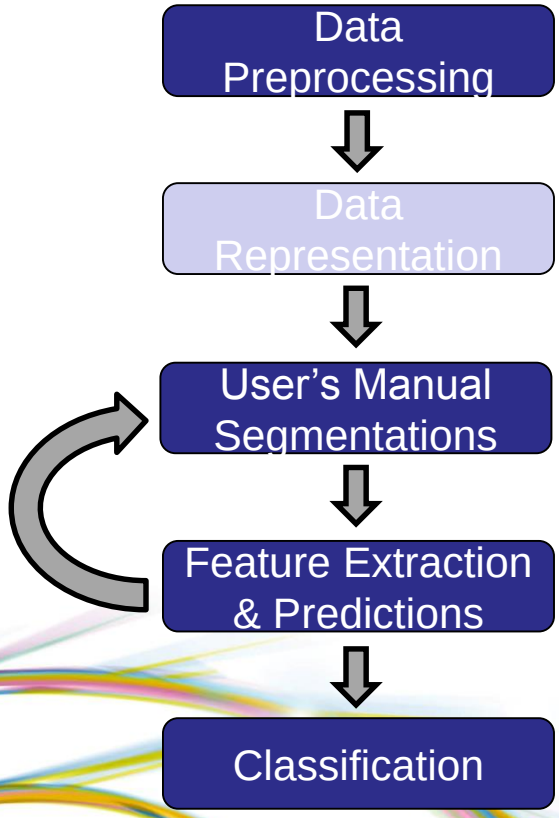
SuRVoS – Super Region Volume Segmentation Workbench



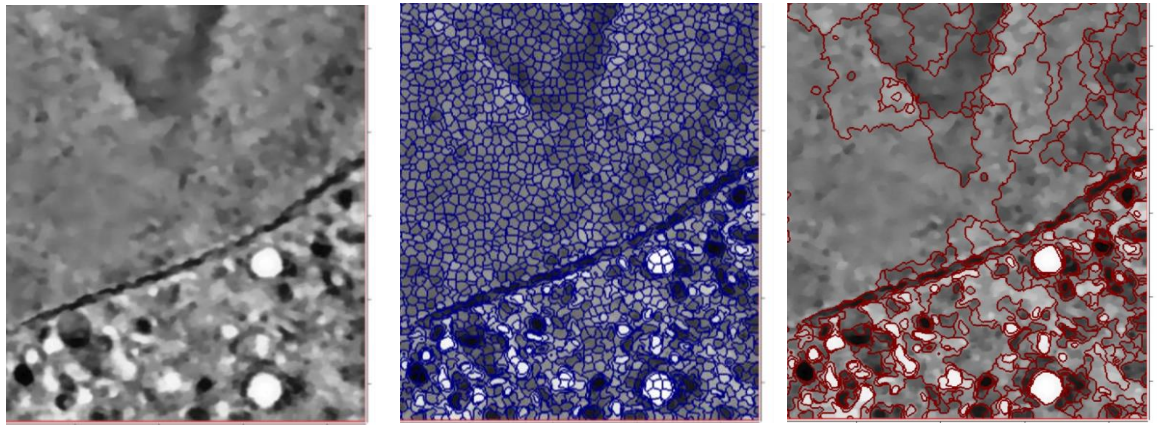


Luengo I., et al. 2017, J Struct Biol; Darrow, M., et al, 2017, JoVE

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.

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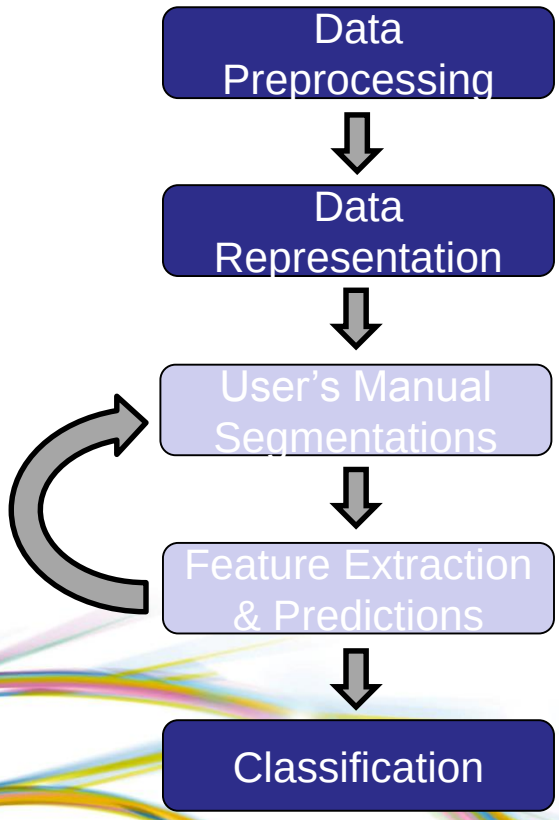
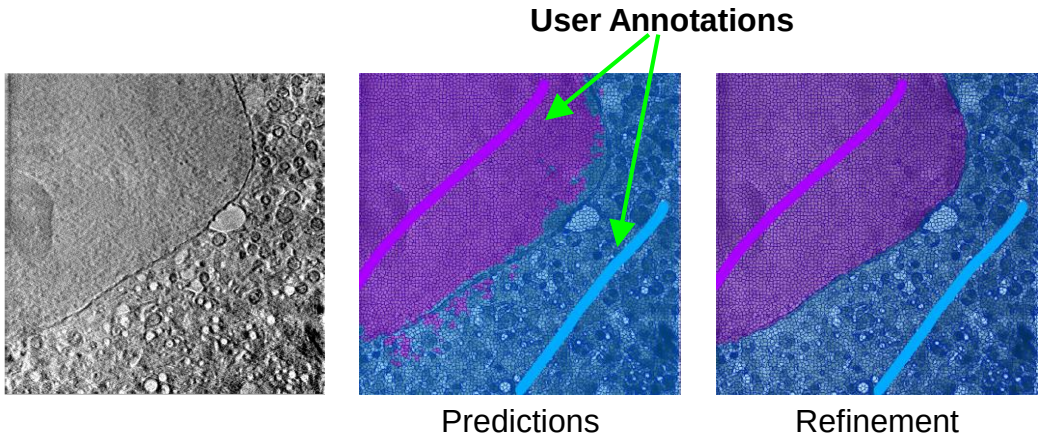
SuRVoS – Super Region Volume Segmentation Workbench





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.

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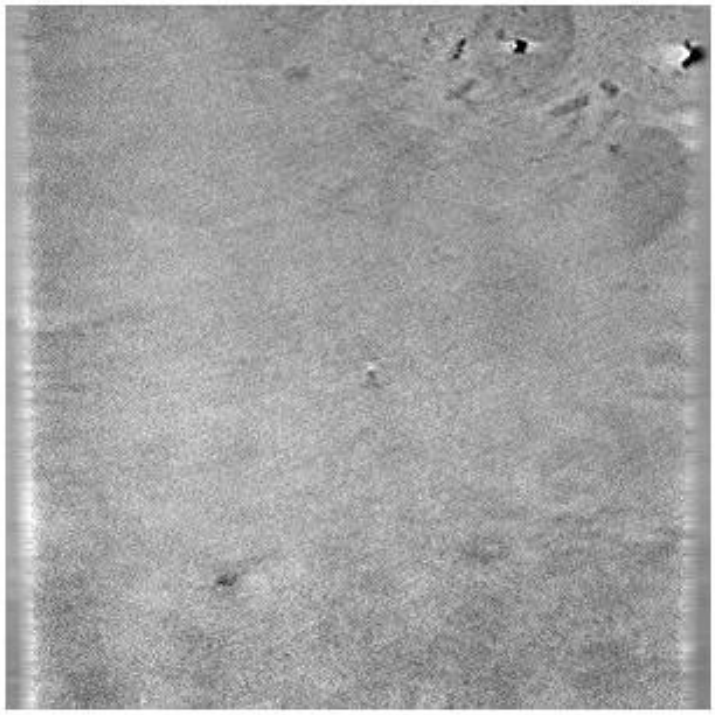
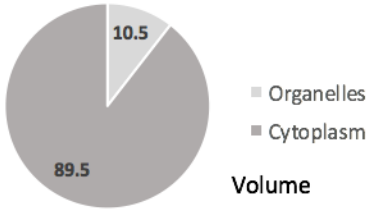
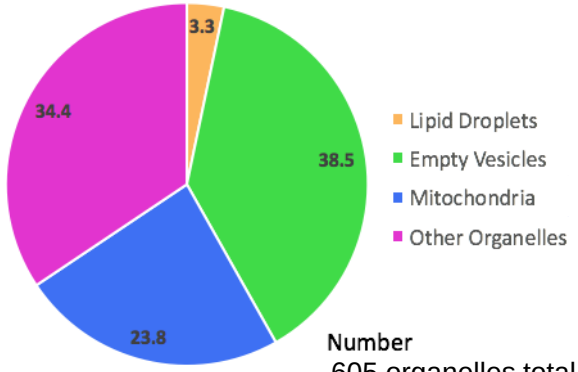
Segmented PC-12 mHTT-Ex1 (97O)

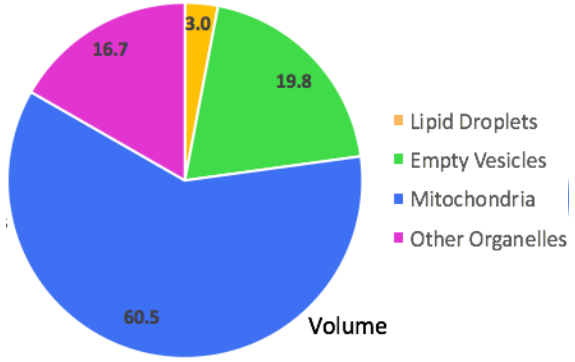
- Nucleus
- Nucleolus
- Lipid Droplets
- Mitochondria
- Empty Vesicles
- Other Organelles







605 organelles total



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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 capapble 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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