Karlsruhe Institute of Technology

MATTER AND TECHNOLOGIES

Big Data Applications and Challenges for Photon Science

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„Big Data“

- Expression coined by John R. Mashey
- Definition today

  Big data is a term for data sets that are so large or complex that traditional data processing applications are inadequate to deal with them. […] (Wikipedia)

J R Mashey, 1998

„Big Data is such a simple term, it's not much a claim to fame.“

- What is big?
  - 10^ 9 Giga = GB/s rate of fast detectors
  - 10^12 Tera = 10 TB size of largest harddisks
  - 10^15 Peta = ~1 PB size of photon science data
  - 10^18 Exa = 3..12 EB NSA data center Utha
  - 10^21 Zetta = capacity of harddisk world-wide

Data-Intense Applications in Photon Science and Machine Physics

- Facilities
  - PETRA3
  - XFEL
  - Acc. Test Platform ATP: ANKA, FLUTE, ..
- Data-intense methods
  - Tomography
  - Scattering
  - Electron Beam monitoring
  - …
- Detectors
  - Commercial cameras
  - X-ray detectors
  - Fast digitizers

High-speed cameras (e.g. pco.dymax)

Large-area X-ray detectors (e.g. Pilatus 6M)

Custom detectors (e.g. KAPTURE)

Detector Rates in Photon Science and Machine Physics

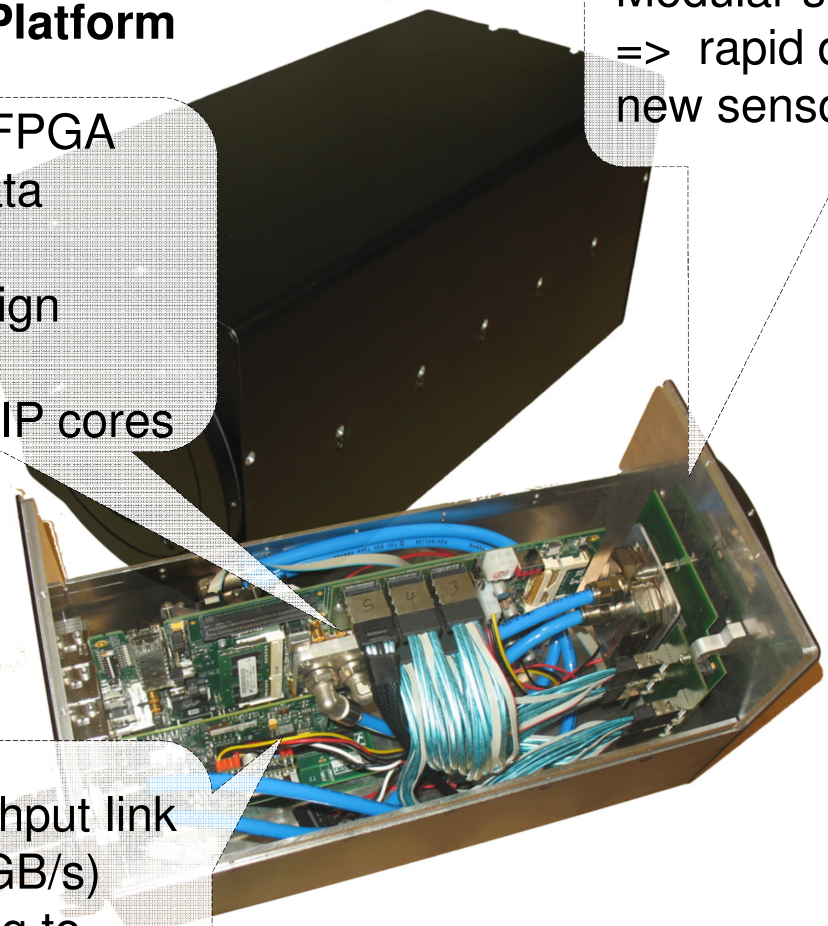
Device	Rate MB/s	Rate TB/8h	Ch.	ADC bit	Rate Hz	Beamline
"CL Base"	255	7				e.g. pco.dymax
"CL Full"	800	22	4M	16	100	e.g. pco.edge
Pilatus 6M	223	6	6M	20	10-12,5	P11
UFO Camera	1125	31	20M	12	30	P05/07
KAPTURE	3815	105	4	12+4	500M	ANKA
KAPTURE2	15259	419	4-8	12+4	1G	
KALYPSO2	4883	134	512	14	5MHz	

- CL = Camera Link
- All devices without compression

Custom DAQ Electronics

Karlsruhe Institute of Technology

UFO DAQ Platform



Embedded FPGA for online data analysis
⇒ open design
⇒ library of standard IP cores

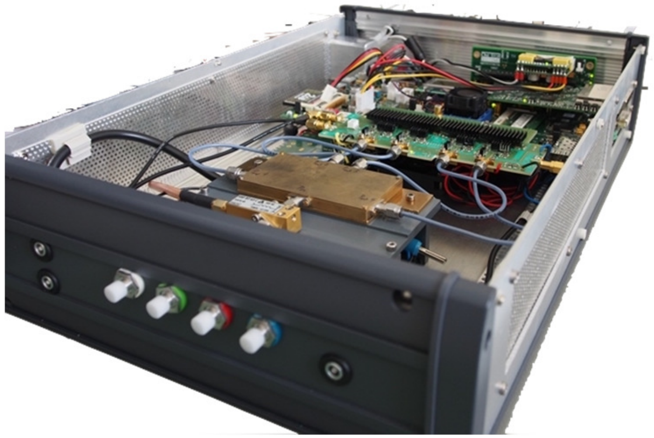
Modular sensor interface
=> rapid development for new sensors

High-throughput link (PCIe, <15GB/s)
=> streaming to GPU for processing

Applications:

Helmholtz-Zentrum Geesthacht
Centre for Materials and Coastal Research

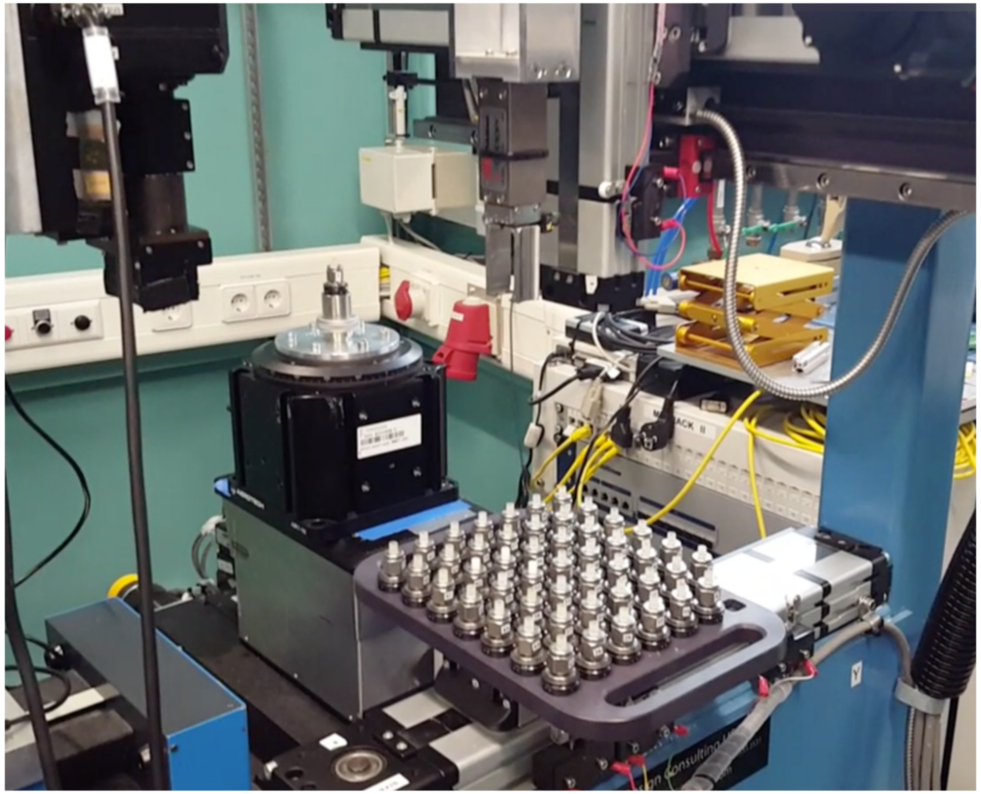
- Phase contrast tomography P05/07
- KAPTURE electron beam characterization, ATP
  see M Caselle, next session



DAQ frameworks match detector performance

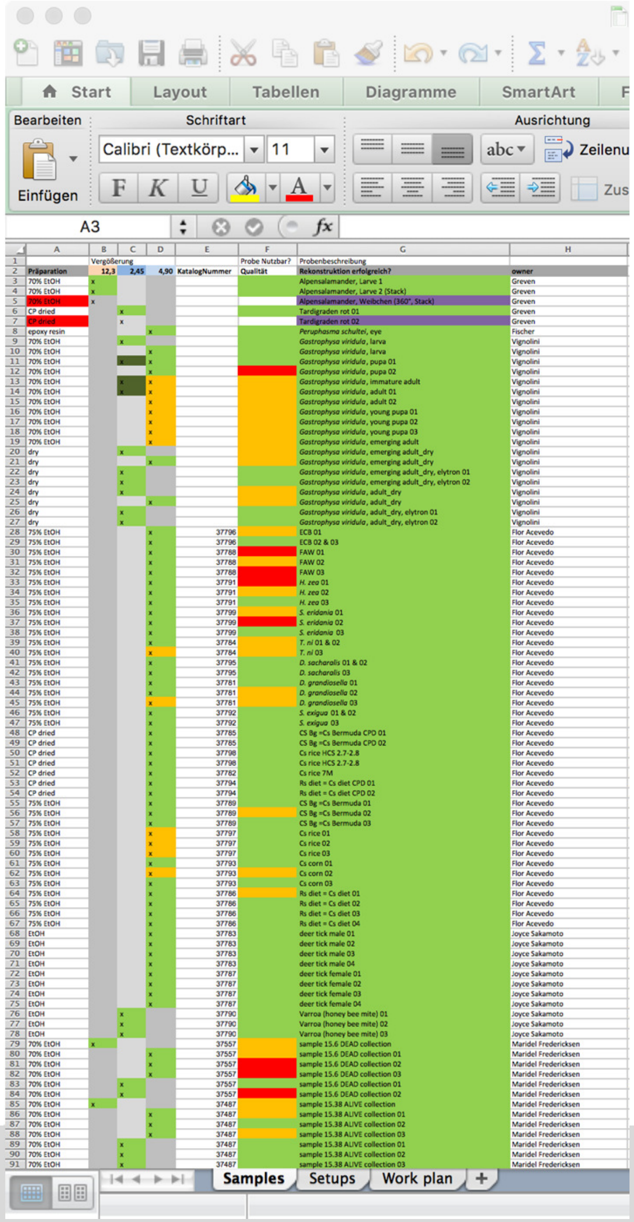
Beamline Automation

- Robots for sample changers
- Sample identification (e.g. by QR code)
- Camera revolver, lenses
- Advanced control systems



Tomography Services for Morphology

- ANKA domain expert collects samples
  - Check of sample quality
- Measurement at ANKA
  - Beamtime 6 days (e.g. Nov 2015)
  - Up to 300 samples from 14 scientists
  - Methods: Radiology, Tomography, Cine-Tomography
  - Samples: in alcohol, dried, amber, …
  - More than 90% of the samples are usefull
  - Interested scientists might join
- Datasets are automatically transfered to processing storage
  - Analysis by users

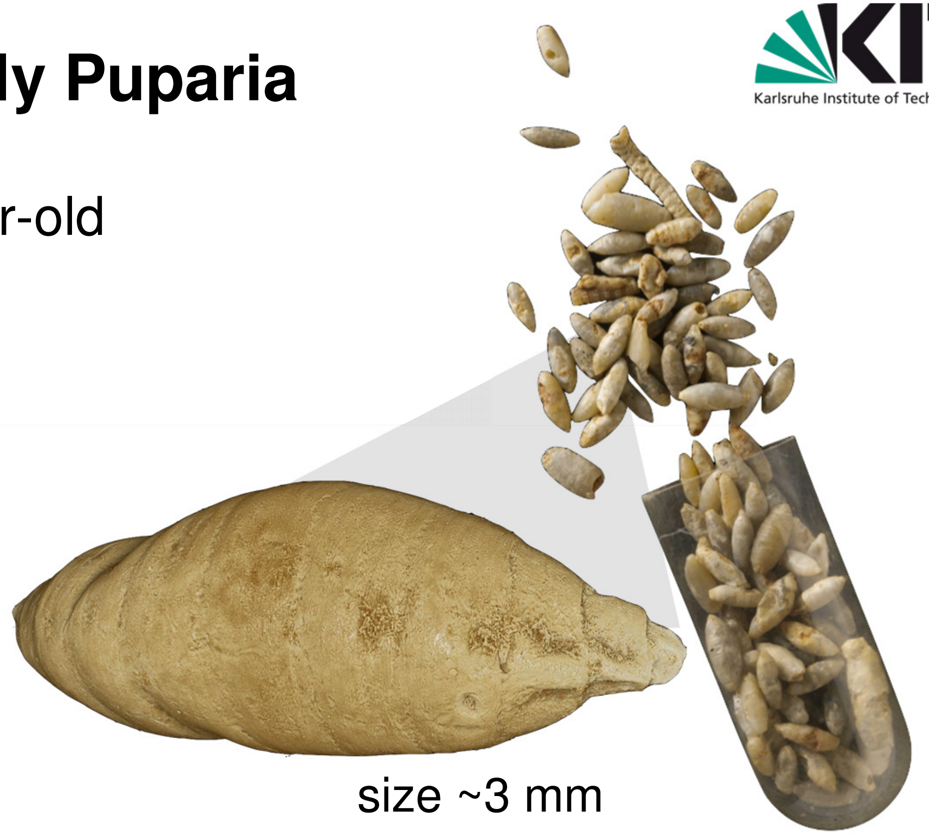


Quantitative Studies of Fly Puparia

- Digitalization of 30 million-year-old phosphatized insects
- Little-known fossil type!

Scanning:

- February 2016: 29 puparia
- August 2016: 1379 puparia



Result: 1408 scanned puparia!

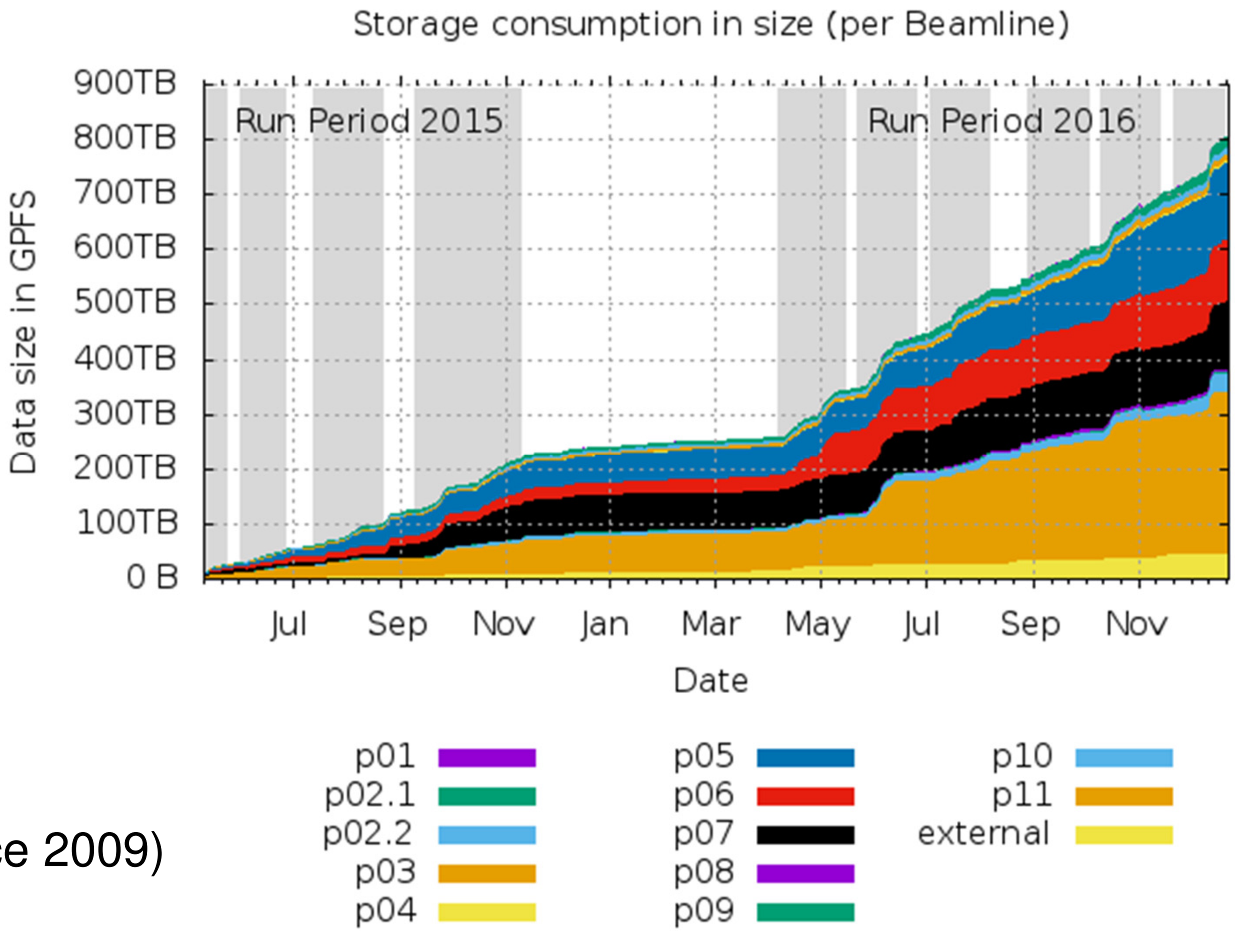
Datasets: ~60 TB

Automation enables quantitative studies

"Real-life" Data Rates

PETRA3 storage system

- PETRA3
  - Total 800 TB
  - Mean 500 TB/a
  - Max 750 TB/a



for comparison

- ANKA
  - Total 800 TB (since 2009)
  - Mean 150 TB/a

source: DESY IT

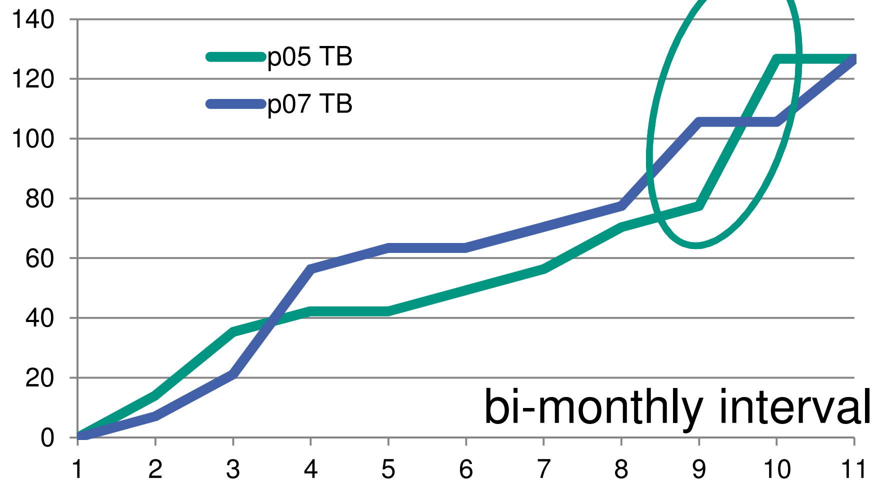
“Real-life” Data Rates (details)

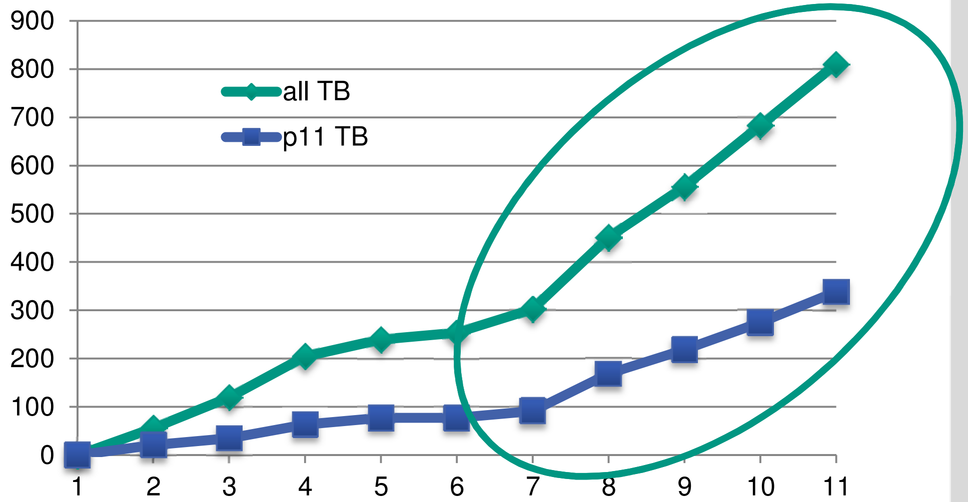
PETRA3

- Tomography (P05/P07)
  - Mean 75 TB/a
  - Max 300 TB/a (eq. 75h op)

- Imaging / Diffraction (P11)
  - Mean 200 TB/a
  - Max   370 TB/a (eq. 500h op)

extracted from previous chart



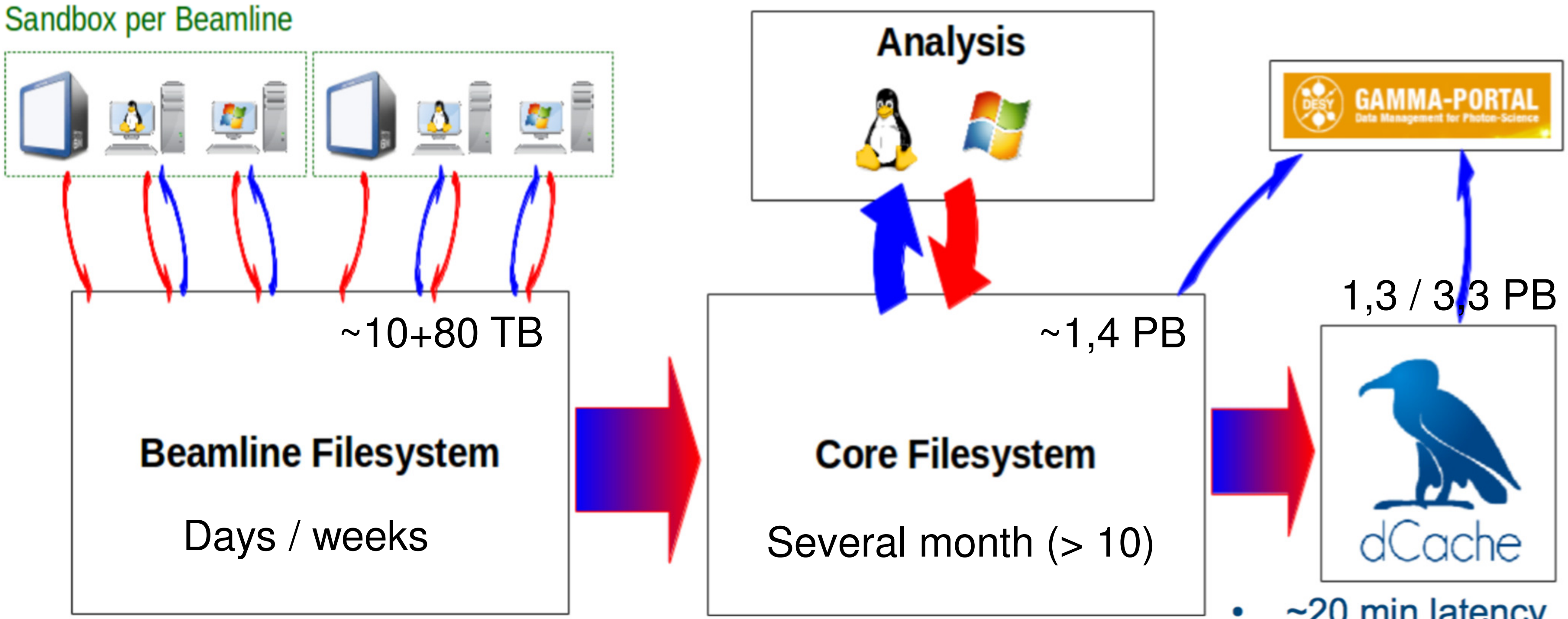


ANKA

- Tomography (TopoTomo)
  - Mean   40 TB/a (eq. 42h op.)
- KAPTURE
  - Mean   10 TB/a (eq. 1h op.)

Data Taking Petra3

Logical Dataflow



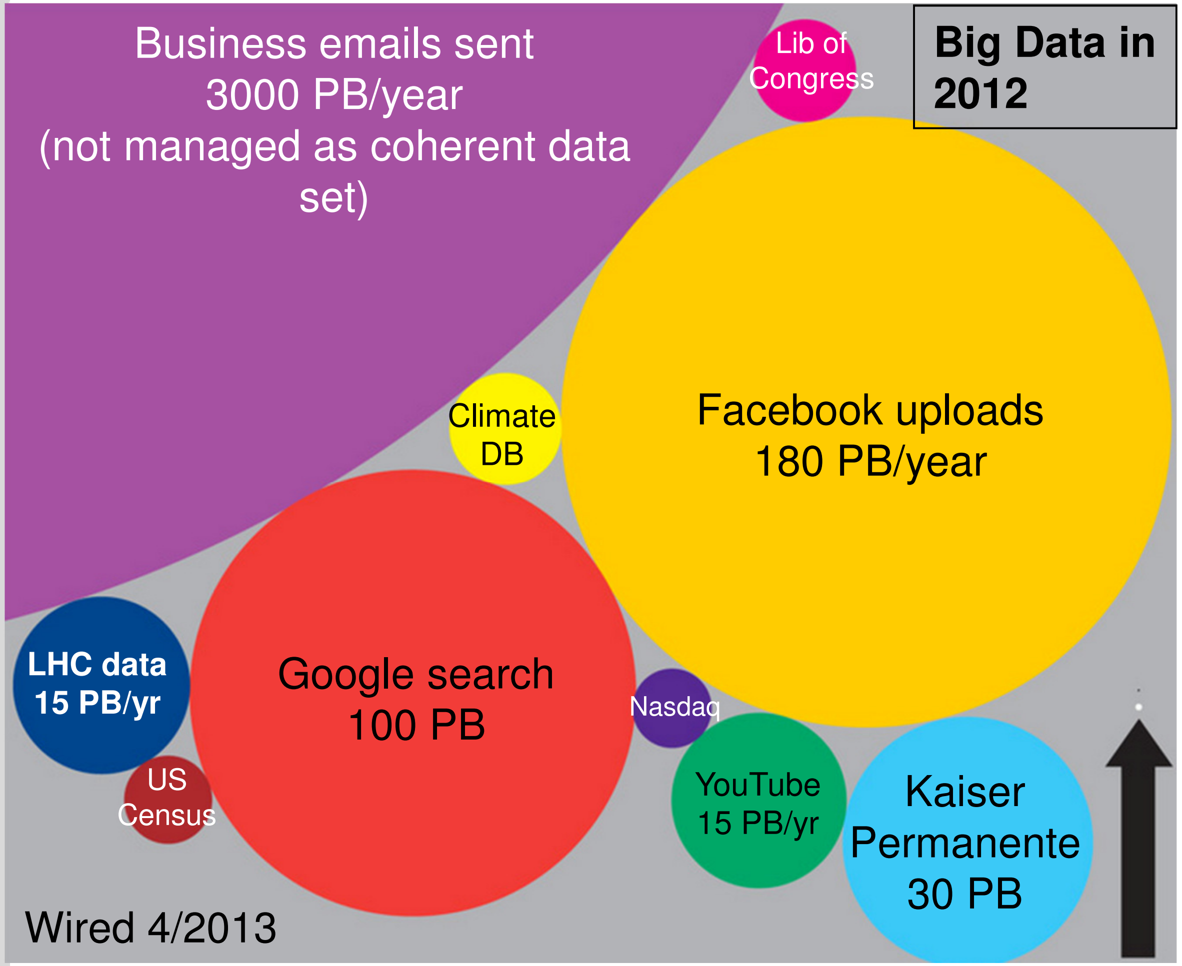
- ~20 min latency
- Very high capacity, tape

- Low latency
- Low capacity

- 4 min latency
- High capacity

Online Processing | **Data Analysis** | **Archive**

Digital Data World-wide



http://www.wired.com/magazine/2013/04/bigdata/

- Commercial services approach Exascale level
- NSA Data Center Utah 3-12 Exabytes
- Helmholtz Data Federation aims for Exascale storage

- IPhones Q1 2017: 78,3M -> 5 EB SSD
- Harddisk Q3/2016: 100M -> 800 EB over 3 years: 7500 EB

Data Challenges:
1. Reduce Data as Early as Possible

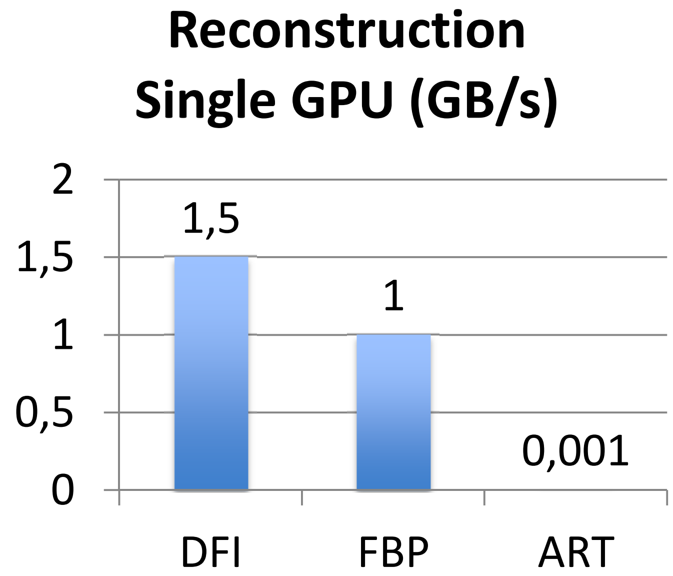
- Adopt pre-processing, reconstruction to detector rates
- Avoid user interaction, define workflows
- Make use of trigger to filter relevant data
- Assess quality of data

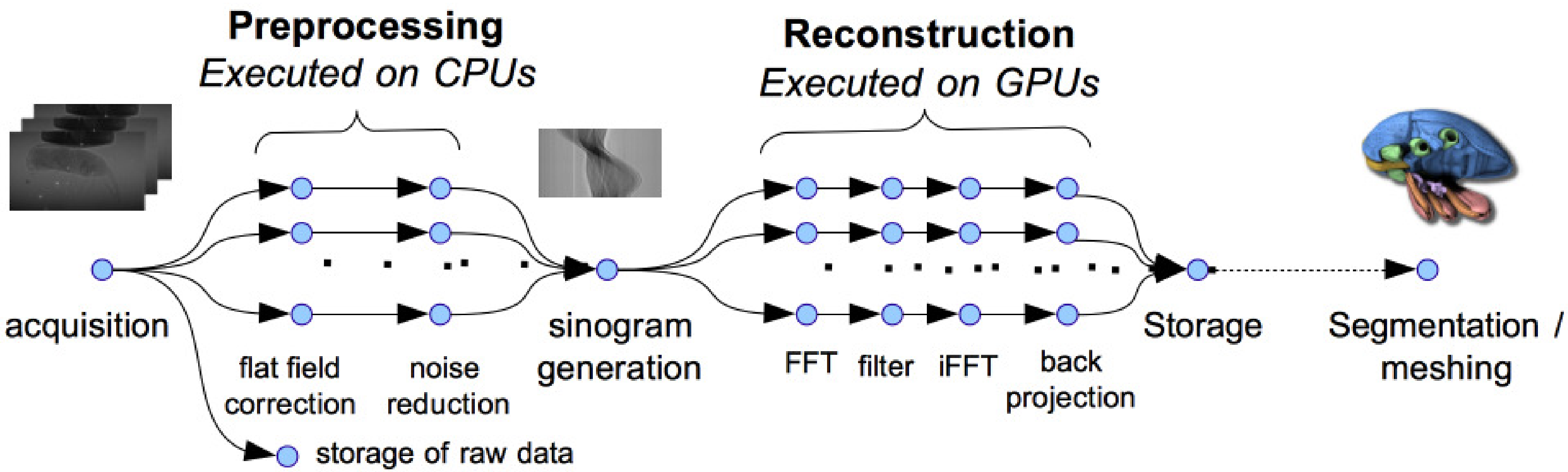
- Heterogeneous FGPA-GPU computing is very powerful
- But tasks are often domain specific

- Solution:
  Modularity and frameworks with core functionality

Tools for GPU Computing: The UFO Parallel Processing Framework

- **Free and open-source**
- Supports OpenCL parallel hardware
- **Remote DMA access to FPGA electronics**
- Fast pipelined architecture
- Scheduling across multiple devices and nodes
- Introspection interface to Python and other scripting languages
- Integrated in control systems





2. Adopt Analysis for Large Datasets

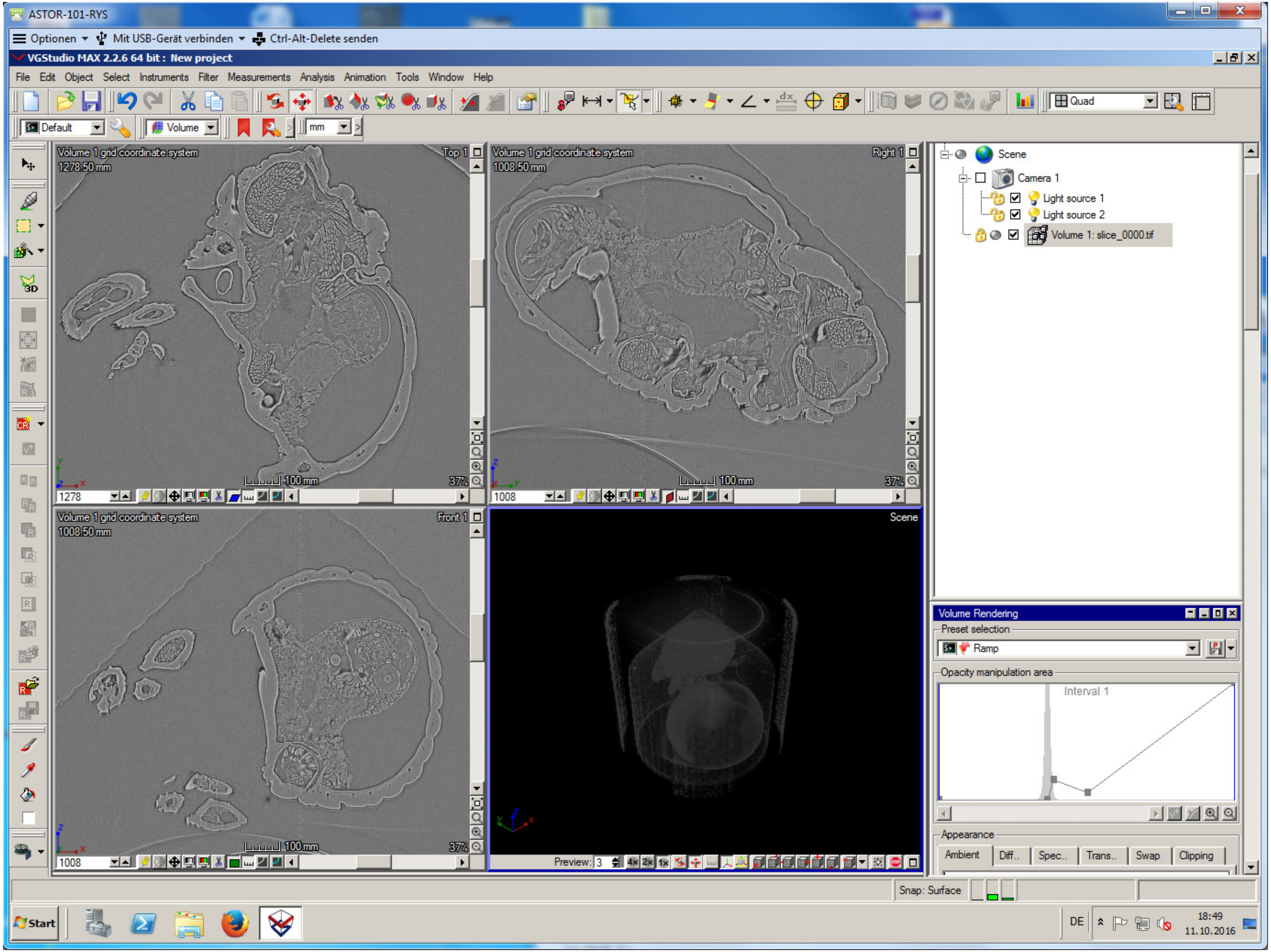
- Huge amount of data
  - User often do not have the necessary resources (computers, memory, software) available in order to process the tomograms at their home institutions

Verbundforschung:

astor --> nova

- Data analysis is still very time-consuming
  - Segmentation of tomographic datasets is usually done manually

- Solutions:
  - Establish analysis centers at the facilities
  - Involve more scientists by collaborative analysis and open data
  - Re-evaluate known algorithms with recent computing performance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VGStudio MAX 2.2.6 64 bit : New project
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Quad
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1008.50 mm
Right 1
100 mm
37%
1008
Volume 1 grid coordinate system
1008.50 mm
Front 1
100 mm
37%
1008
Scene
Preview: 3
Scene
Camera 1
Light source 1
Light source 2
Volume 1: slice_0000.tif
Volume Rendering
Preset selection
Ramp
Opacity manipulation area
Interval 1
Appearance
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Trans..
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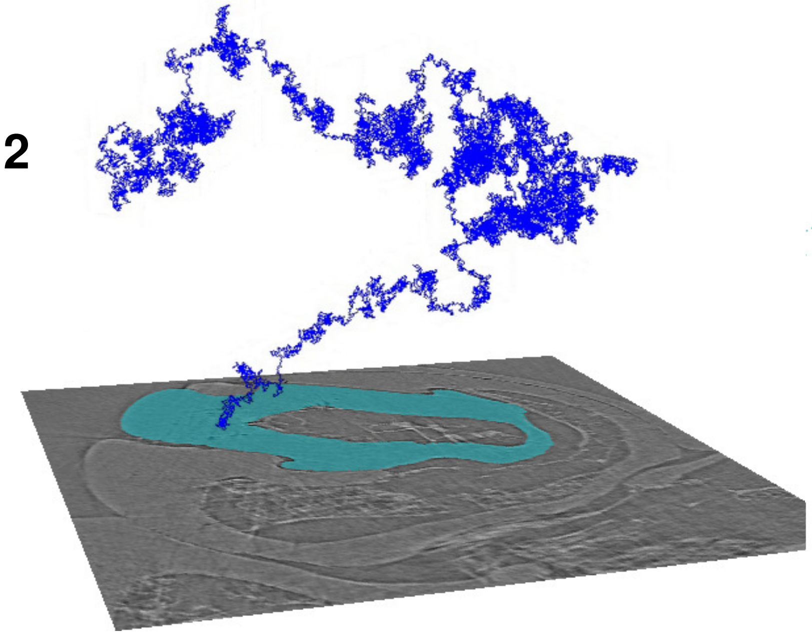
3D Segmentation Algorithms

- Algorithm – *requires performance of GPUs*
  1. Preprocess: Label the segments in some well chosen slices.
  2. Start a great number of weighted random walks at each labeled pixel.
  3. The number of hits by random walks which were started in the same segment leads to the probability that a voxel belongs to this segment.
  4. Postprocessing using Active Contour Method in 3D.

2



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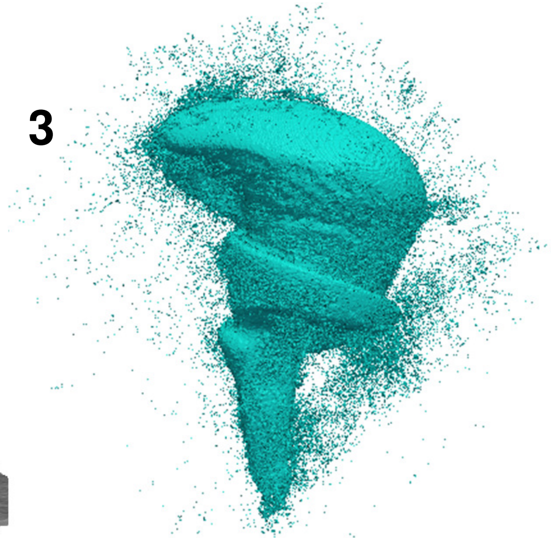

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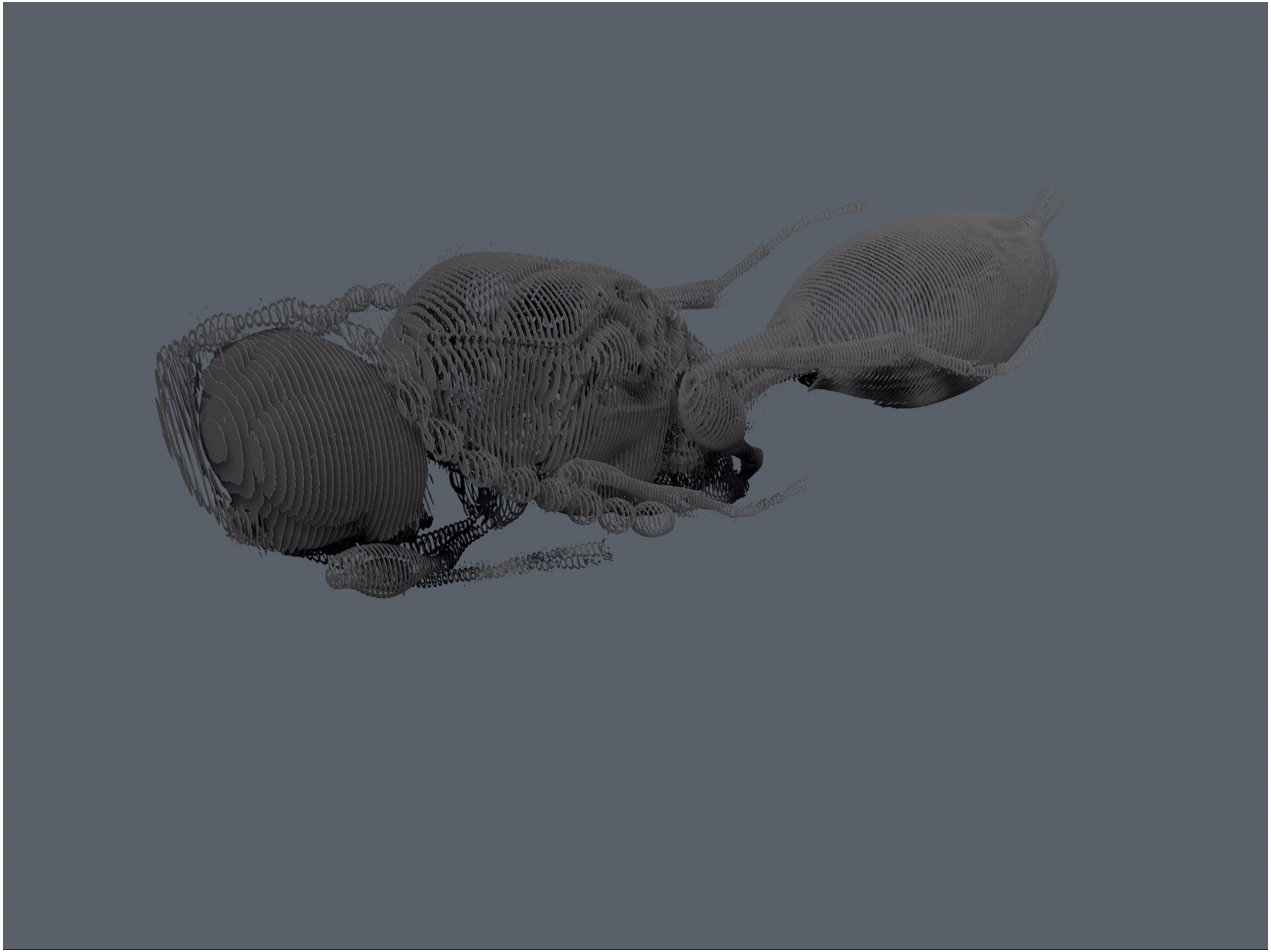
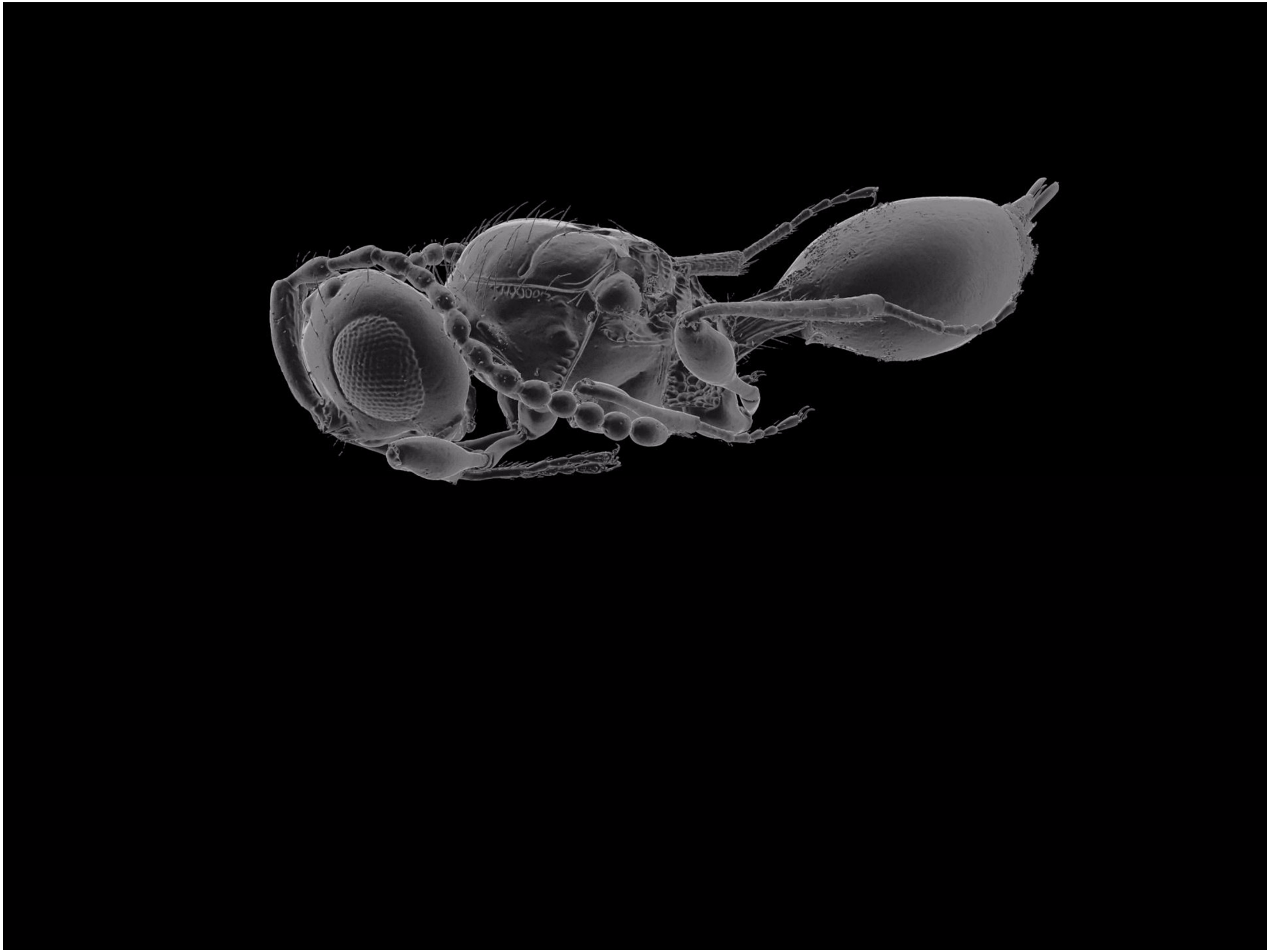
P Lösel, V Heuveline, SPIE 2016, Paper 9784-92



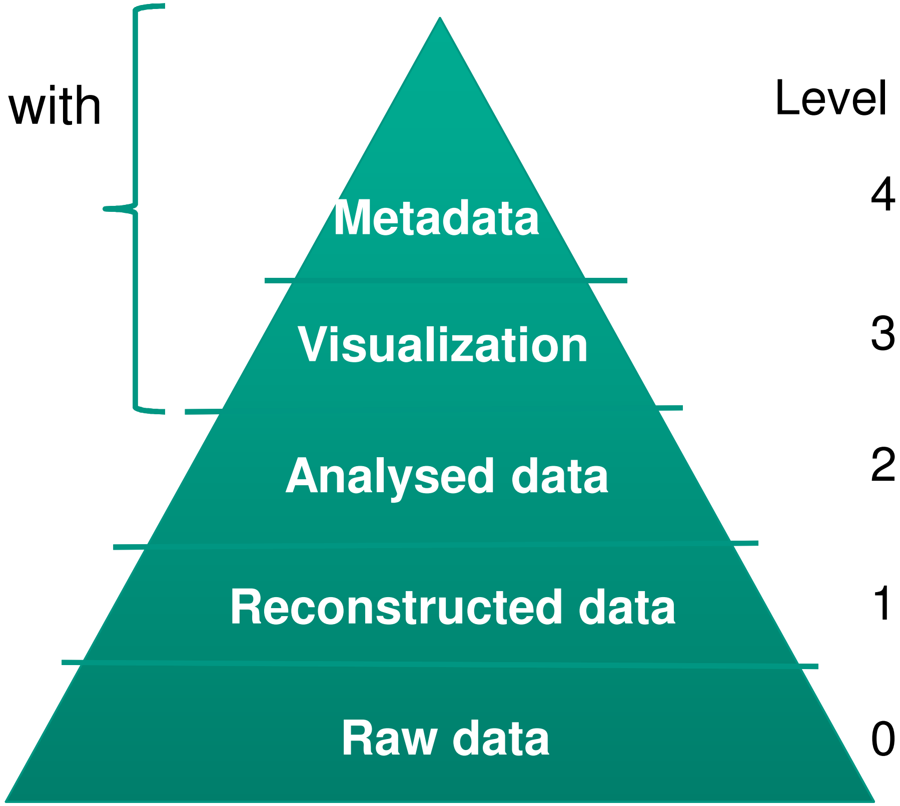


3. Hierarchical Organization of Datasets

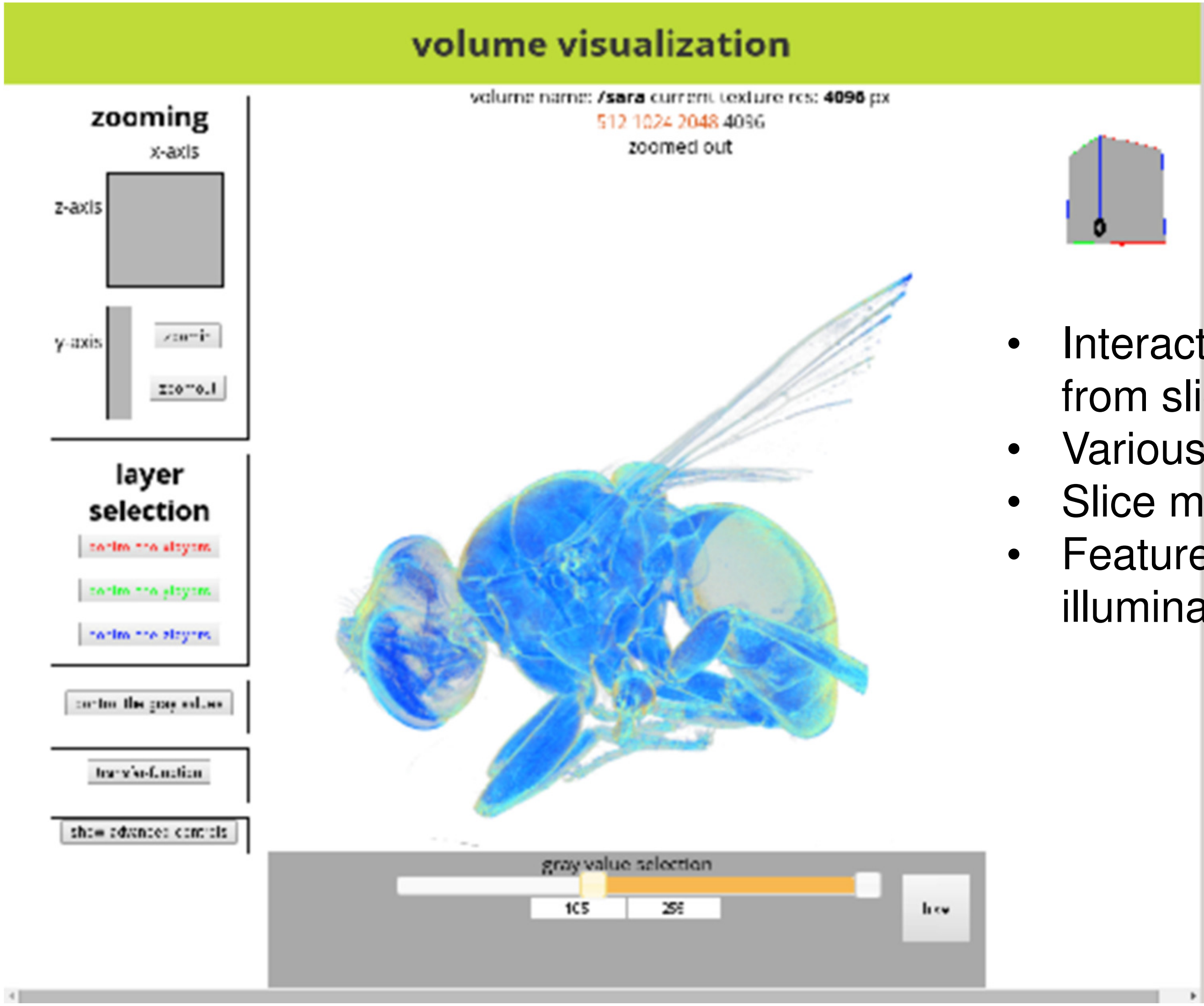
- **Long-term archive have long access times**
- Organize large dataset in levels with decreasing size is needed
- Only metadata is available in data catalogs

Solution:

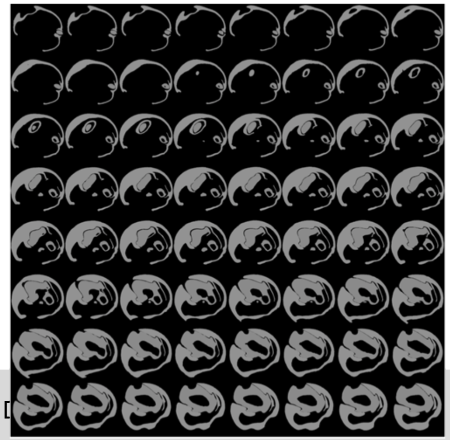
- **Extend classical metadata by visualization data**
- **Develop 3D-visualization for data catalogs**



WAVE - 3D Web-Visualization



- Interactive 3D visualization from slice maps
- Various levels of resolution
- Slice maps
- Features: cuts, thresholds, illumination models , …



Conclusion

- Data rates will reach 1PB/a soon
- Exascale data center will come
- Still datasets will have different access times

If you really care for your data, organize it properly!

  - Online data assessment
  - Improve Analysis methods for large datasets
  - Scalable data formats with extended metadata
    + scalable visualization

Solutions might not appear automatically
by generic "Big Data" research