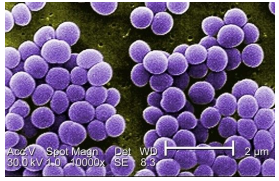
Remote on-the-fly analysis and cloudification of the cryo-electron microscopy data

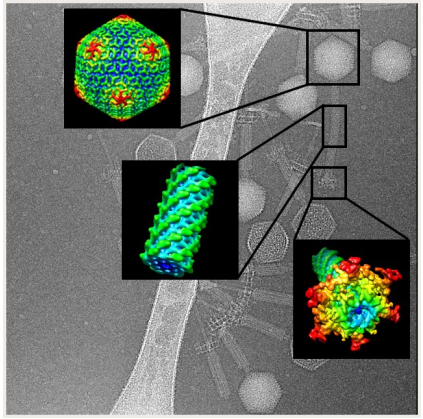
Jiri Novacek

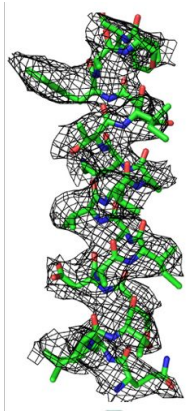
CEITEC, Masaryk University

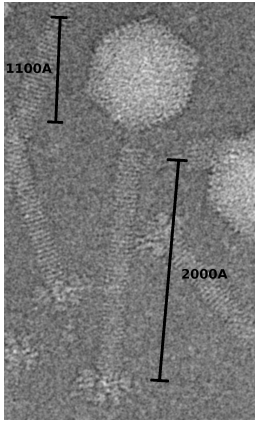
CEMCOF

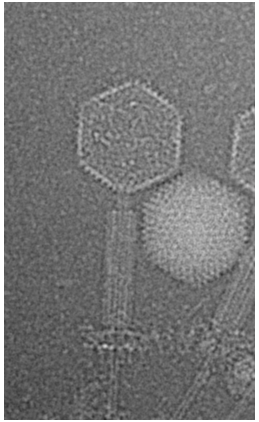
- 6 partners
- 500 researchers
- 7 research programs
- 63 research groups
- 25,000 m2 of lab area
- 13 core facilities











- Staphylococcus Aureus
- Bacteriophage phi812
- Active against 75% MRSA and 95% MSSA

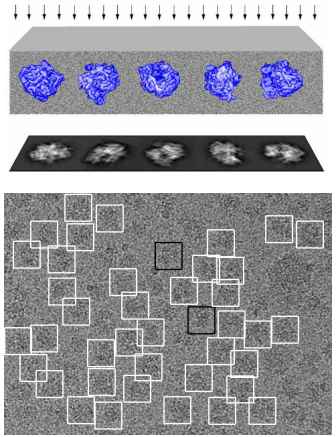
IO-SEA

Goals

- Facilitate management of the raw cryo-electron microscopy data
  - Data annotation directly on the instrument
  - Deployment of the data to the federated cloud solution
  - Automated archival and publication of the raw data
- Real-time data analysis on the remote HPC resources

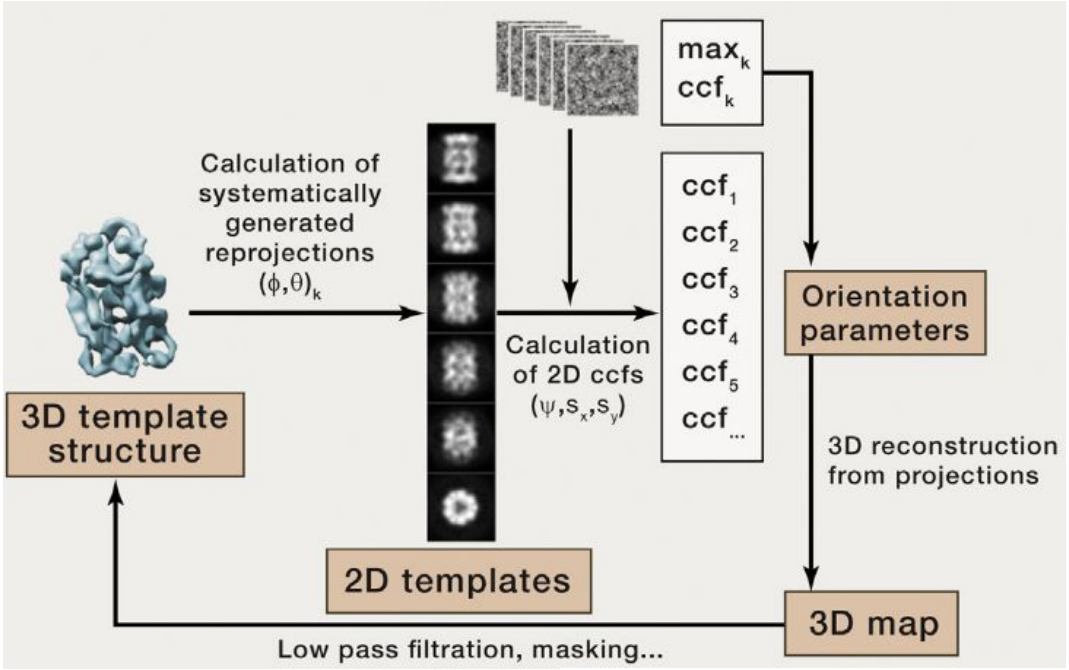
Motivation

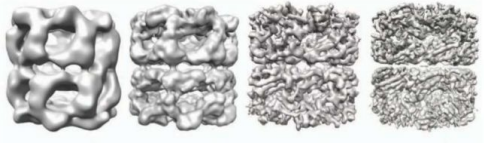
Single particle cryo-EM workflow description



- micrograph (image), particle (ROI)
- 2D projection of a 3D object -> projection orientations not known
- very low signal to noise -> large number o images
- sample drift and beam induced motion during imaging
- convolution with microscope point spread function

-> data intensive

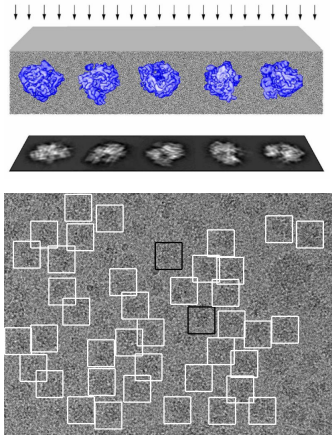




IO-SEA

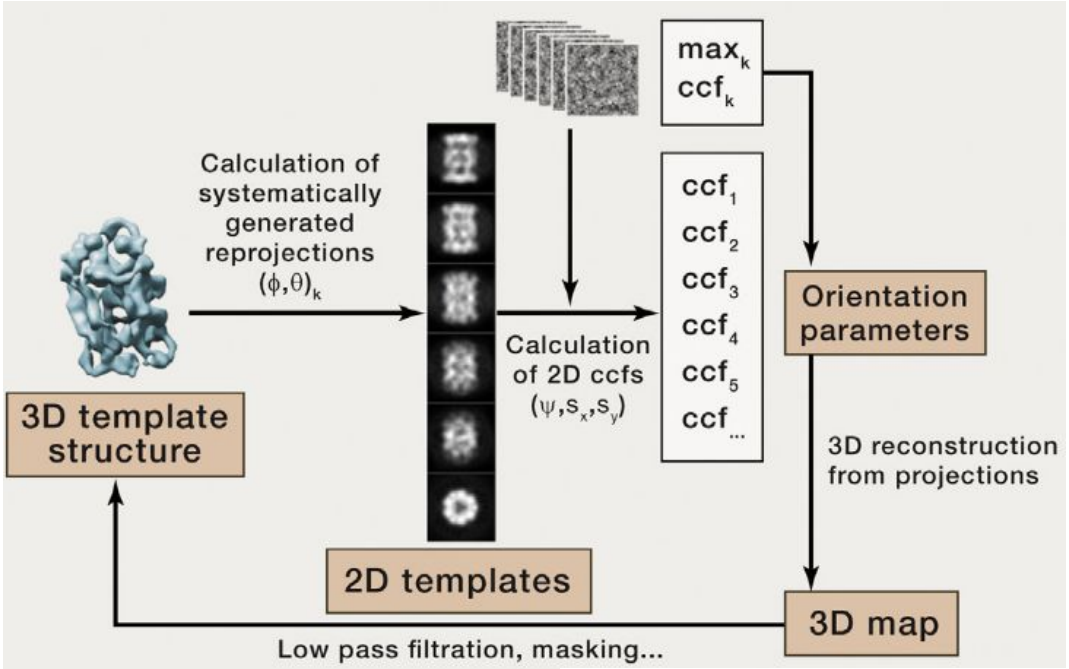
Motivation

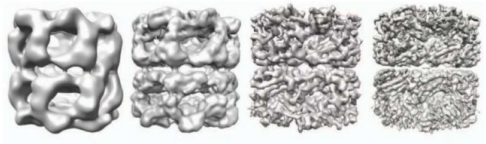
Single particle cryo-EM workflow description



- compare experimental images to all reference projections
- assign the projection angles of the best matching reference to the particle
- calculate 3D model
- project 3D model and use it as a new reference
- iterate

-> computationally intensive





IO-SEA

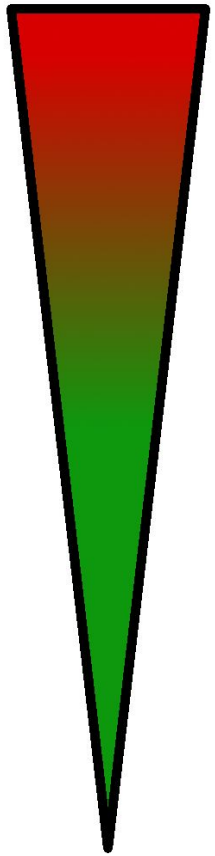
Motivation

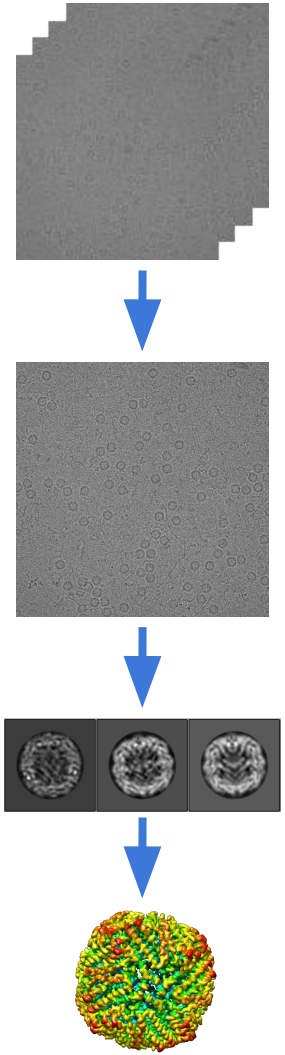
2-4 TB

~400GB

~40GB

~40MB





raw data

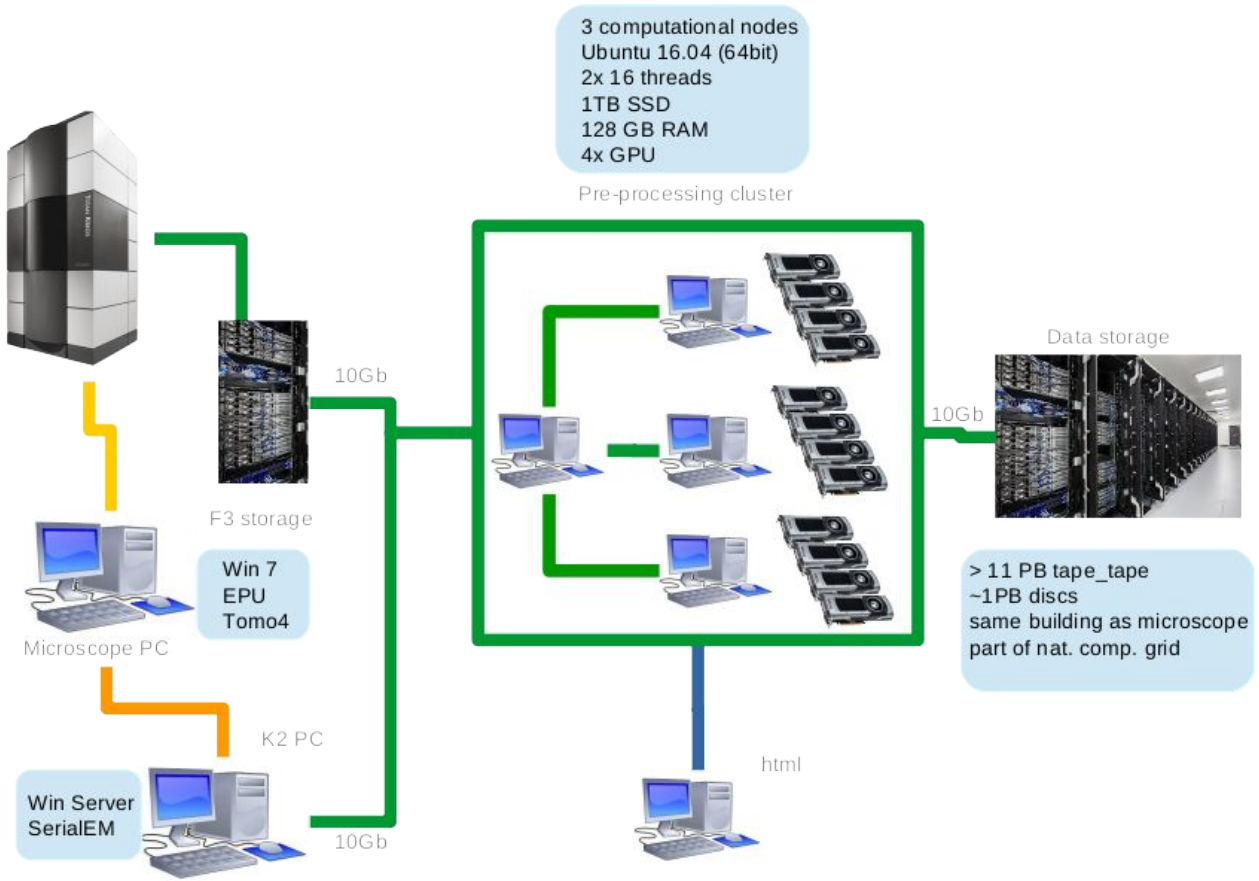
preprocessed data

ROIs/particles

Final 3D structure

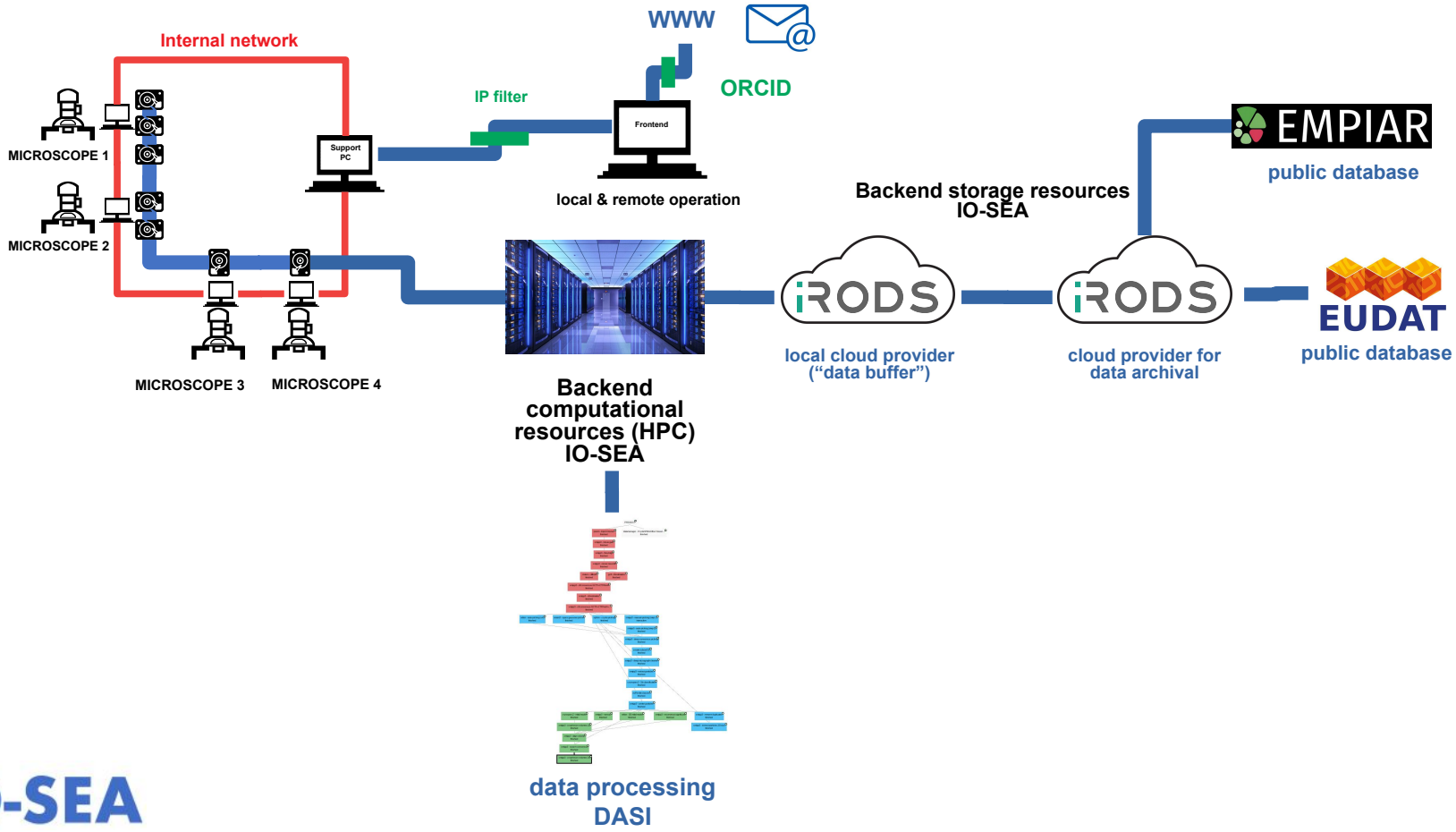
IO-SEA

Motivation



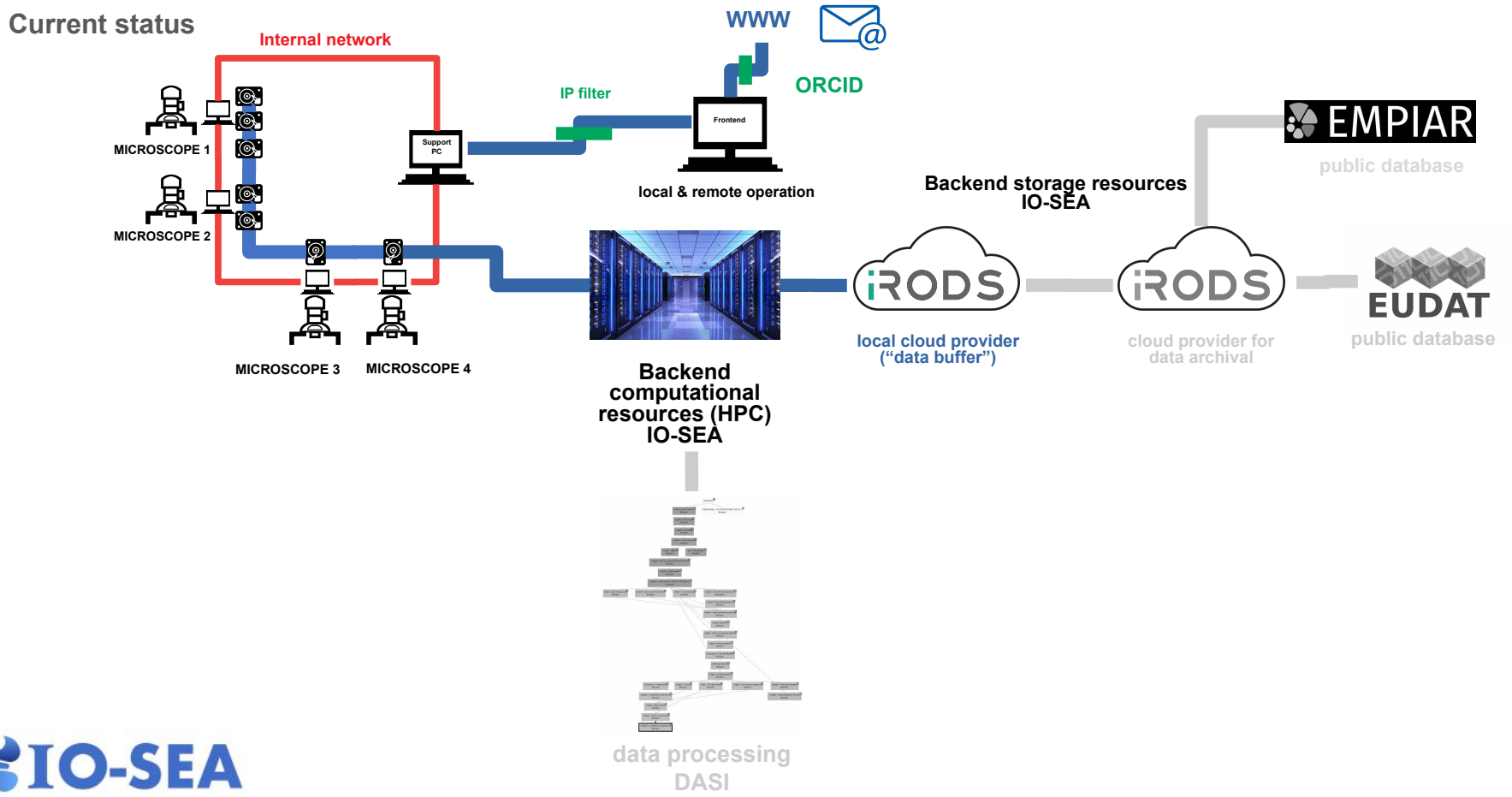
IO-SEA

Proposed solution



IO-SEA

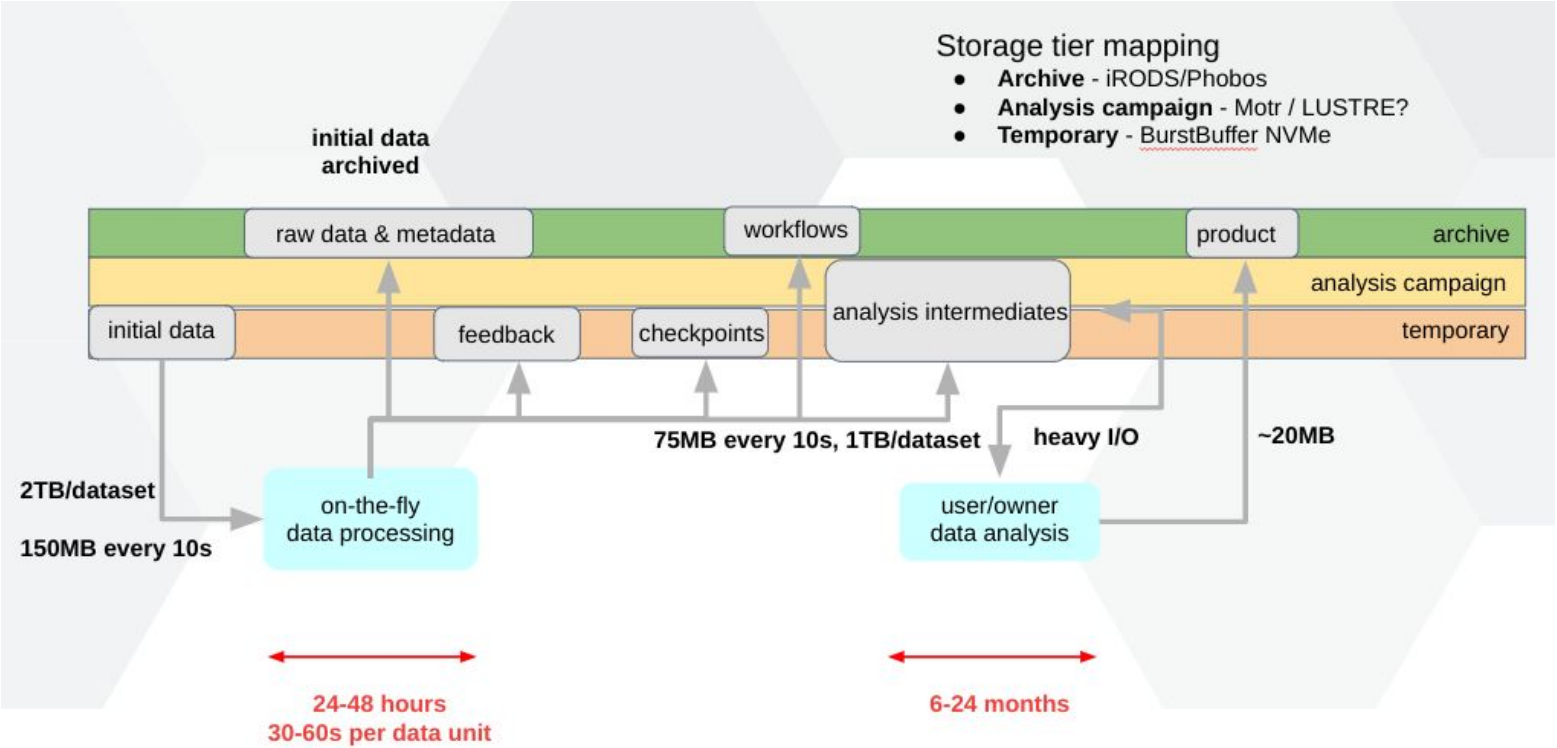
Proposed solution



IO-SEA

Proposed solution

Data cycle



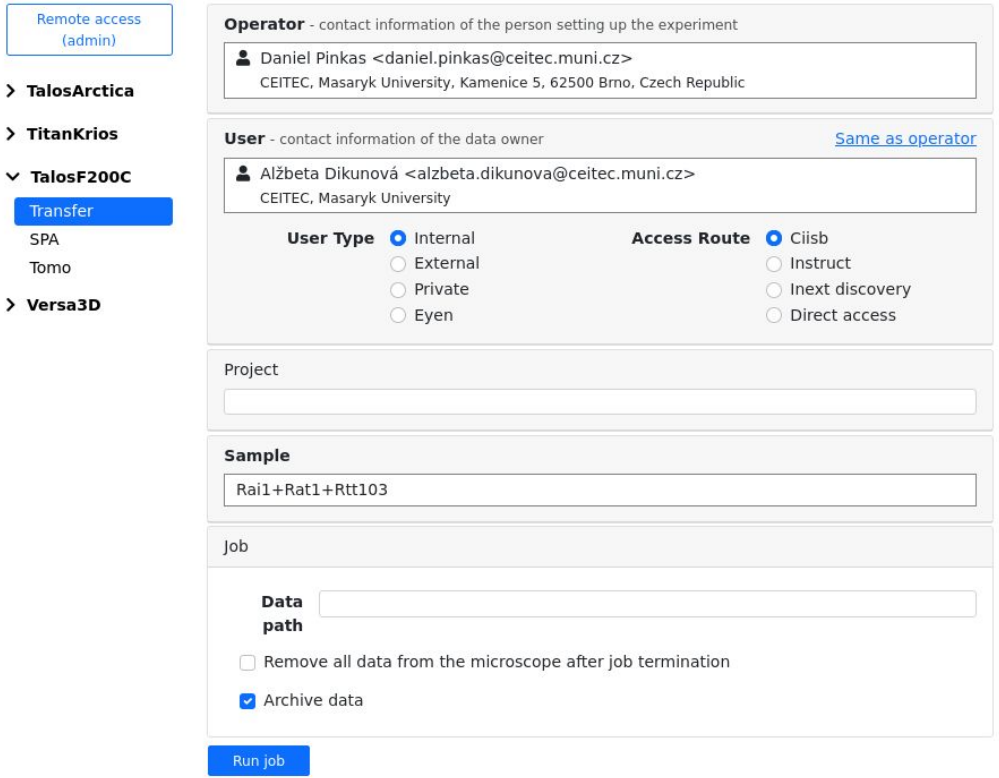
IO-SEA

Proposed solution

Front end

- web-browser based operation
- accessible directly from the instrument/microscope
- secure access from outside the microscope network:
  - Google
  - eduID
  - ORCID

- instrument specific setup
- Implementation of different data analysis workflows
- data-model with four different components:
  - the laboratory (center)
  - the user (data owner)
  - the sample
  - the data
- real-time job status
- automated user notification (email)
- local database of the projects



DEMO

Summary

- automated annotation of the raw cryo-EM data
- real-time data transfer to the remote storage resources (iRODS)
- on-the-fly data analysis on the remote HPC resources
- database entry for data publication (FAIR)

Acknowledgements

- Radek Veverka
- Radek Furmanek
- Martin Golasowski
- Jan Martinovic