

Towards a Collaborative Computational Project for Volume Electron Microscopy

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Volume Electron Microscopy

Also, workflows will change for different microscopes, samples, sample preparations and imaging configurations!

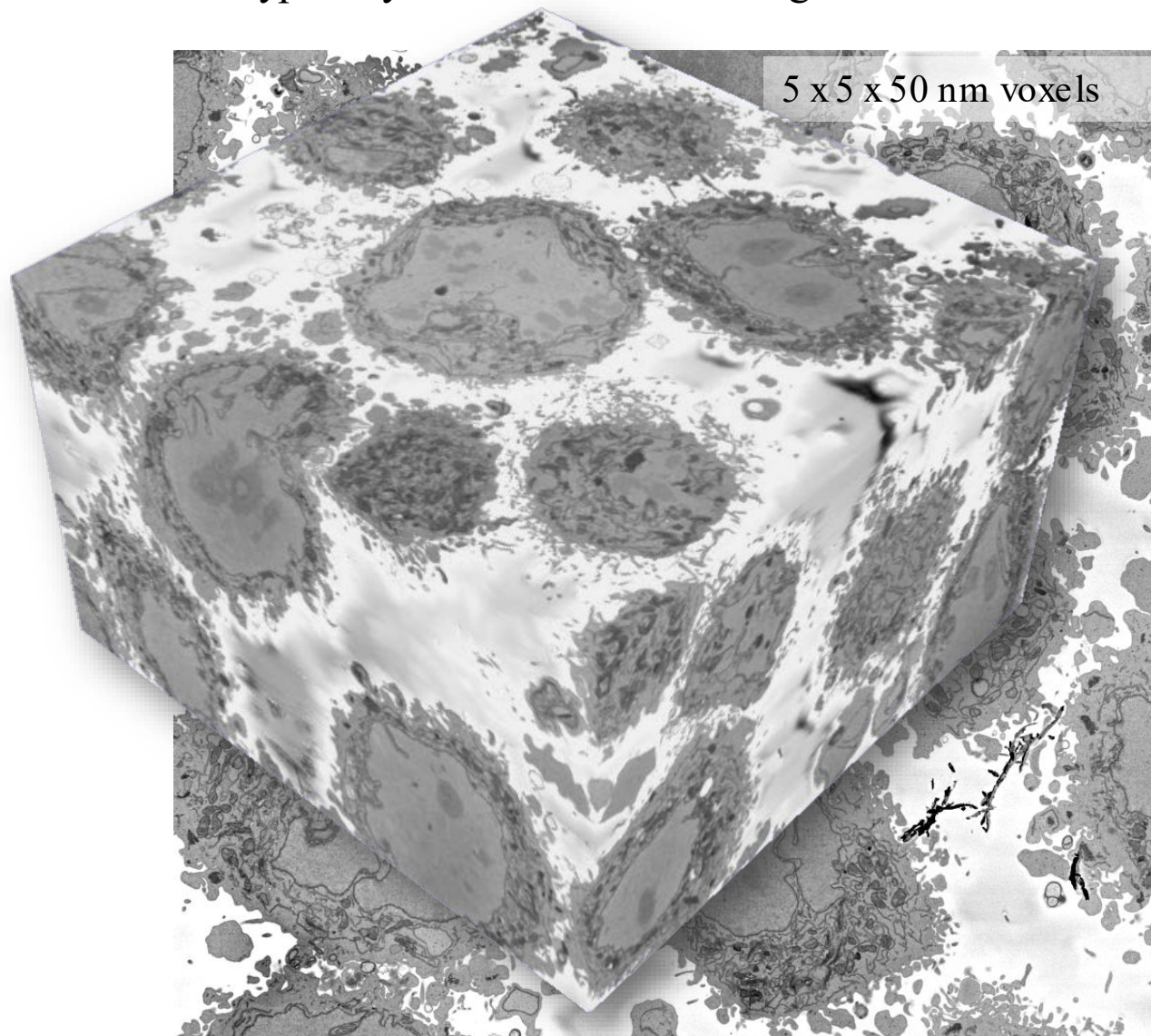
- Each approach requires specific processing, reconstruction and analysis methods
- E.g.
 - ssTEM or Array tomography non-linear stack alignment
 - ssET tomographic reconstruction
 - SBF/FIB-SEM jitter correction
 - Contrast adjustment
 - ...

Volume Electron Microscopy: Serial Block Face SEM

Typically in the 0.1-10+ TB range

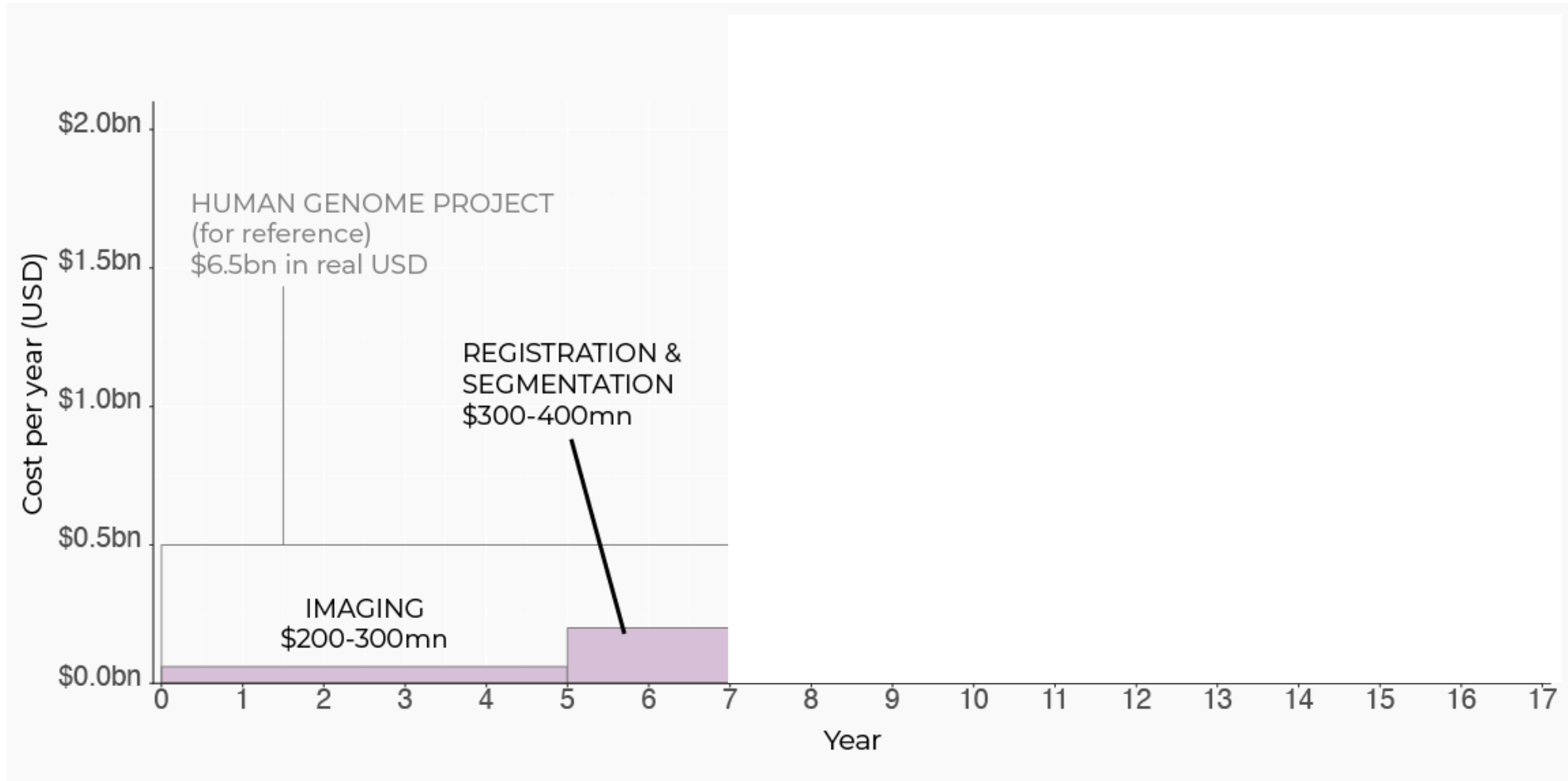


<http://www.gatan.com/products/sem-imaging-spectroscopy/3view-system>



The importance of high-quality analysis is ...

- Connectomics in the mouse brain



<https://e11.bio/news/roadmap> adapted from <https://wellcome.org/reports/scaling-connectomics>

The problems of scale

- Single datasets can be much larger than RAM, even on a big workstation
- All types of processing are challenging at terabyte-scale, even very routine operations
- Storage and compute costs can be significant
- Environmental implications of computationally intensive processing

I want to study the phenotype of knocking down the SHH gene

I want quantify the shape of the mitochondria

I have imaged my drosophila in FM, XR and EM

I want to extract functional and ultrastructural information at nm scale



Is your data in Zarr format?
We could use Dask!

Have you tried fine-tuning a pre-trained ViT?

How much vRAM do you have?

Just SSH to your HPC and launch this slurm job



- Differences in domain knowledge can lead to missed opportunities or unreasonable expectations
- Deep domain knowledge allows for the creation of long-term plans as well as reactively solving current problems
- Lack of long-term view can hamper the adoption of new technologies as the initial effort is high



What we need to do

- Limit the (perceived) need for reinventing the wheel
- Support the use of modern tools, techniques and libraries
- Promote software engineering best-practice for sustainability and reproducibility
- Encourage FAIR Data
(Findable, Accessible, Interoperable, Reusable)

Collaborative Computational Projects (CCP)

- A Collaborative Computational Project at CoSeC is a community-driven initiative that builds and supports computational tools and expertise for specific research areas in the UK scientific community
 - Develop, maintain, and support scientific software for research communities
 - Provide training, workshops, and support for users and developers
 - Foster collaboration between academics, research institutions, and national computing services

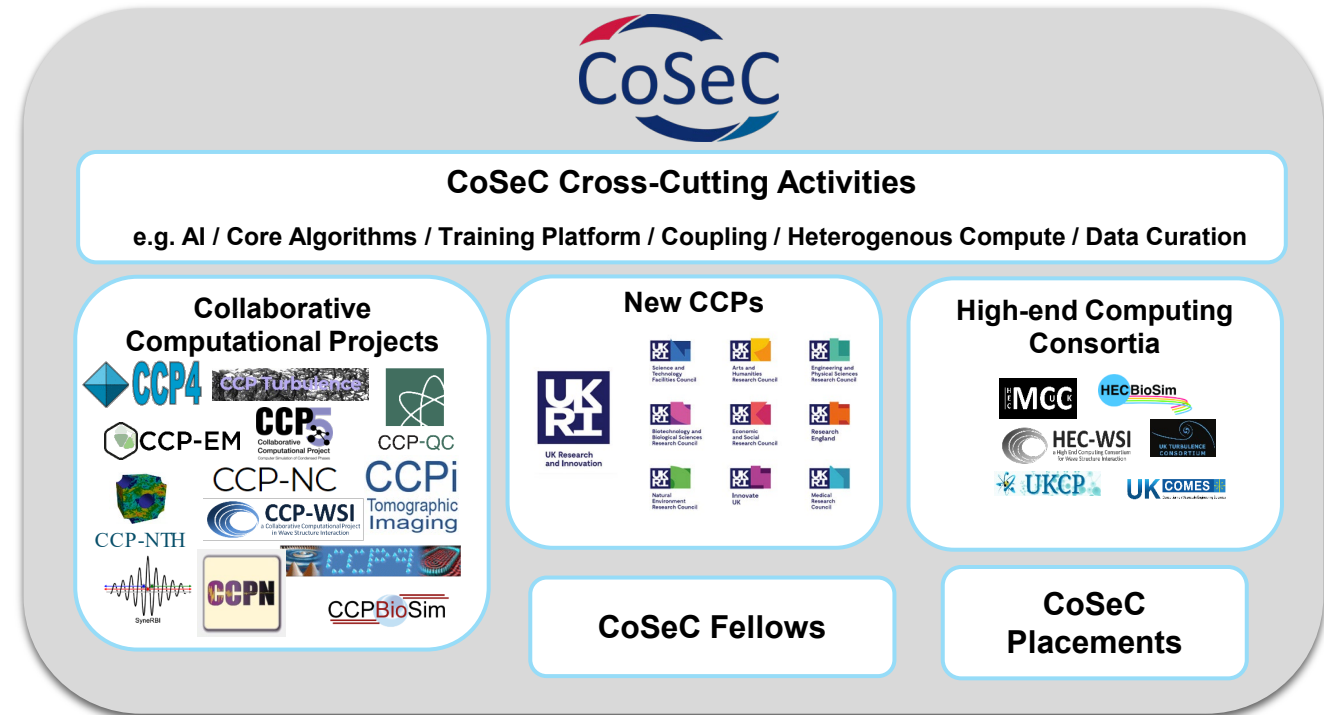


Computational Science Centre
for Research Communities

www.cosec.ac.uk



- Large and skilled group of Research Technical Professionals (scientists, RSEs, management and support) within UKRI-STFC.
- Based in national labs at Daresbury and Harwell campuses.
- Cross-cutting capabilities within the Centre
- Creation of CoSeC Fellowships and placement schemes



Some current CCPs

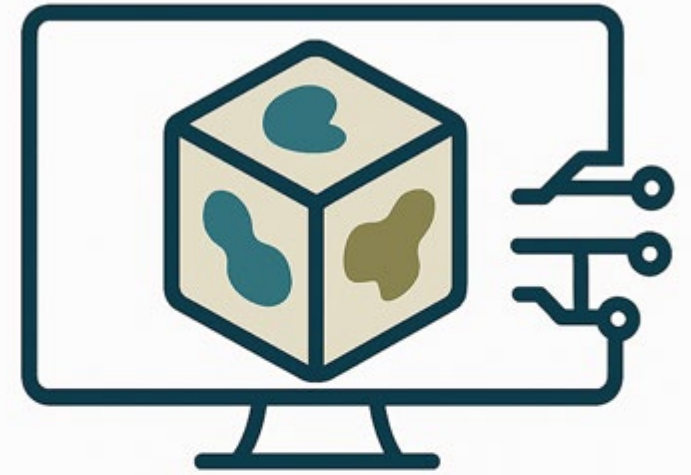
Range of activities, including

- Community coordination
- Domain-critical software support and development
- Interaction with researchers and developers from different domains
- Deployment of software on new hardware infrastructure
- Code efficiency
- High Performance Computing
- AI best-practice
- Ensuring FAIR data

Name	Research Area		
CCP4	Macromolecular x-ray crystallography		
CCP5	Computer simulation of condensed phases		
CCP9	Computational electronic structure of Condensed matter		
CCPBioSim	Biomolecular simulation		
CCP-EM	Electron cryo-Microscopy		
CCPi	Tomographic imaging		
CCPN	Nuclear magnetic resonance		
CCP-NC	Nuclear magnetic resonance for crystallography		
CCP-NTH	Nuclear thermal hydraulics		
CCP-QC	Quantum computing		
CCPSyneRBI	Synergistic reconstruction for biomedical imaging		
CCP-Turbulence	Turbulence modelling for fluid dynamics		
CCP-WSI	Wave structure interaction		
Materials Chemistry Consortium	Materials chemistry		
UKCar-Parrinello	Developing 'first principles' quantum mechanical techniques for studying atomistic systems	Dr Phil Hasnip	Dr Dominik Jochym
HEC-WSI	World-class wave structure interaction using national High-End Computing resources	Professor Deborah Greaves	Dr Wendi Liu
UK-COMES	UK Consortium on Mesoscale Engineering Sciences	Professor Kai Luo	Dr Michael Seaton
HECBioSim	Biomolecular simulation	Professor Syma Khalid	Dr James Gebbie-Rayet
UKTC	Understanding, predicting and controlling turbulent flows using High Performance Computing	Professor Sylvain Laizet	Dr Stefano Rolfo

CCP-volumeEM

- CoSeC funded 2 year project to develop the computational community for volume EM with a view to creating a long-term CCP
- Integrated with CoSeC to join-the-dots with related efforts and access huge knowledge-base for scientific computing



CCP-volumeEM

Collaborative Computational Project
for Volume Electron Microscopy



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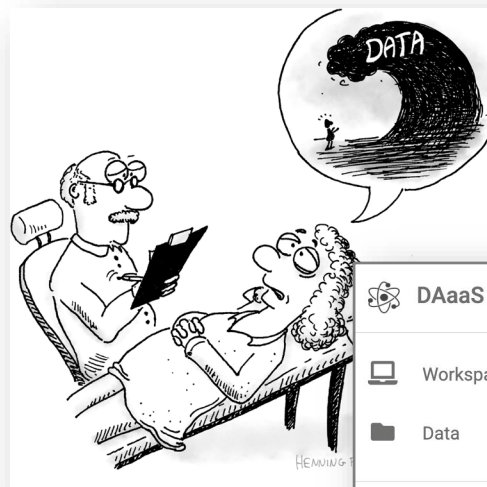
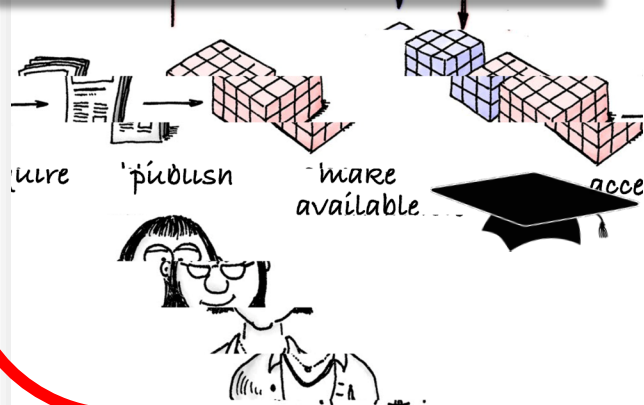
Work Package 1: Community building

- Existing communities
volumeem.org
[RMS](https://rms.euroimaging.org/)
[BioImagingUK](https://www.bioimaginguk.org/)
- Survey
- Mailing list
- Community events
→ Roadmap
- Website (soon!)
- Slack
- BlueSky



Work Package 2: Research Software and Data Management

FAIR data
Next Generation File Formats
Exemplar workflows
Reproducibility via containerisation



Work Package 3: Training and Skills

DaaS Training

Workspaces

Data

Attendee
Workspaces

My Courses

Resources

12 CPUs

90 GB RAM

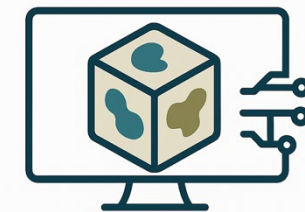
GPU1

Software

► Napari - Latest

► Fiji - 06-02-2024

CREATE WORKSPACE



CCP-volumeEM
Collaborative Computational Project
for Volume Electron Microscopy

Standing on the shoulders of giants



MicroscopyDB

How to get involved

- Save the date!
Monday 3rd November
Francis Crick Institute (London)
- One day meeting to discuss the draft roadmap for a collaborative computational project in volume EM (CCP-volume EM)
- Talks from vEM and computing experts, plus breakout sessions to discuss priorities



How to get involved

- JISC Mailing list: bit.ly/ccp-volume-em



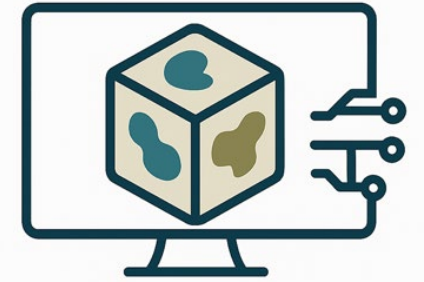
How to get involved

- Survey on software needs in vEM
<https://forms.office.com/e/eMAJGCKUnc>



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- JISC Mailing list: bit.ly/ccp-volume-em
- BlueSky: ccp-volumeem.bsky.social
- Email: CCPvolumeEM@gmail.com



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Attend the Community event
at the Crick on 3rd Nov!

