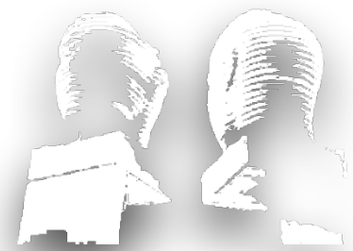
TEM data is not FAIR, how to make it play well with others?

Andy Stewart
University of Limerick

University of Limerick
Ollscoil Luimnigh

Bernal Institute

andy.stewart@ul.ie



Where is Limerick?

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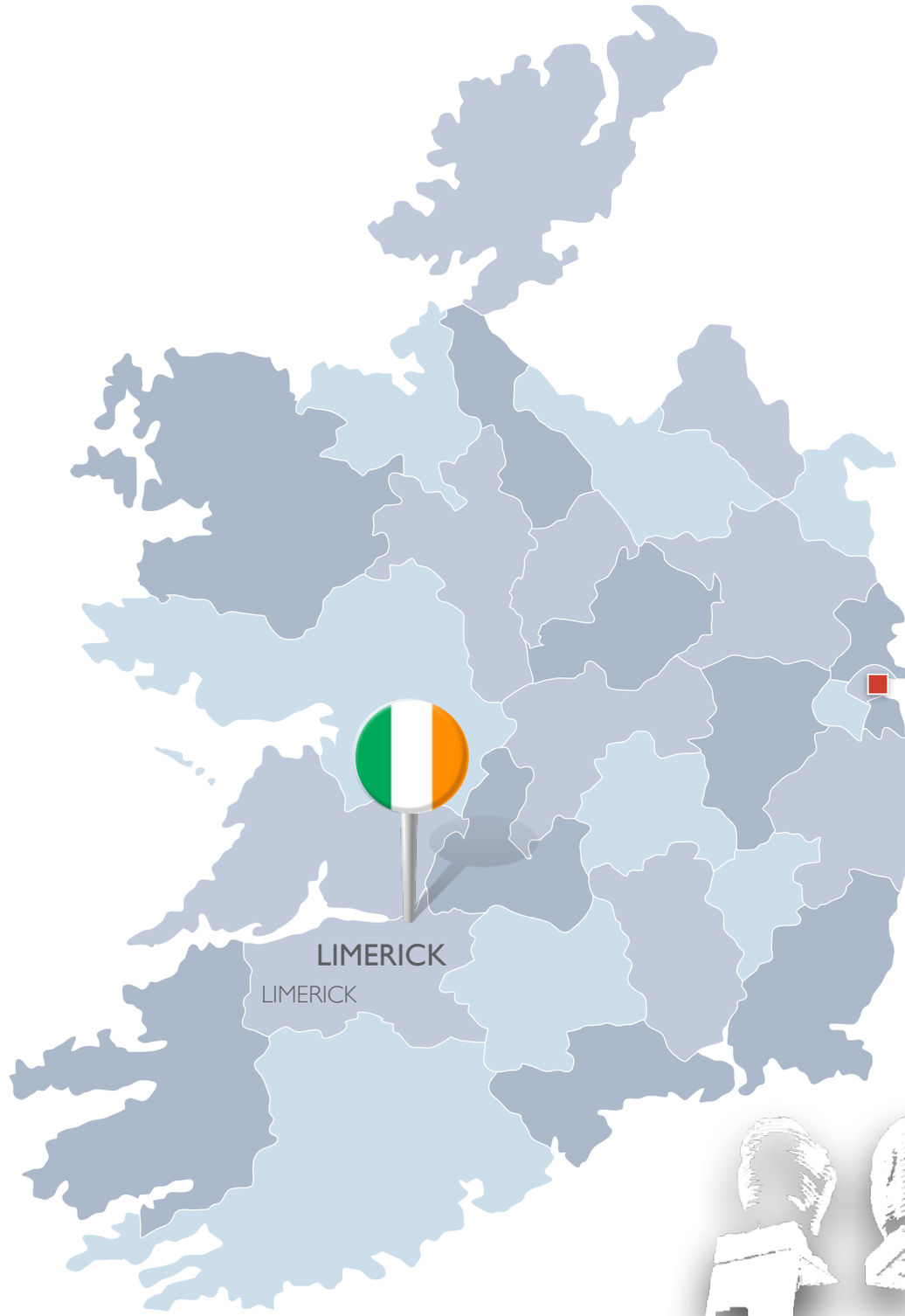
Where is Limerick?



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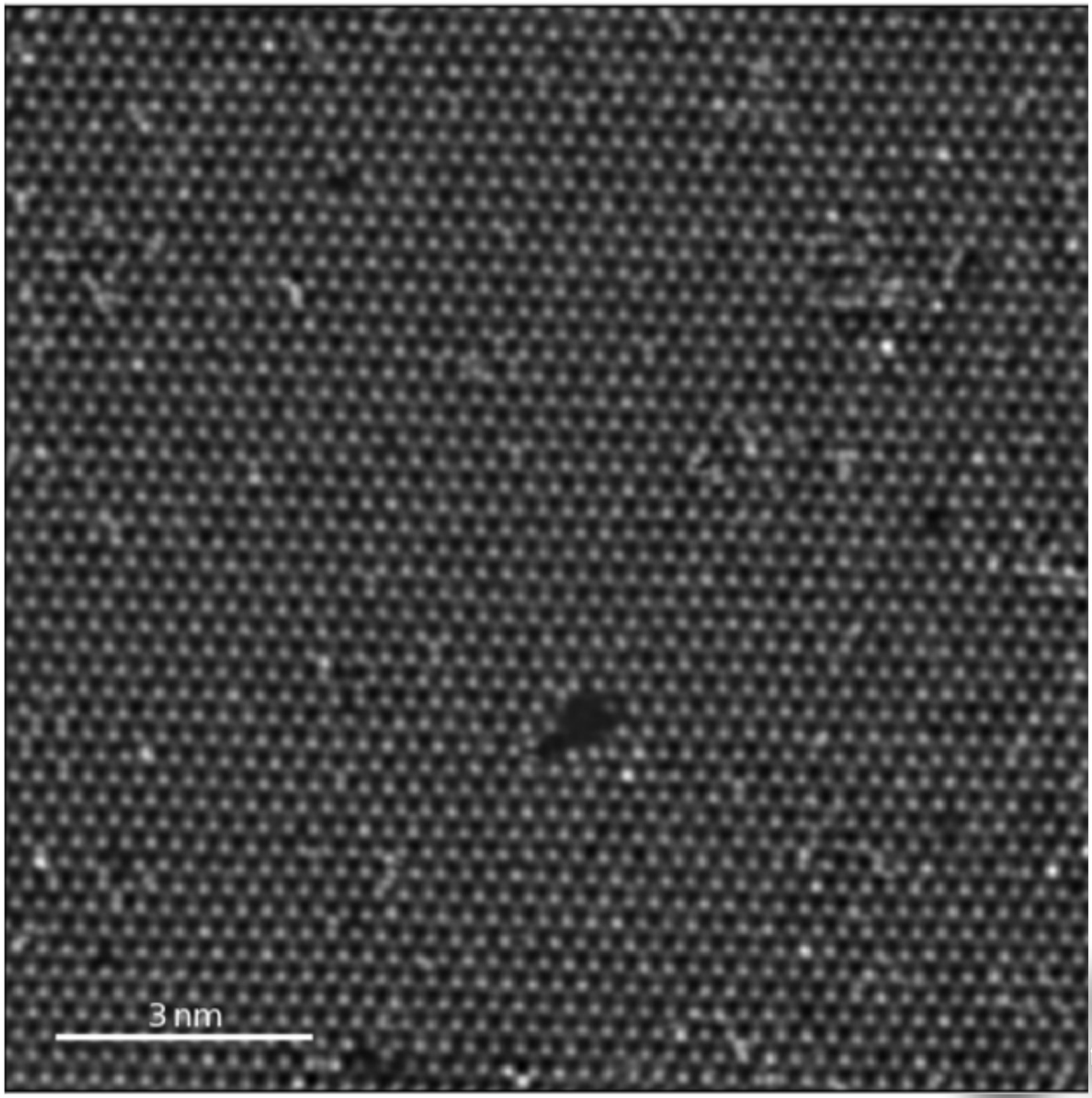
TEM image



Courtesy of Eoghan O'Connell, University of Limerick

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Data Processing Metadata

Data Processing Metadata

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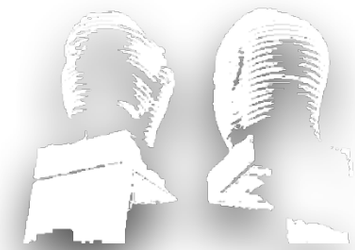
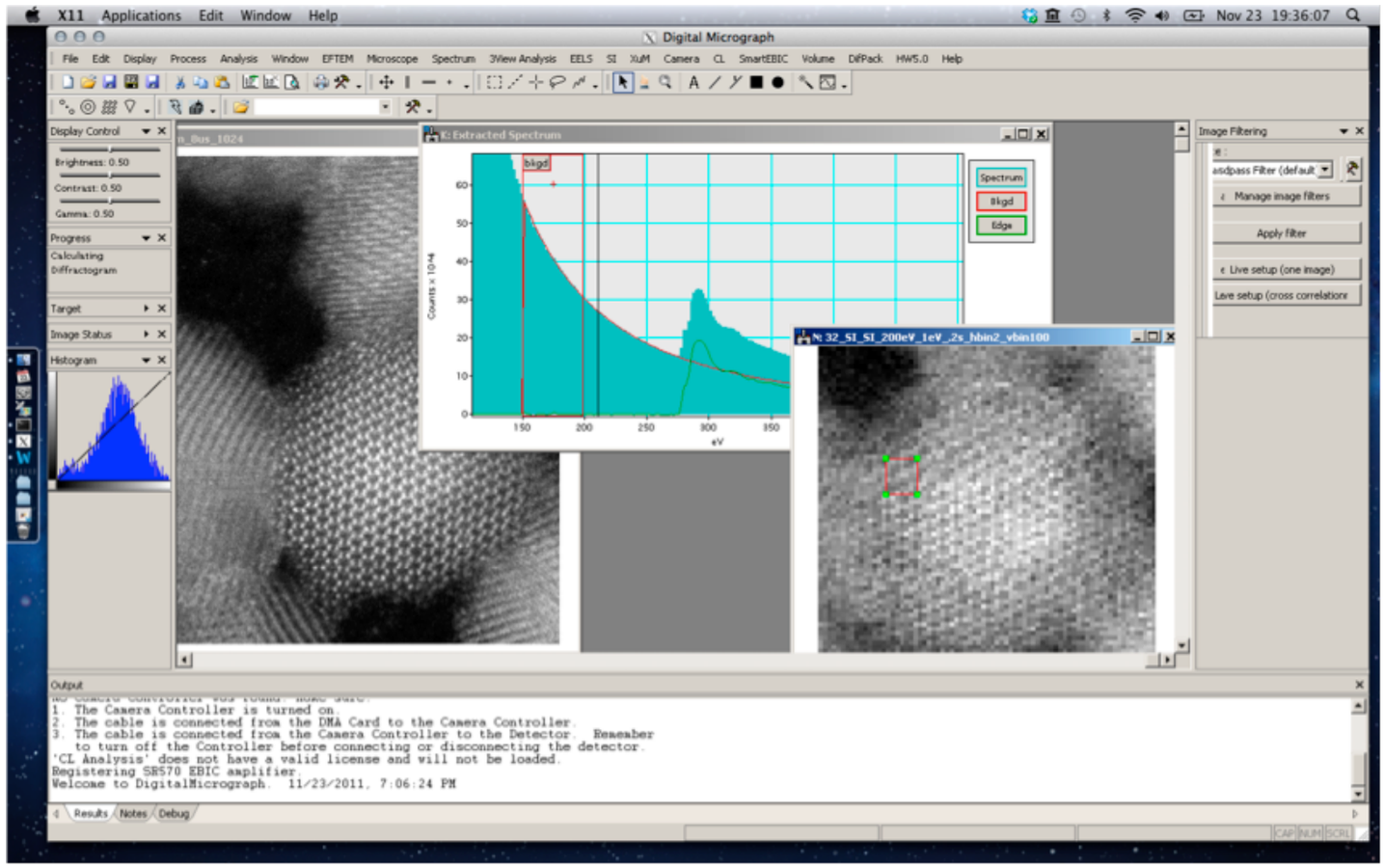


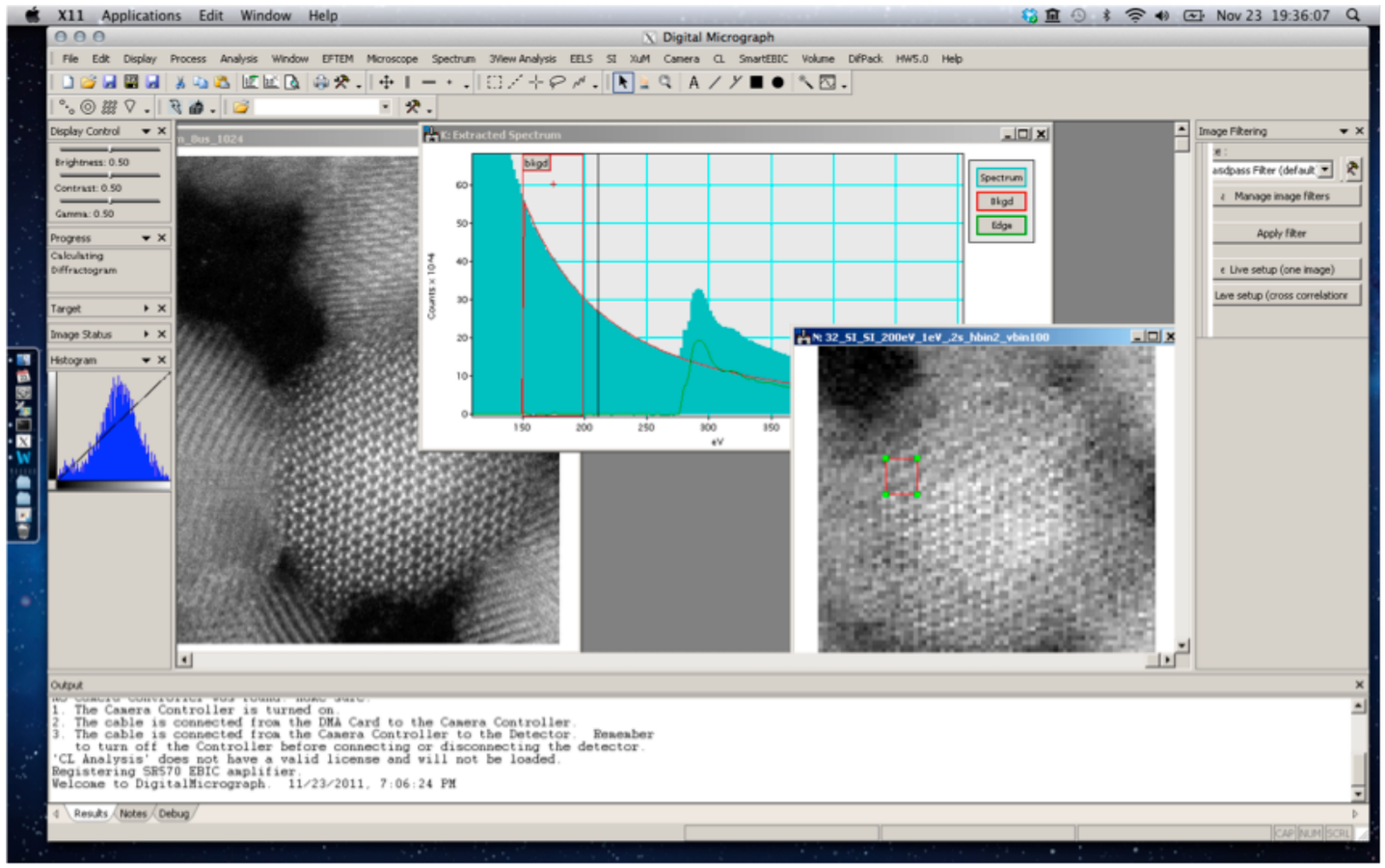
Data formats

Currently dm3/dm4



Data formats

Currently dm3/dm4



23 versions of the TIFF

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TEM Metadata

- Acquisition
  - Device
    - Active Size (pixels): (4096,4096)
    - Camera Number: 2
    - CCD
      - Pixel Size (um): 15.0+i15.0
    - Configuration
      - Location: high_resolution
      - Transpose
    - Name: One View Camera
    - Source: One View Camera
    - Source ID: OneView-46565850035
    - Source Model: OneView
    - Temperature (C): -5.03906
  - Frame
    - Area
    - CCD
    - Intensity
    - Reference Images
  - Parameters
    - Acquisition Write Flags: 4294967295
    - Base Detector
    - Detector
    - Environment
    - High Level
    - Objects
    - Parameter Set Name: Record
    - Parameter Set Tag Path: Imaging:Acquire:Record
    - Version: 34078720
  - Calibration
  - DataBar
    - Acquisition Date: 12/21/2018
    - Acquisition Time: 11:31:32 AM
    - Acquisition Time (OS): 1.31899e+17
    - Binning: 2
    - Collection Number: 1
    - Device Name: One View Camera
    - Exposure Number: 2175
    - Exposure Time (s): 4.0
    - Signal Name: One View Camera
  - GMS Version
    - Created: 3.31.2169.1
    - Saved: 3.31.2169.1
  - Microscope Info
    - Actual Magnification: 1069.74
    - Cs(mm): 0.0
    - Emission Current (µA): 0.0
    - Emission Current (µA): 0.0
    - Formatted Actual Mag: 1kx
    - Formatted Indicated Mag: 580x
    - Formatted Voltage: 300kV
    - Illumination Mode: TEM
    - Illumination Sub-mode: 1
    - Imaging Mode: DIFFRACTION
    - Indicated Magnification: 580.0
    - Magnification Interpolated: false
    - Name: FEI Tecnai Remote
    - Operation Mode: DIFFRACTION
    - Operation Mode Type: 2
    - Probe Current (nA): 0.0
    - Probe Size (nm): 0.0
    - STEM Camera Length: 145.0
    - Stage Position
      - Stage Alpha: 0.00878402
      - Stage X: -90.0588
      - Stage Y: -40.6173
      - Stage Z: -35.5413
    - Voltage: 300000.0
  - Session Info
    - Items
    - Microscope:

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Sample Metadata missing?

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Sample Metadata missing?

Sample

Preparation methods and details

Specimen composition

Date and time of production

Colour

Shape

Thickness

Defects

Grain boundaries

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Sample Metadata missing?

Sample

Preparation methods and details
Specimen composition
Date and time of production
Colour
Shape
Thickness
Defects
Grain boundaries

Sample Storage

Environment
Relative humidity
Temperature
Light/Dark

Any variable which may cause sample to change over time

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Sample Metadata missing?

Sample

Preparation methods and details
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Sample Storage

Environment
Relative humidity
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Light/Dark
Any variable which may cause sample to change over time

Relationship between images and spectroscopy data

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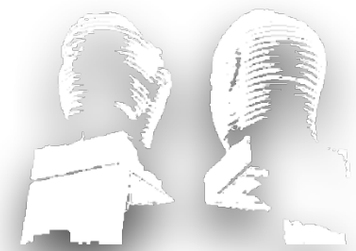

Sample Metadata missing?

Sample

Preparation methods and details
Specimen composition
Date and time of production
Colour
Shape
Thickness
Defects
Grain boundaries

Sample Storage

Environment
Relative humidity
Temperature
Light/Dark
Any variable which may cause sample to change over time

Relationship between images and spectroscopy data

Record any value/detail which will be necessary for evaluating with any other dataset or technique

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TEM Missing Metadata

TEM Missing Metadata

<u>TEM variables</u>

TEM Environment
Relative Humidity of room
Temperature of room
Fields in the room
Water temperature
Magnet temperature
Power Supply variability
Beam brightness
Detector temperature

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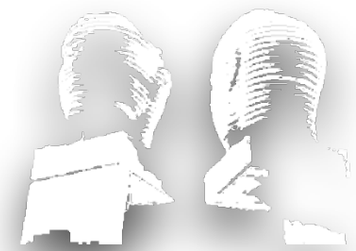

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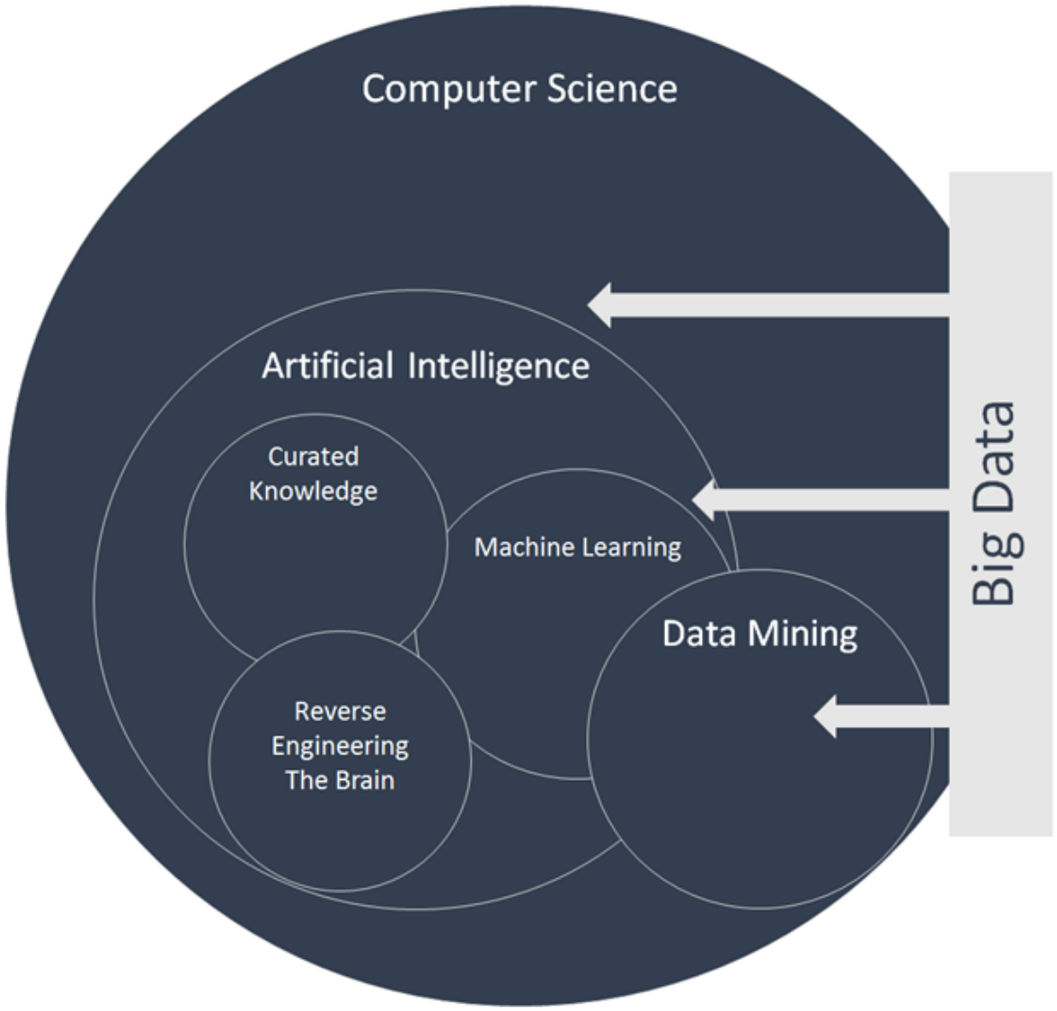

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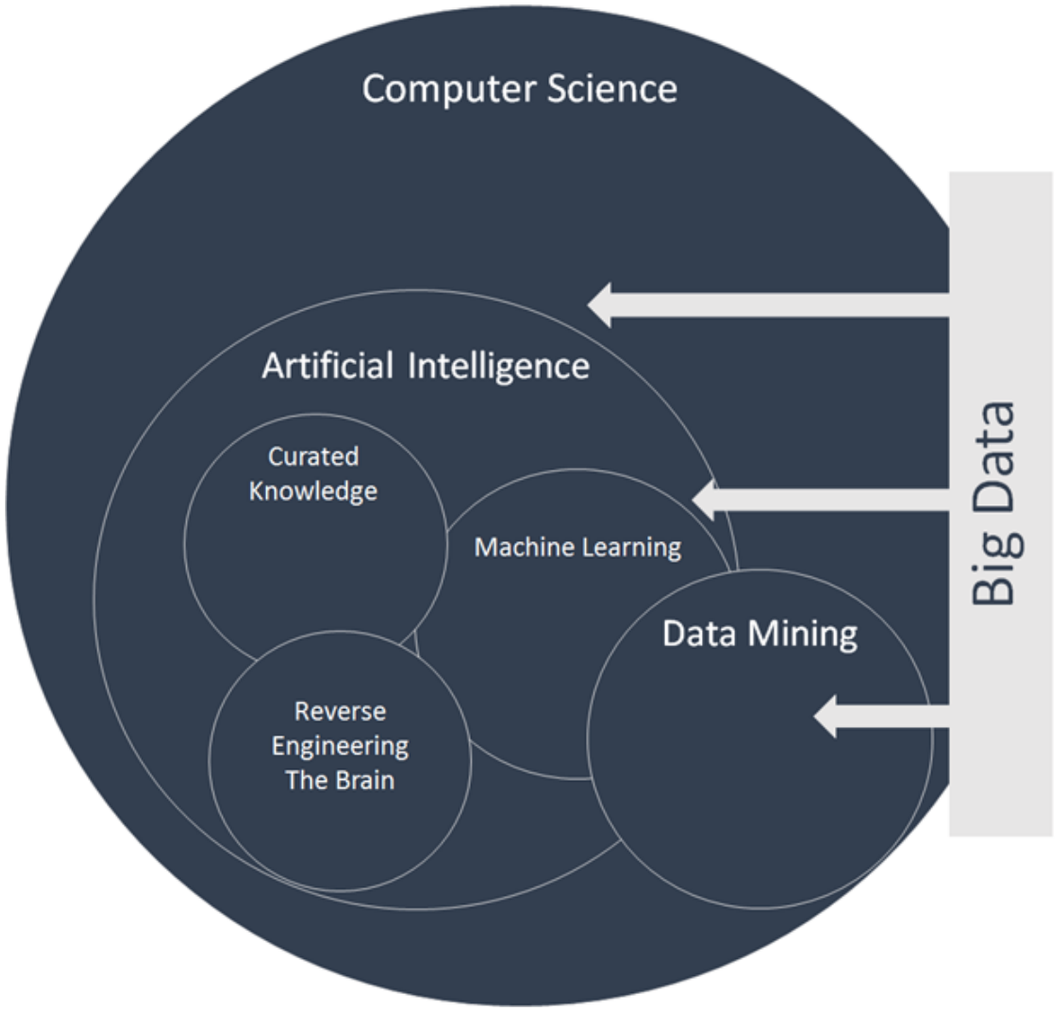
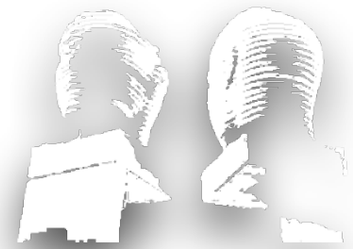
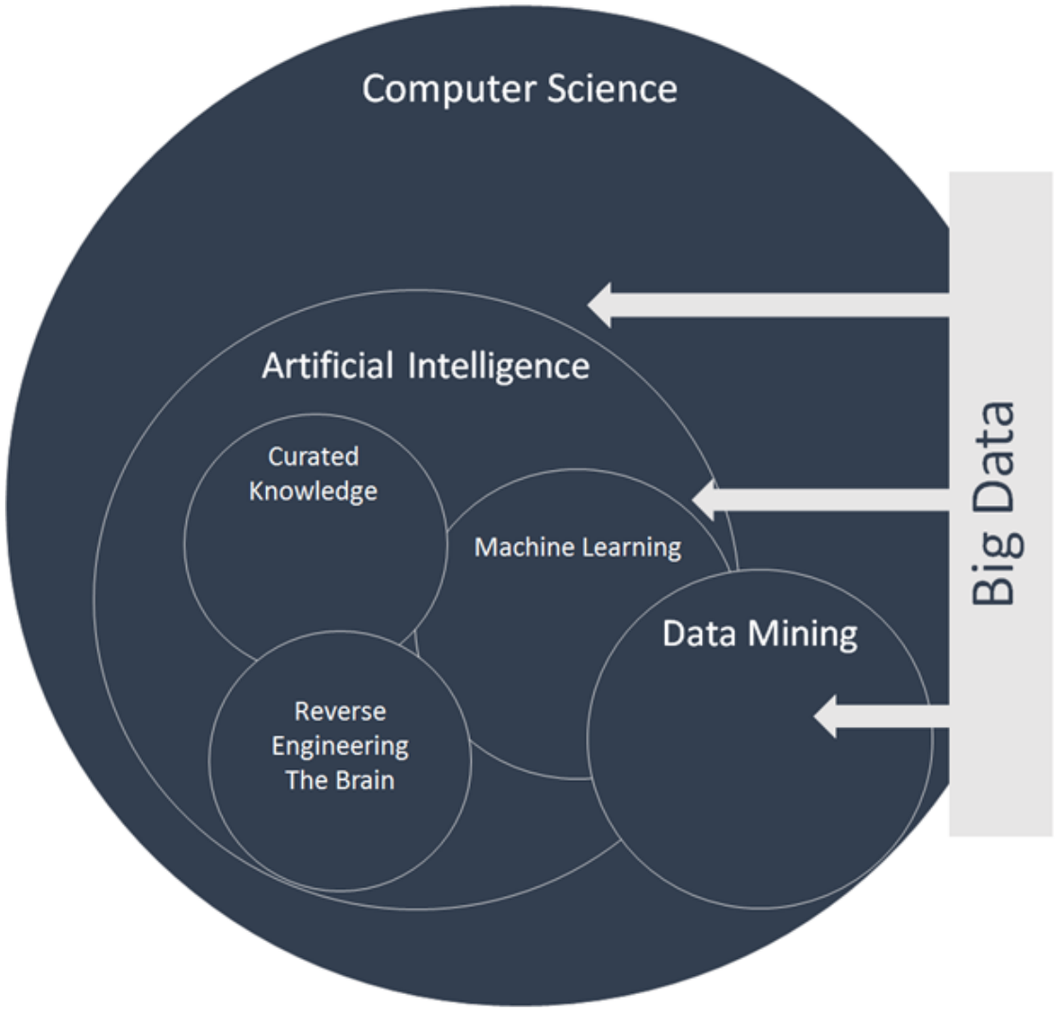


Grow the need for microscopy



Why should we care?



Grow the need for microscopy

More opportunities to be cited

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It’s NOT about you

It’s NOT about you

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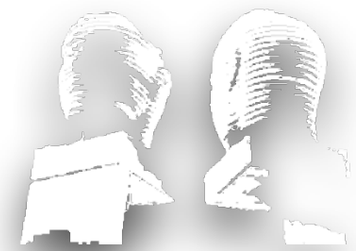

It’s NOT about you

Wellcome Open Research

EPSRC
Engineering and Physical Sciences Research Council

European Commission
HORIZON 2020

HELMHOLTZ ASSOCIATION

Open Science

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For TEM Simulations

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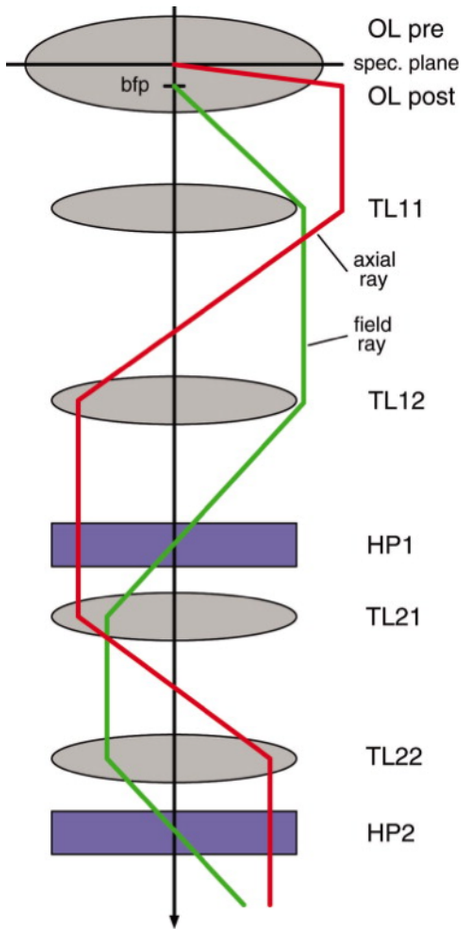
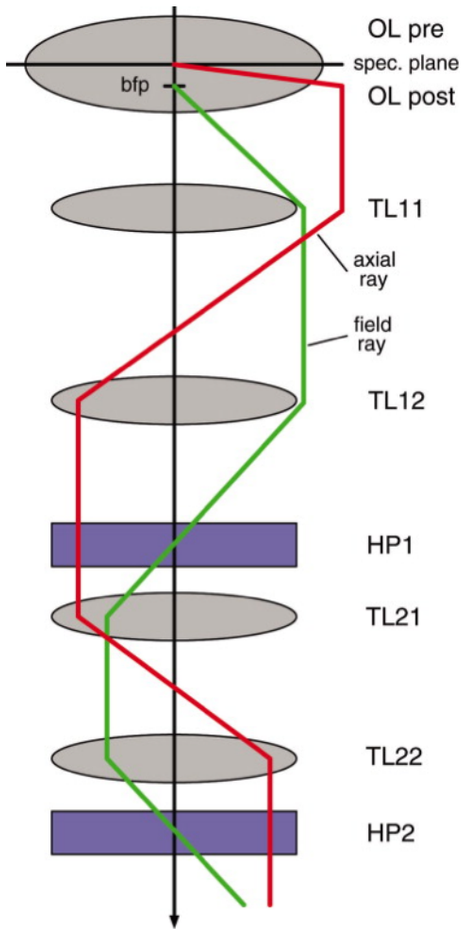
For TEM Simulations

No Corrector aberrations measurements Stored



For TEM Simulations

No Corrector aberrations measurements Stored



Time between aberration measurement and data acquisition

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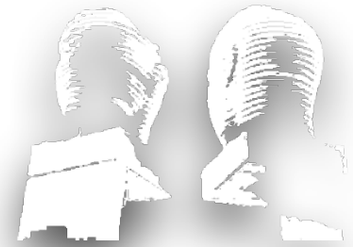
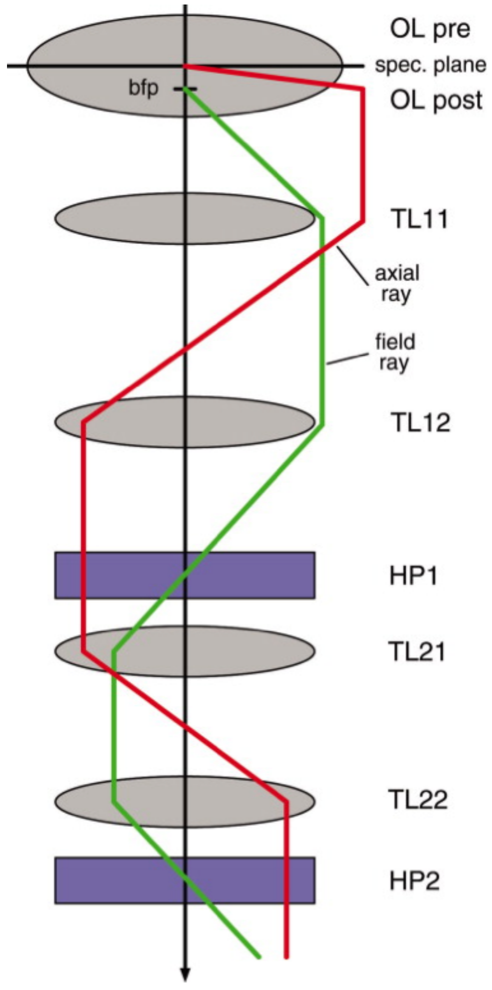


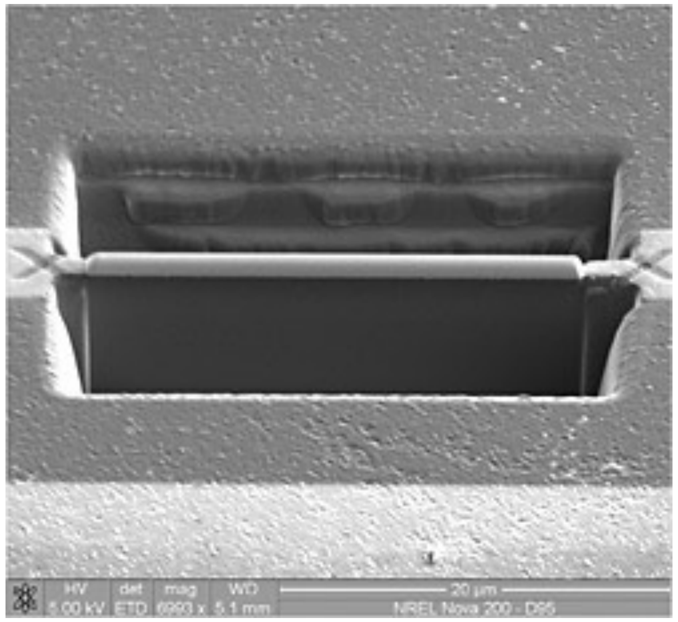
For TEM Simulations

No Corrector aberrations measurements Stored



Time between aberration measurement and data acquisition

Sample thickness estimate/measurement



We are not the first and will not be the last

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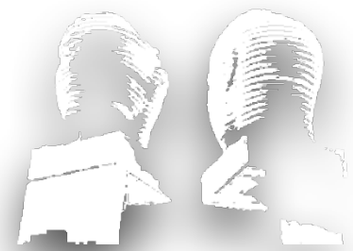

We are not the first and will not be the last

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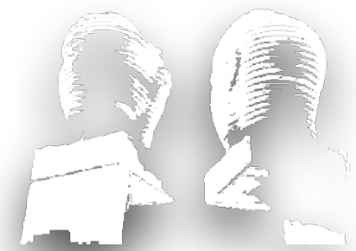
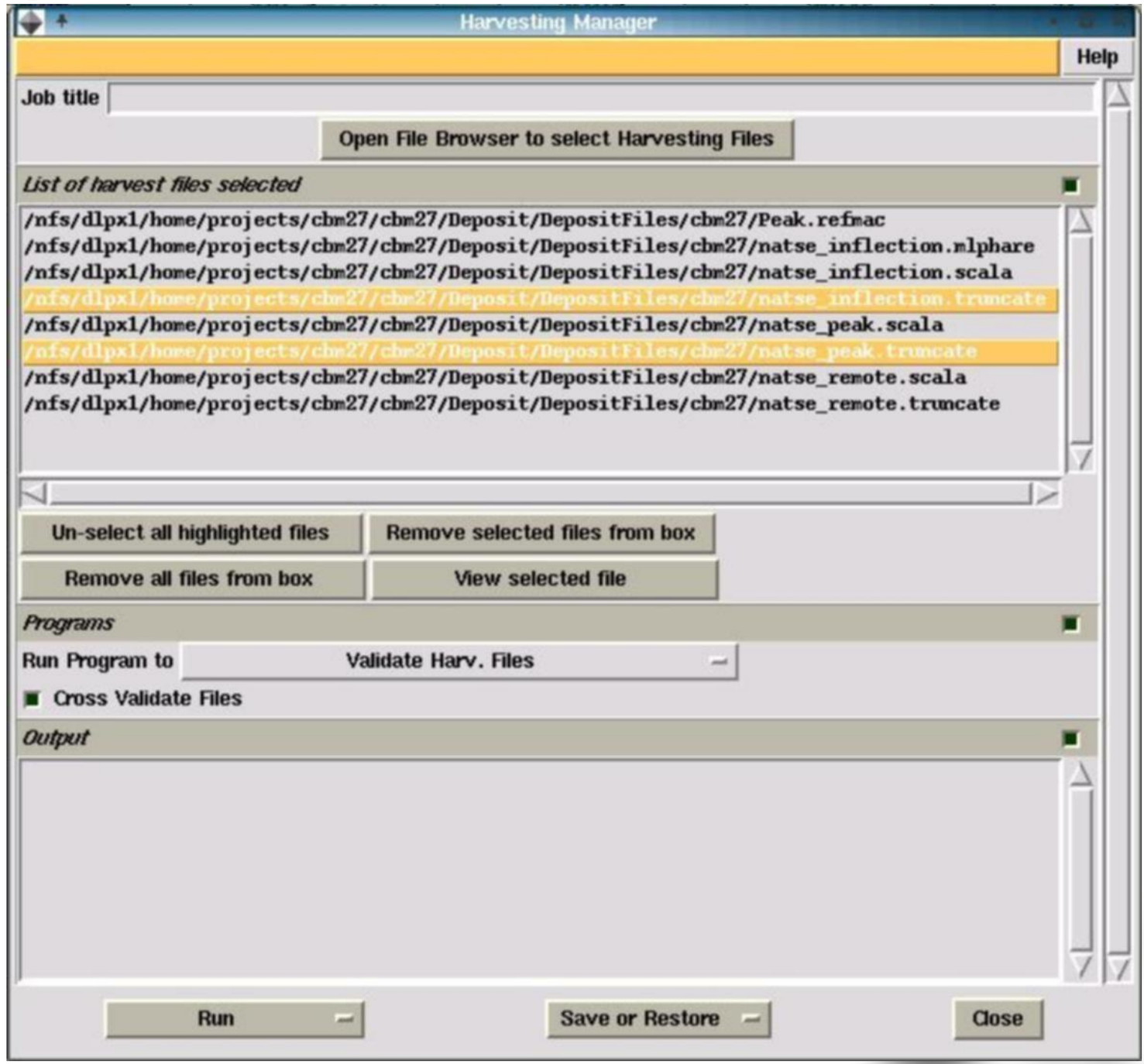


CCP4

MTZ format (1970's)

Data Harvesting (1990's)

Also Nomad



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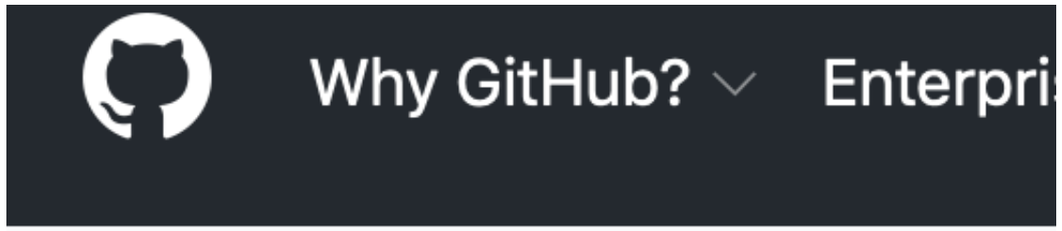
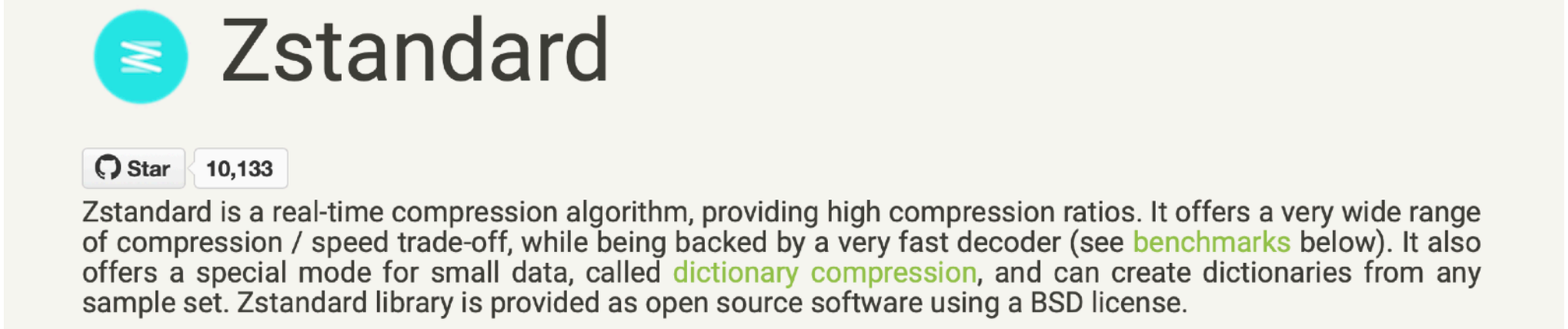
Data compression

MRCZ



XFEL

On the file data compression



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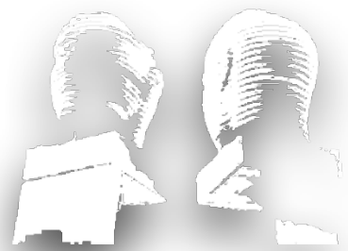
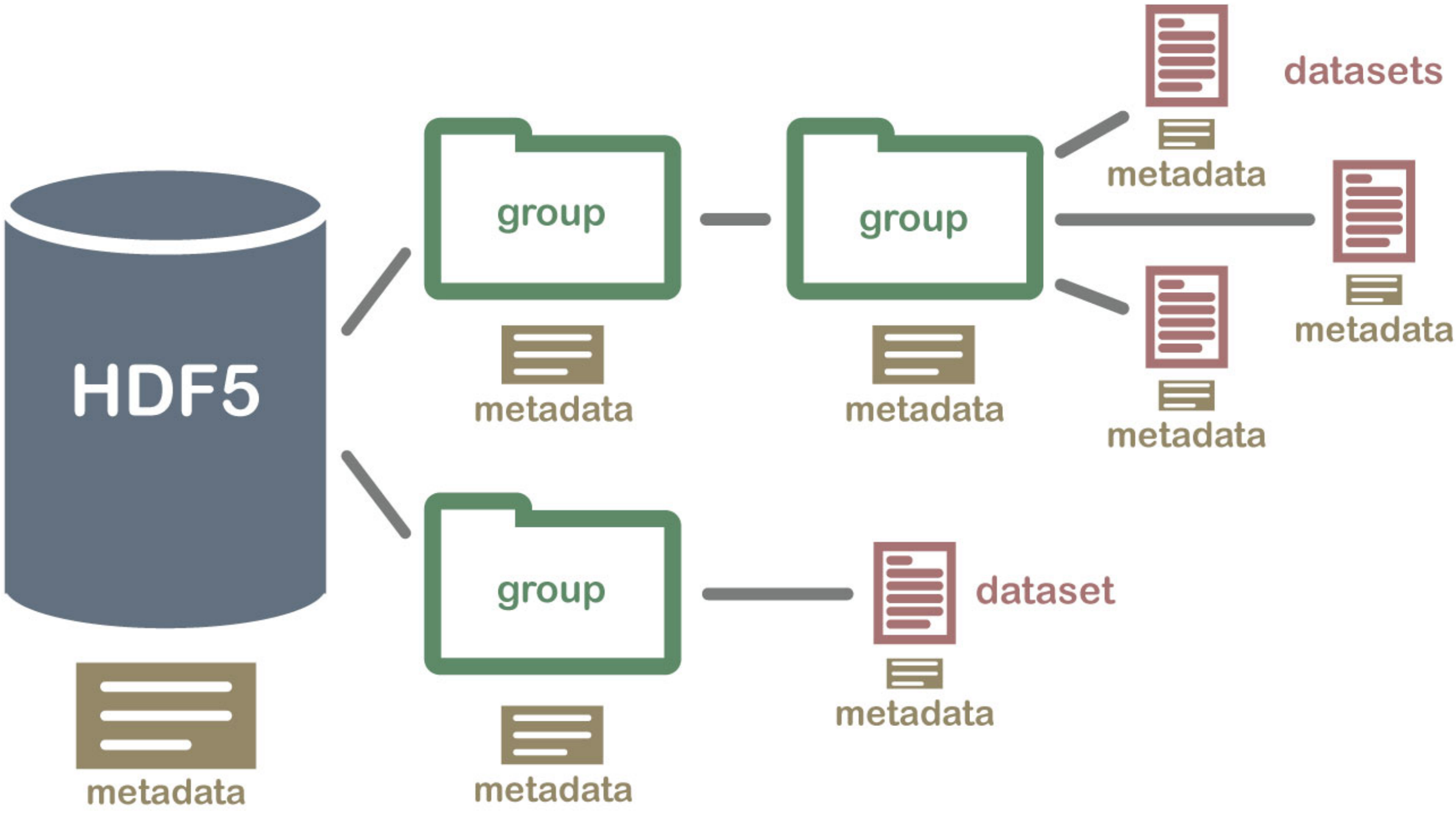


Recognised need for change Hierarchical Data Format #5

Already >25 variants in the EM community



Data format proliferation

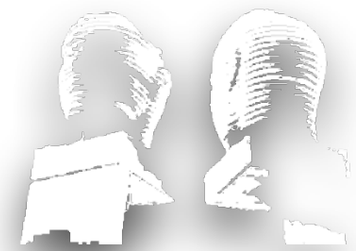
Monty Python, Life of Brian

Data format proliferation

Monty Python, Life of Brian

Adoption

Last thing we need is just another file format



Adoption

Last thing we need is just another file format

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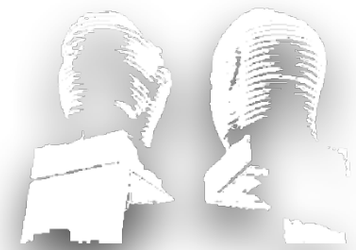

Adoption

Last thing we need is just another file format

- Public databases
- Organisations promote use of format

Adoption

Last thing we need is just another file format

- Public databases
- Organisations promote use of format

- Journals insist on data submission in a specific format
- Funding bodies insist on open data with all meta data

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Community Agreement on a single format

Or a series of convertors like Nomad?

Missing metadata a problem….?

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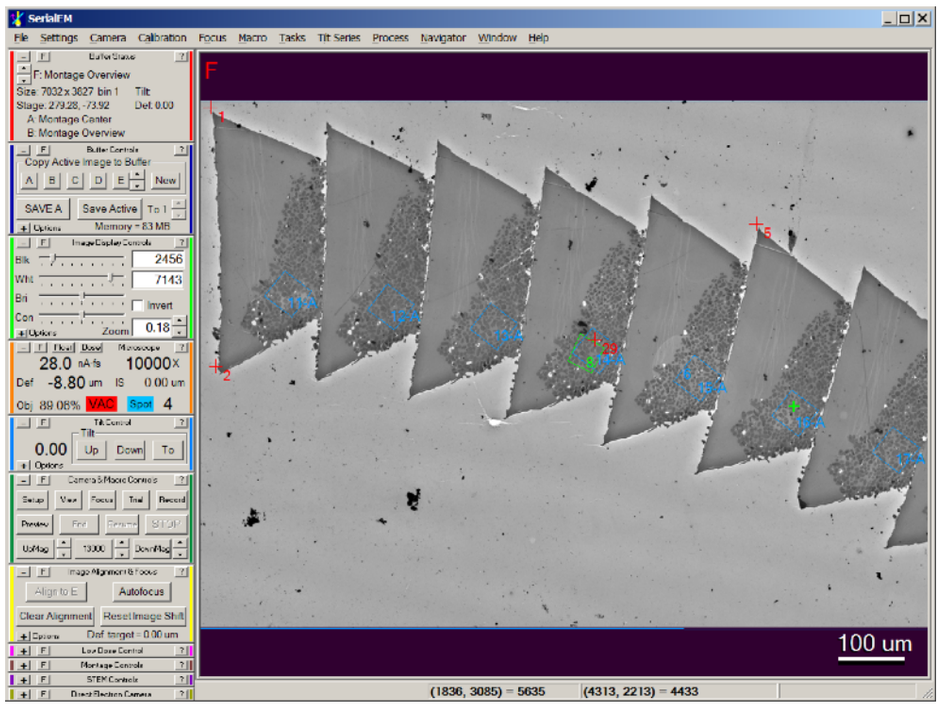
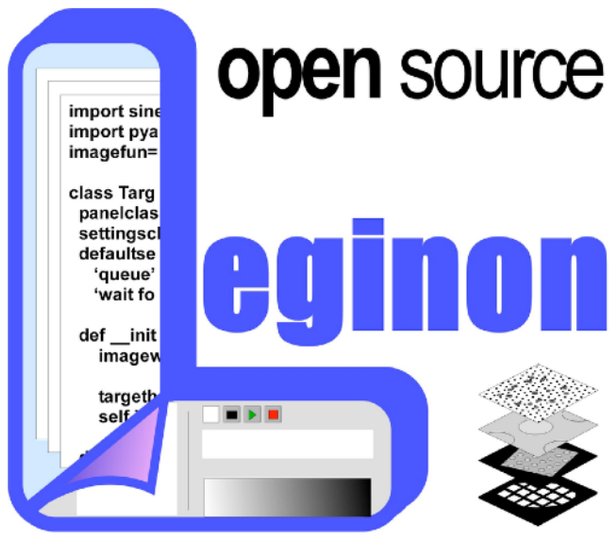
Making Metadata Easier

SerialEM

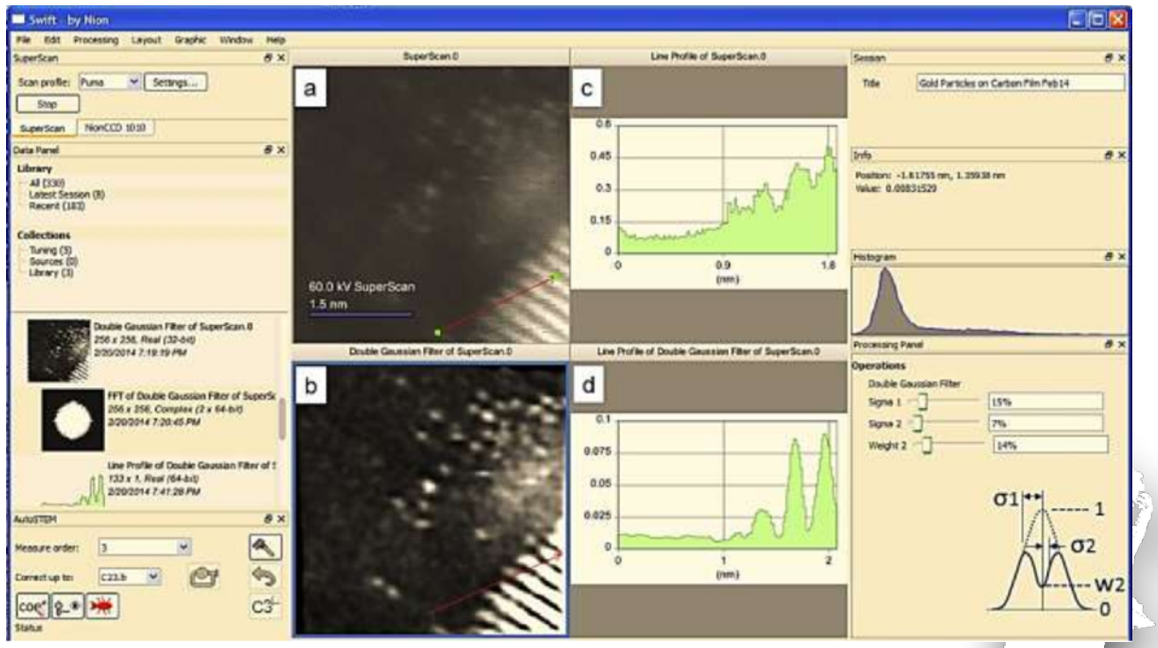


Leginon



LiberTEM

Swift Nion



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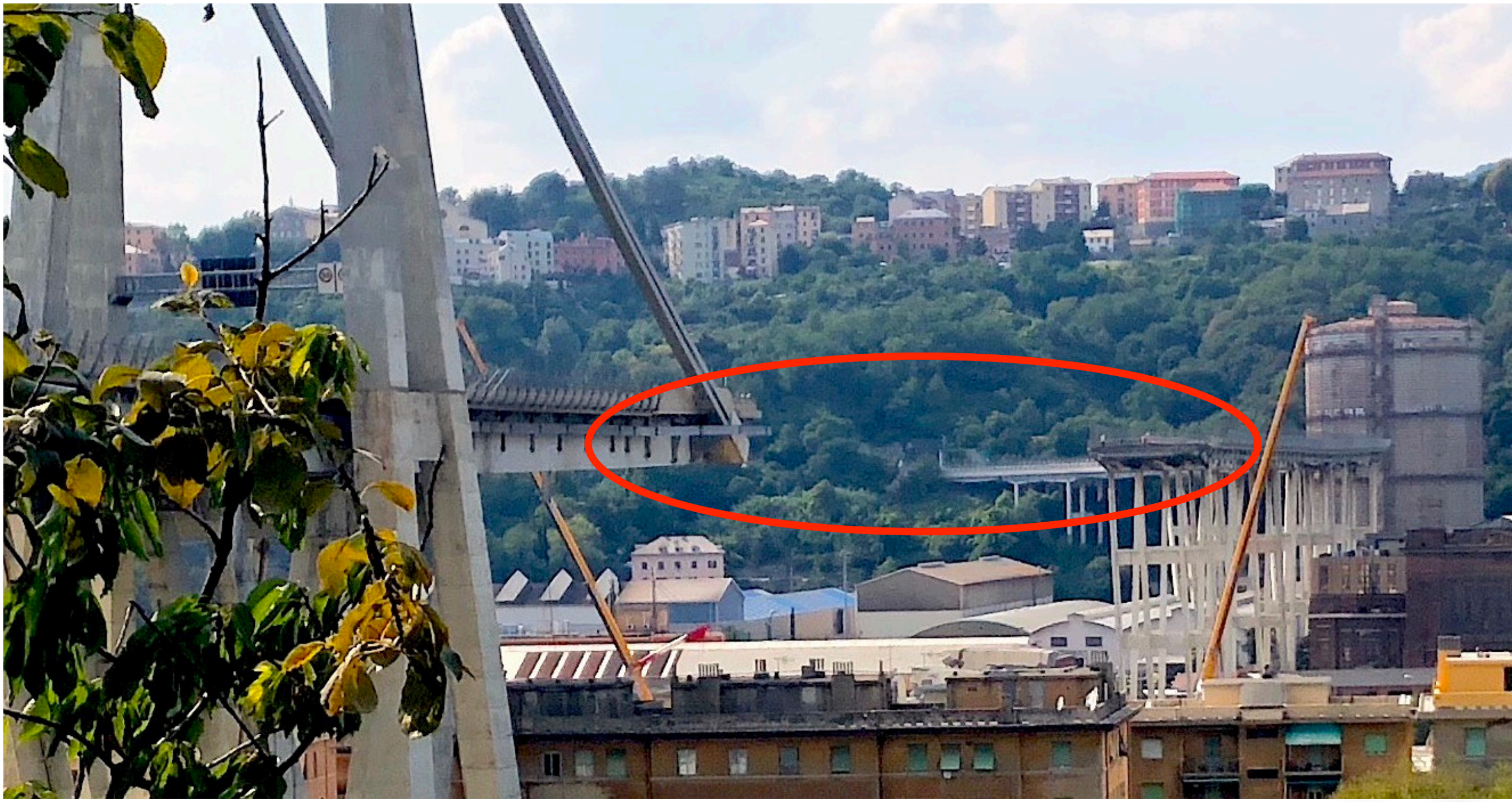
Morandi Bridge Collapse



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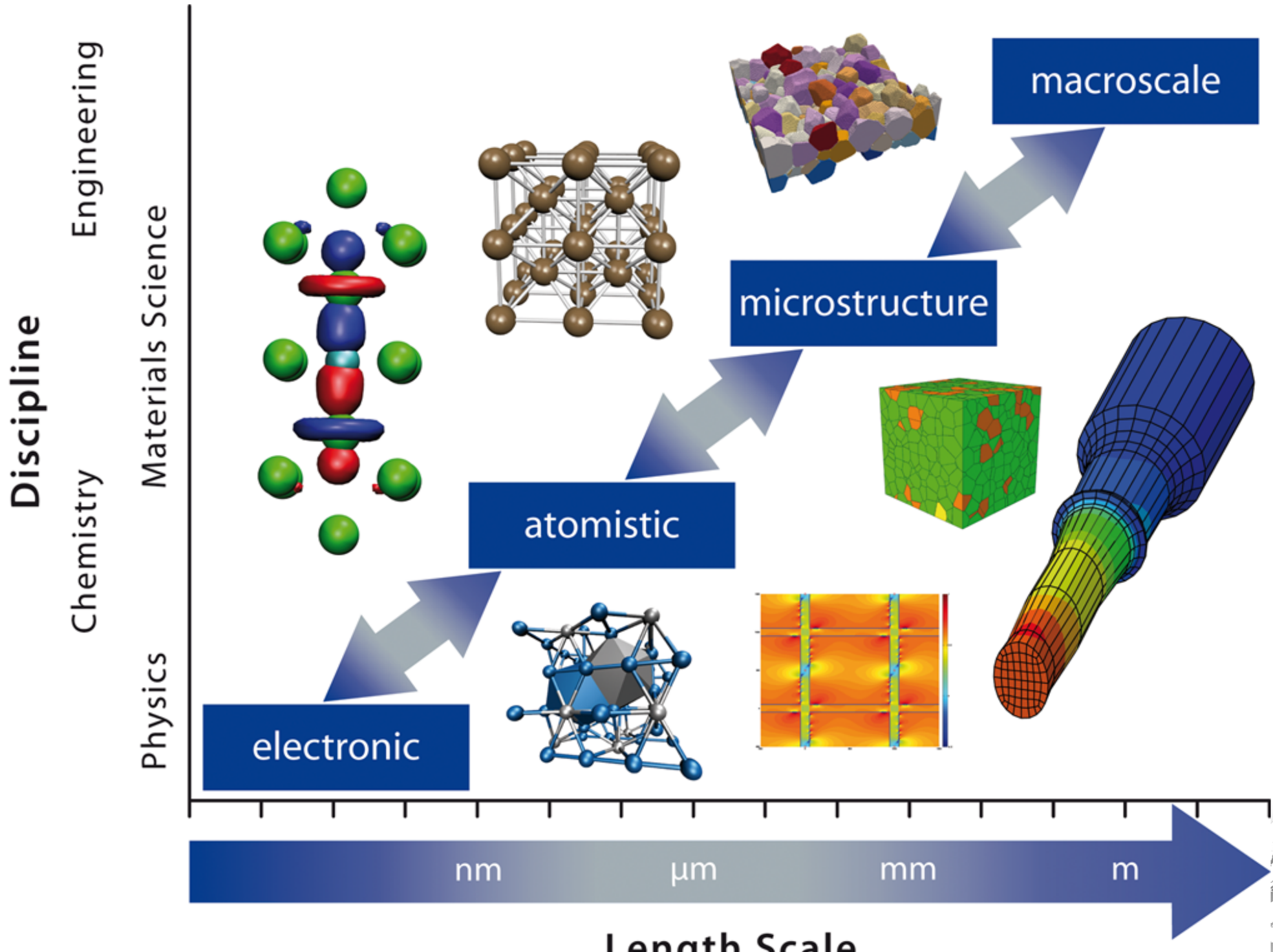
Davide Papalini

Integration across the length scales



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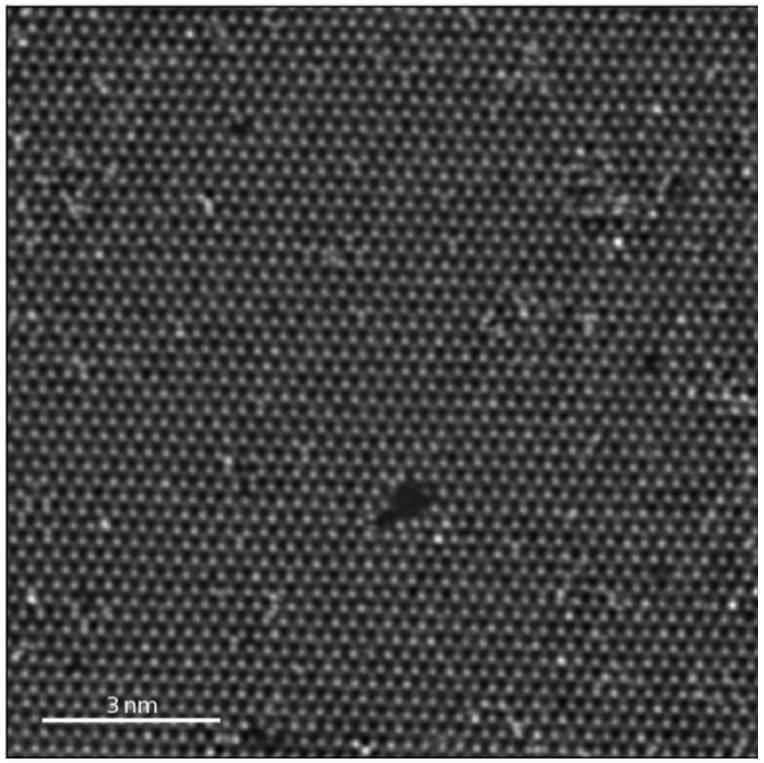
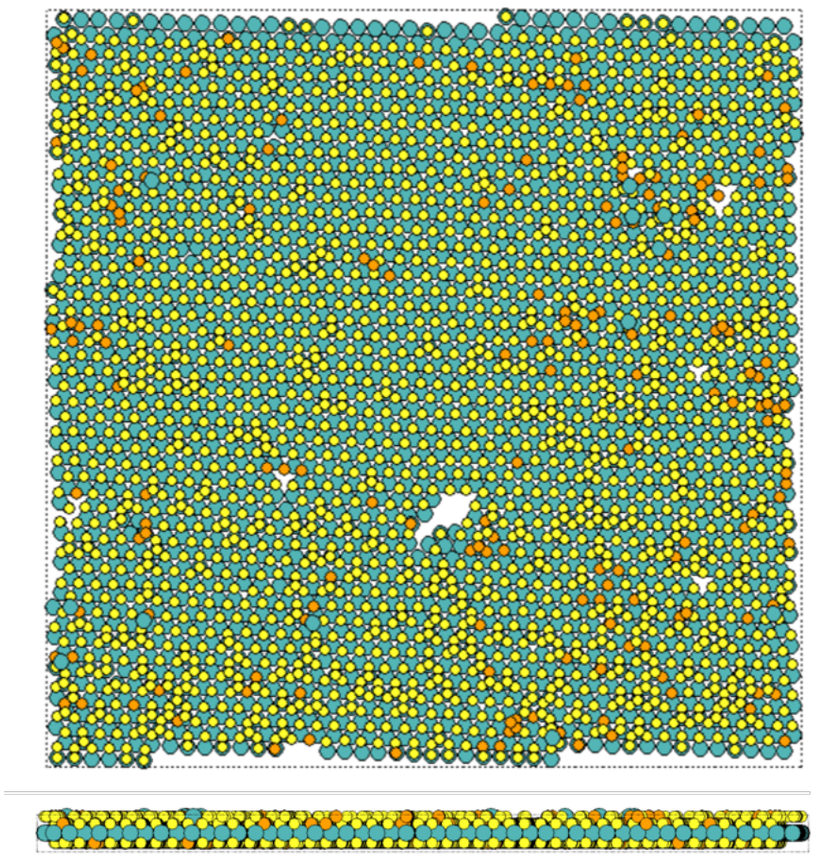
Mixing fields

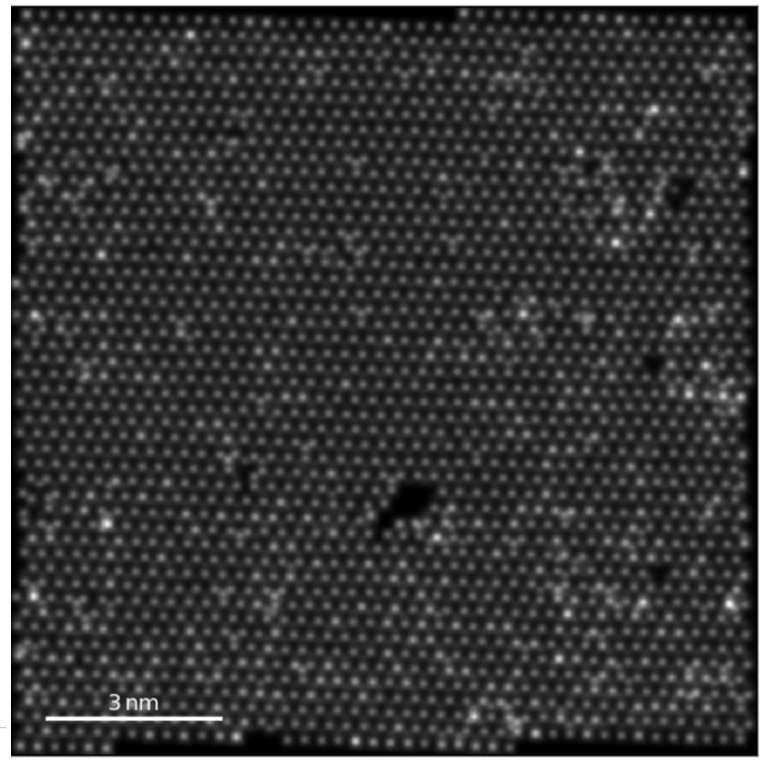
Filtered Experiment



Initial Model



Filtered Simulation



Multislice simulation

For Low Dimensional materials we can easily generate models from TEM data
Next link with simulations

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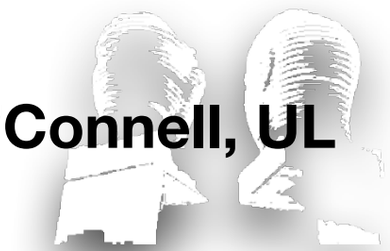
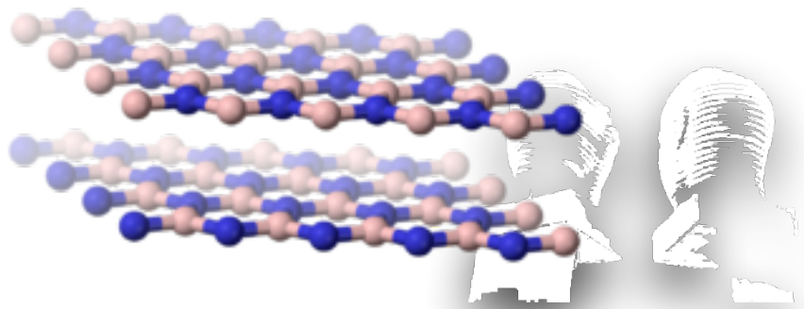
Eoghan O'Connell, UL



Proposal/Suggestion

Experimentally simulate and test a material across the length scales for a demonstration paper

Suggestion Material?
Boron Nitride
Magnesium Alloy…



Proposal/Suggestion

Experimentally simulate and test a material across the length scales for a demonstration paper

Additionally use the experience to define and refine the metadata required to make the exchange of data between experiments and simulation as smooth as possible

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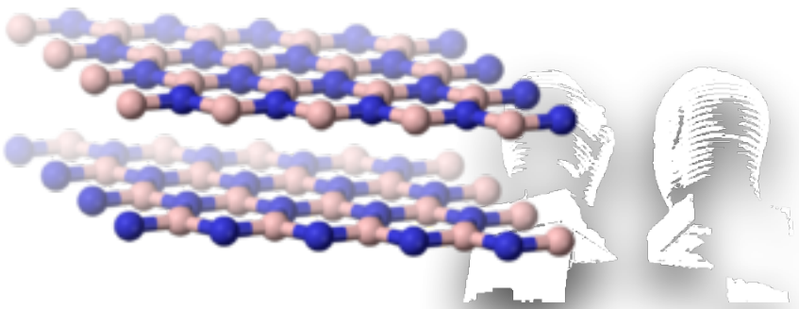
Suggestion Material?
Boron Nitride
Magnesium Alloy…



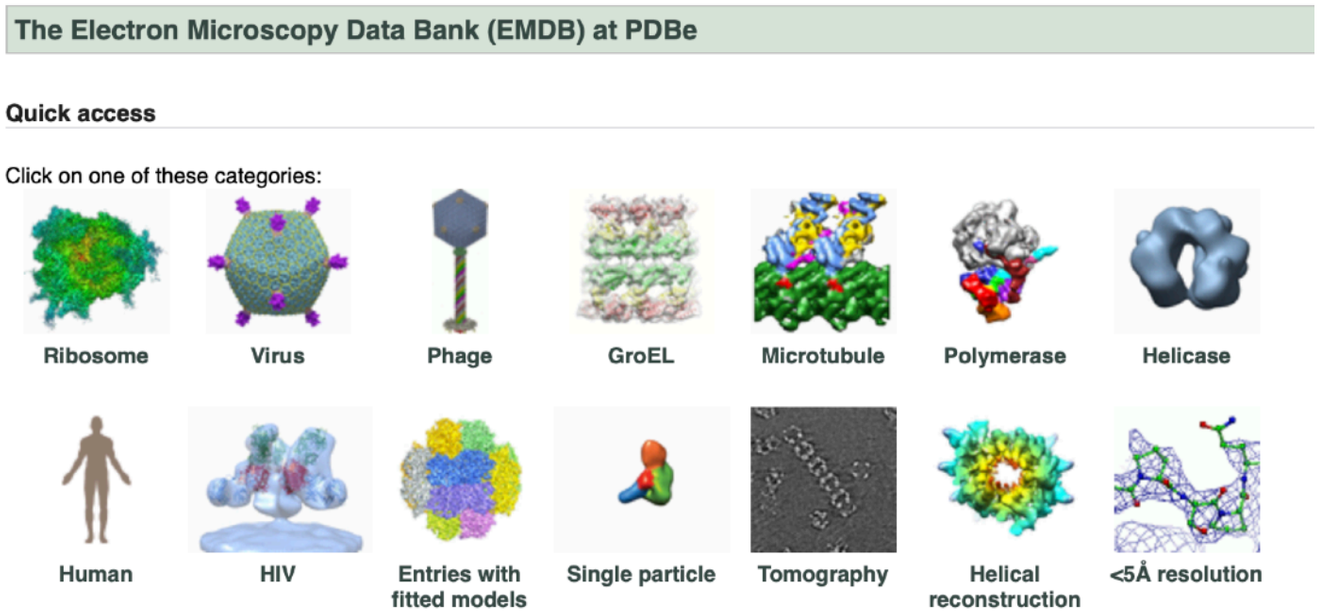
Databases

CCDC

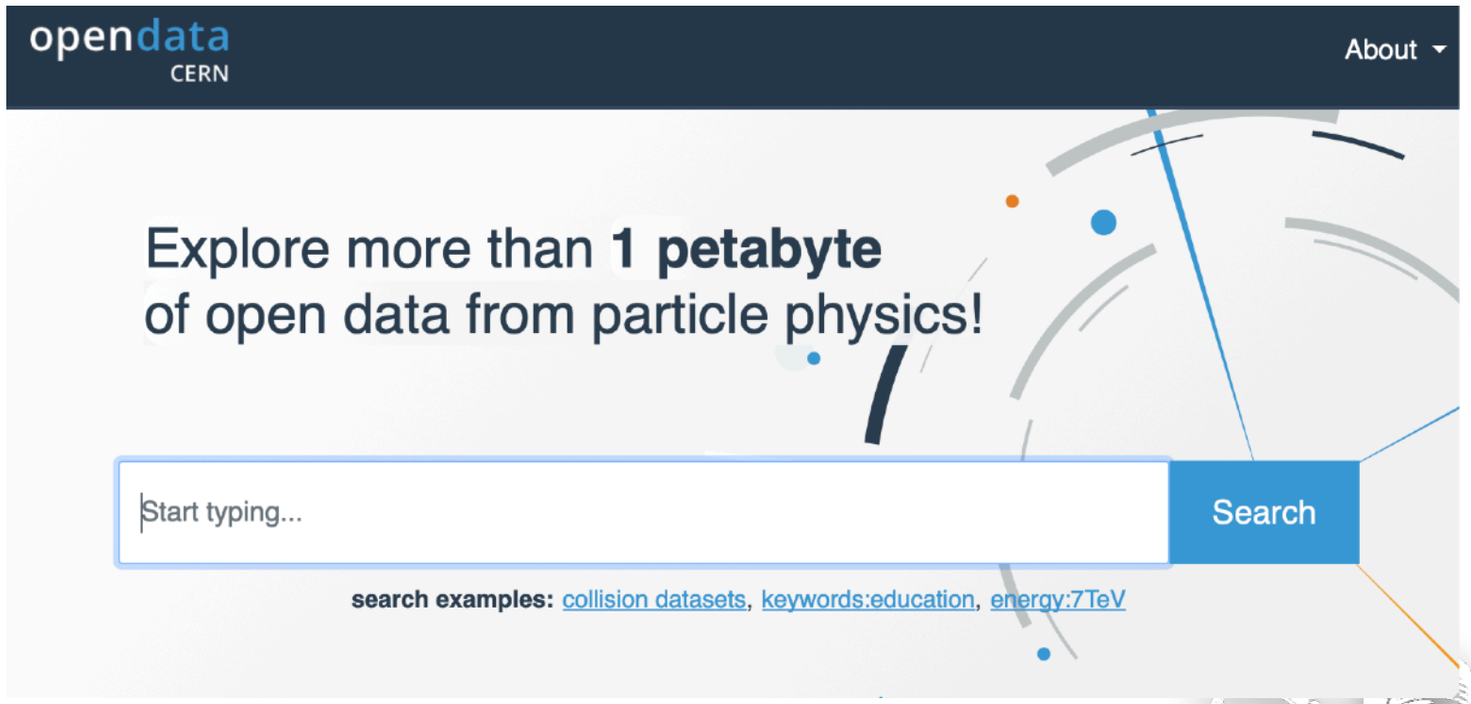
RCSB PDB PROTEIN DATA BANK

153836 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

PDB-101 | WORLDWIDE PDB PROTEIN DATA BANK | EMDataResource Unified Data Resource for 3DEM | ndb NUCLEIC ACID DATABASE | Worldwide Protein Data Bank Foundation



EMPIAR



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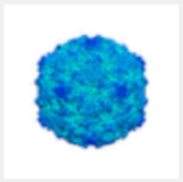
EMPIAR

Dataset	Title	Authors and references	Size	Resolution	Release date
EMPIAR-10284 	Extracellular albumin and endosomal ions prime enterovirus particles for uncoating that can be prevented by fatty acid saturation [multiple data sets in MRC format]	Domanska A, Ruokolainen VP, Pelliccia M, Laajala MA, Marjomäki VS, Butcher SJ [Pubmed: 31189702] [DOI: 10.1128/JVI.00599-19] EMD-4903, EMD-0565, 6rjf, 6o06	2.4 TB	3.5-3.6	2019-06-19
EMPIAR-10281 	Cryo electron micrographs of human cystic fibrosis transmembrane conductance regulator (CFTR) in complex with GLPG [3335 multi-frame micrographs composed of 50 frames each in TIFF format]	Zhang ZZ, Liu FL, Chen JC [Pubmed: 31221859] [DOI: 10.1126/science.aaw7611] EMD-0606, 6o1v	1.4 TB	3.2	2019-06-21
EMPIAR-10270 	Single particle reconstruction of 52 kDa biotin-bound state streptavidin at 3.2 Angstrom resolution [3309 multi-frame micrographs composed of 32 frames each in MRC format]	Fan X, Wang J, Zhang X, Yang Z, Zhang JC, Zhao L, Peng HL, Lei J, Wang HW [Pubmed: 31160591] [DOI: 10.1038/s41467-019-10368-w] EMD-0689, 6j6j	5.5 TB	3.2	2019-06-07

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Block Chain database

Caltech

Caltech Electron Tomography Database

A public repository featuring 11293 electron tomography datasets of intact bacterial and archaeal cells, representing 85 species.

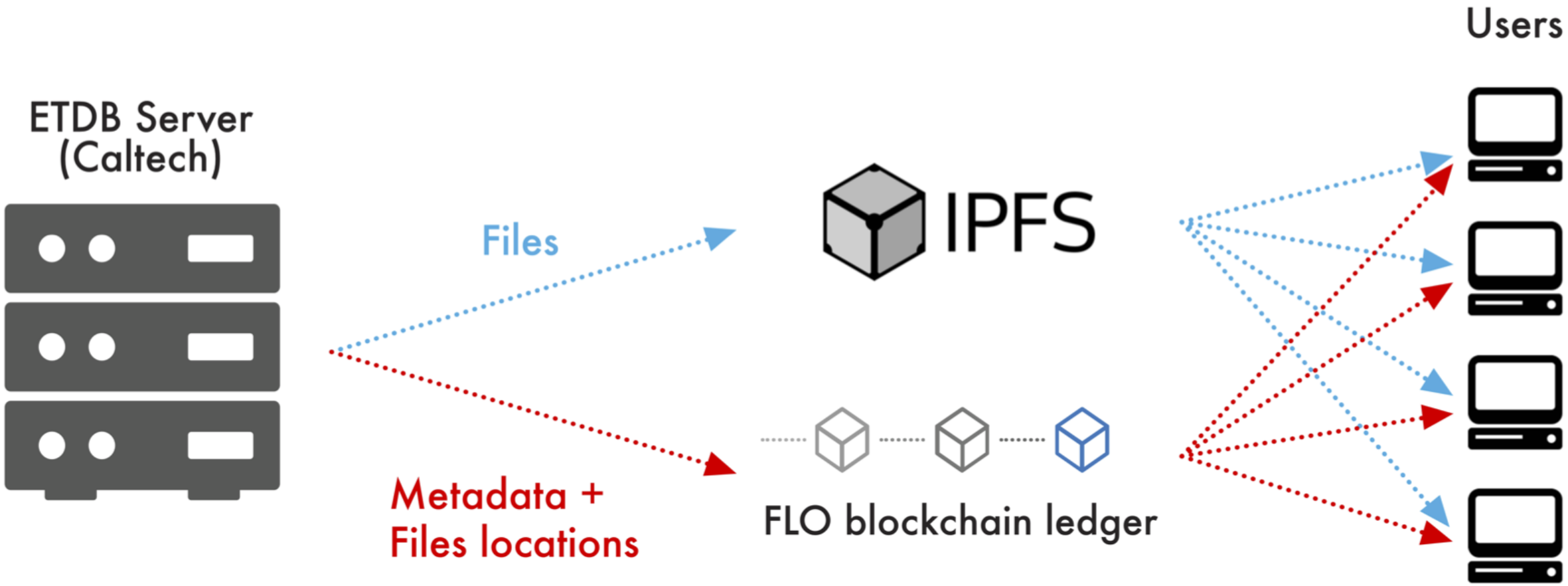
Browse database →

View our terms and conditions

>30TB of Cryo-Tomography data available, variable quality

ETDB-Caltech: A blockchain-based distributed public database for electron tomography
Davi R. Ortega, et al., PLOS ONE
https://doi.org/10.1371/journal.pone.0215531

Block Chain database



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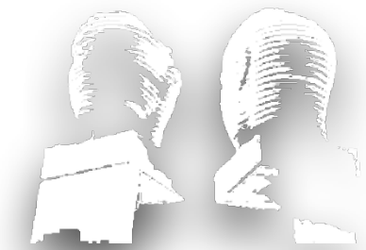
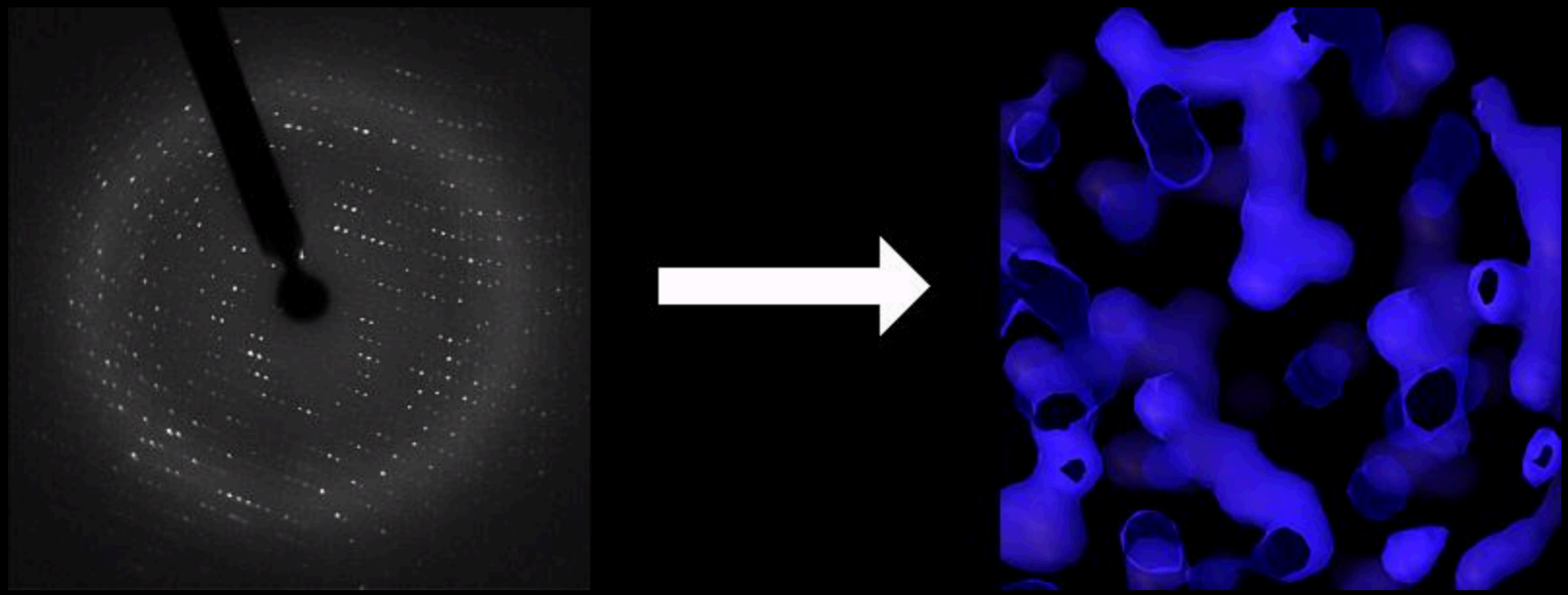


ELVES

"Because You Have Better Things To Do"™



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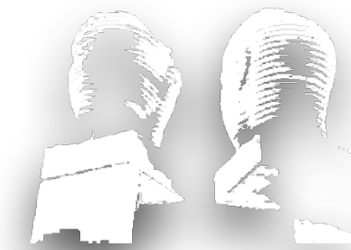
James Holten



Standard Operating Procedures

COMPLIANCE POLICY GUIDE (CPG)

Guidance for Industry, Q7A Good Manufacturing Practice Guidance for Active Pharmaceutical Ingredients

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Food and Drug Administration

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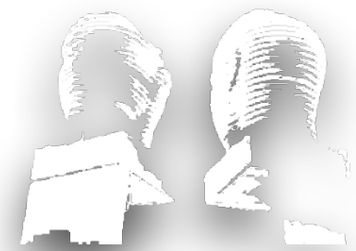

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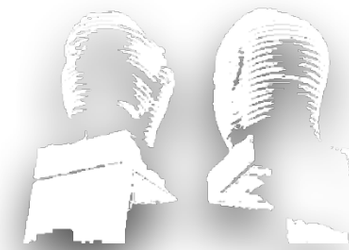

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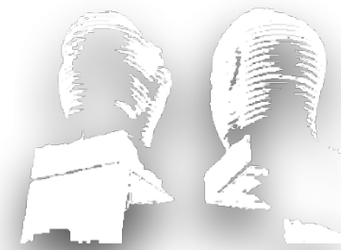

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International Metrology Institutes

European Molecular Biology Laboratory

EMBL

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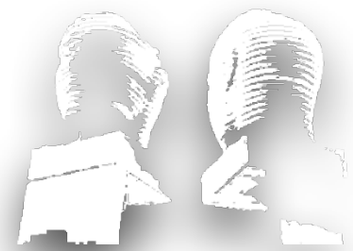

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Biology Laboratory

EM L

European Materials
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European Molecular Biology Laboratory

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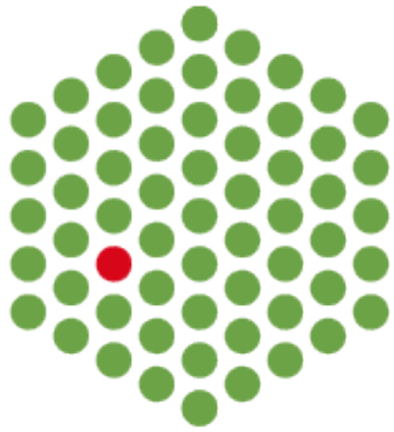
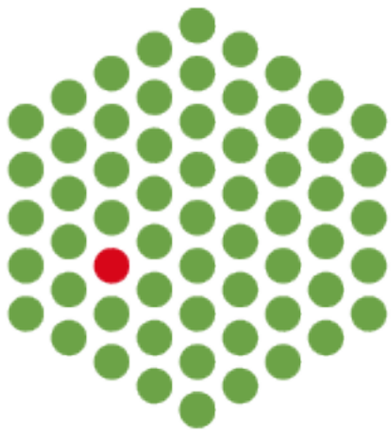


European Molecular
Biology Laboratory

CERN

EM L



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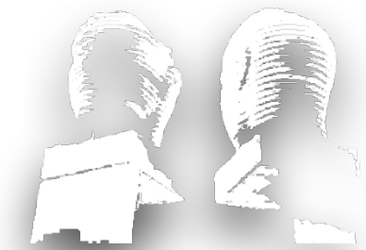

Thank you for listening

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