

New data-intensive experiments and scientific opportunities for x-ray micro-tomography

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APS X-ray Science Division



Outline

From high throughput to real-time micro tomography

- Static to dynamic samples

Computing Challenges

- Large volume data handling
- Real time data analysis
- Data distribution

Data exchange solution

- Meta data information
- Data Provenance

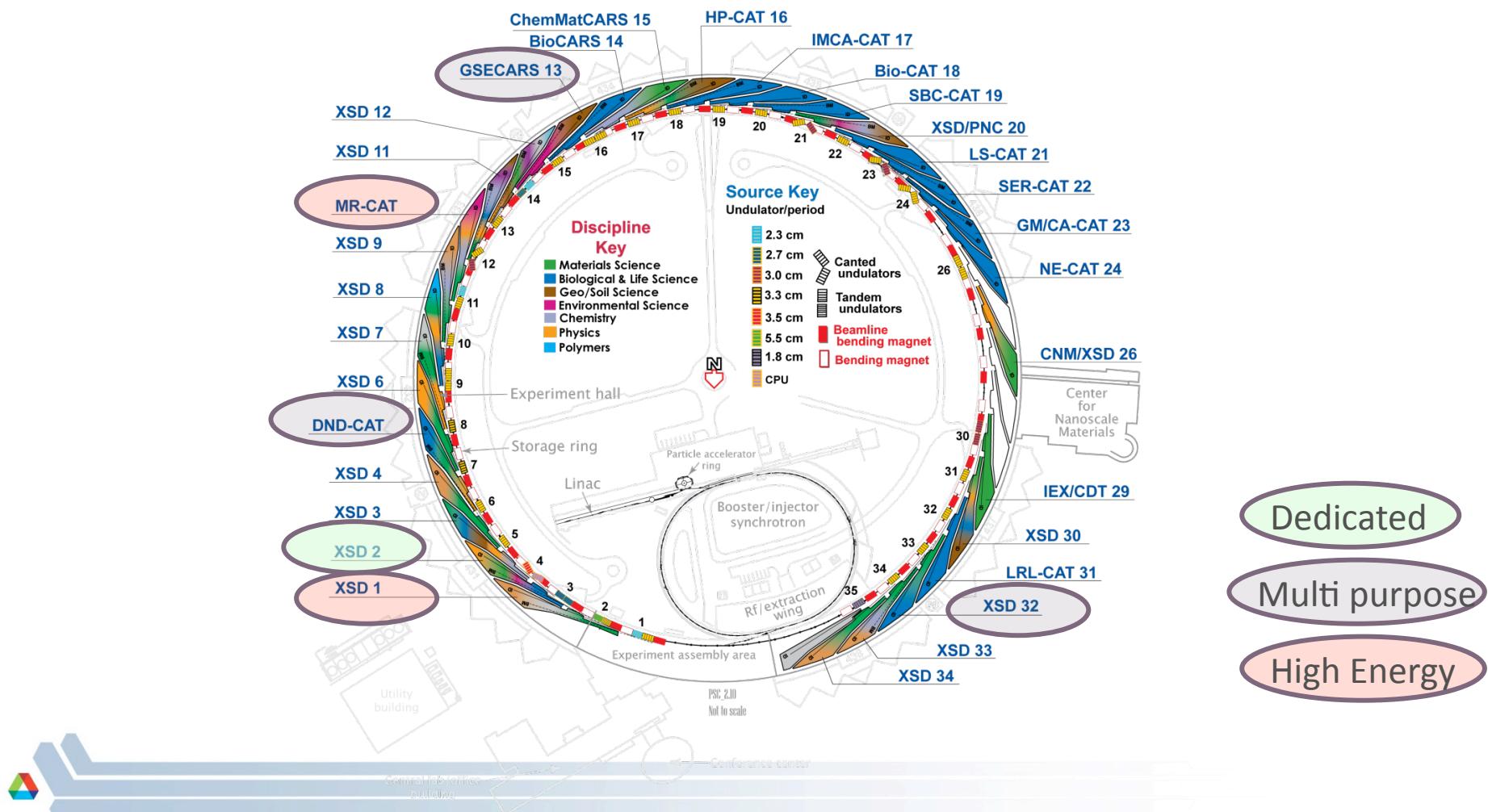
Outlook

- Multiscale and multi technique data integration



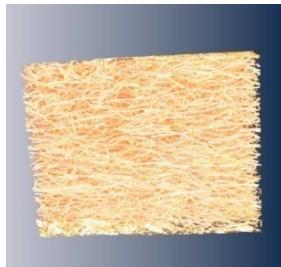
Micro Tomography at the APS

| | |
|-------|--|
| 2-BM | 5-33 keV, 25 x 4 mm ² , Dedicated tomography |
| 13-BM | 7-70 keV, 50 x 4 mm ² , Multipurpose for geosciences |
| 32-ID | 8-35 keV, 2 x 1 mm ² , Multipurpose phase-contrast imaging |
| 5-BM | 10-42 keV, 30 x 2 mm ² , Multipurpose (materials, polymers) |

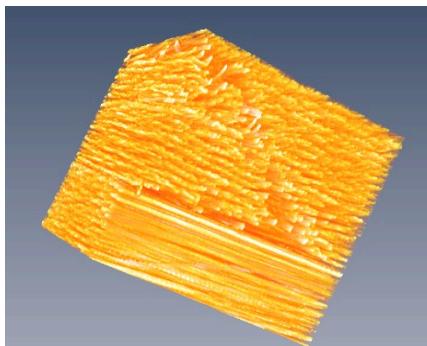


Micro Tomography of Static Samples

High throughput fully automated 1µm resolution tomography



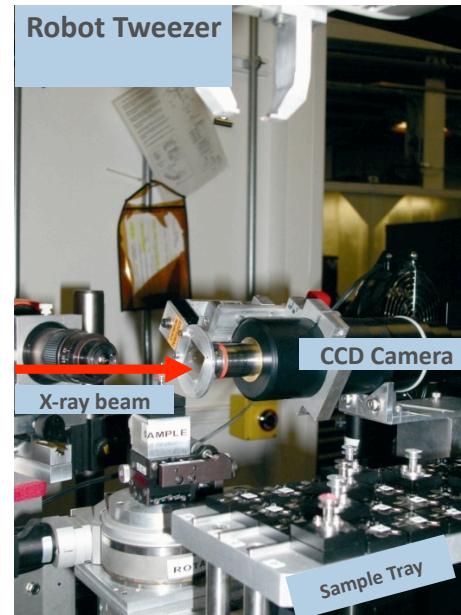
New Reusable Solid Rocket Motors
Insulation



Self healing composite - healing
efficiency

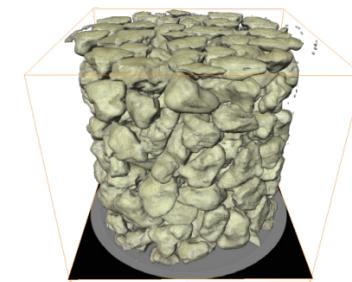


Ceramic coating layers

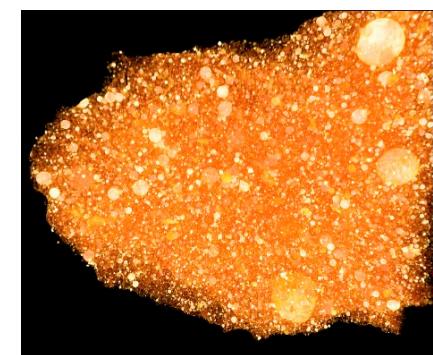


2-BM:

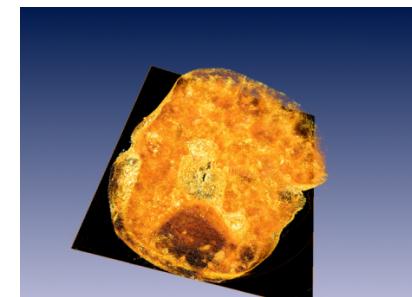
- Dedicated to micro-tomography
- Fully automated
- High throughput (>100 samples/day)
- Real time data analysis



Mechanical behavior of sand
under compression



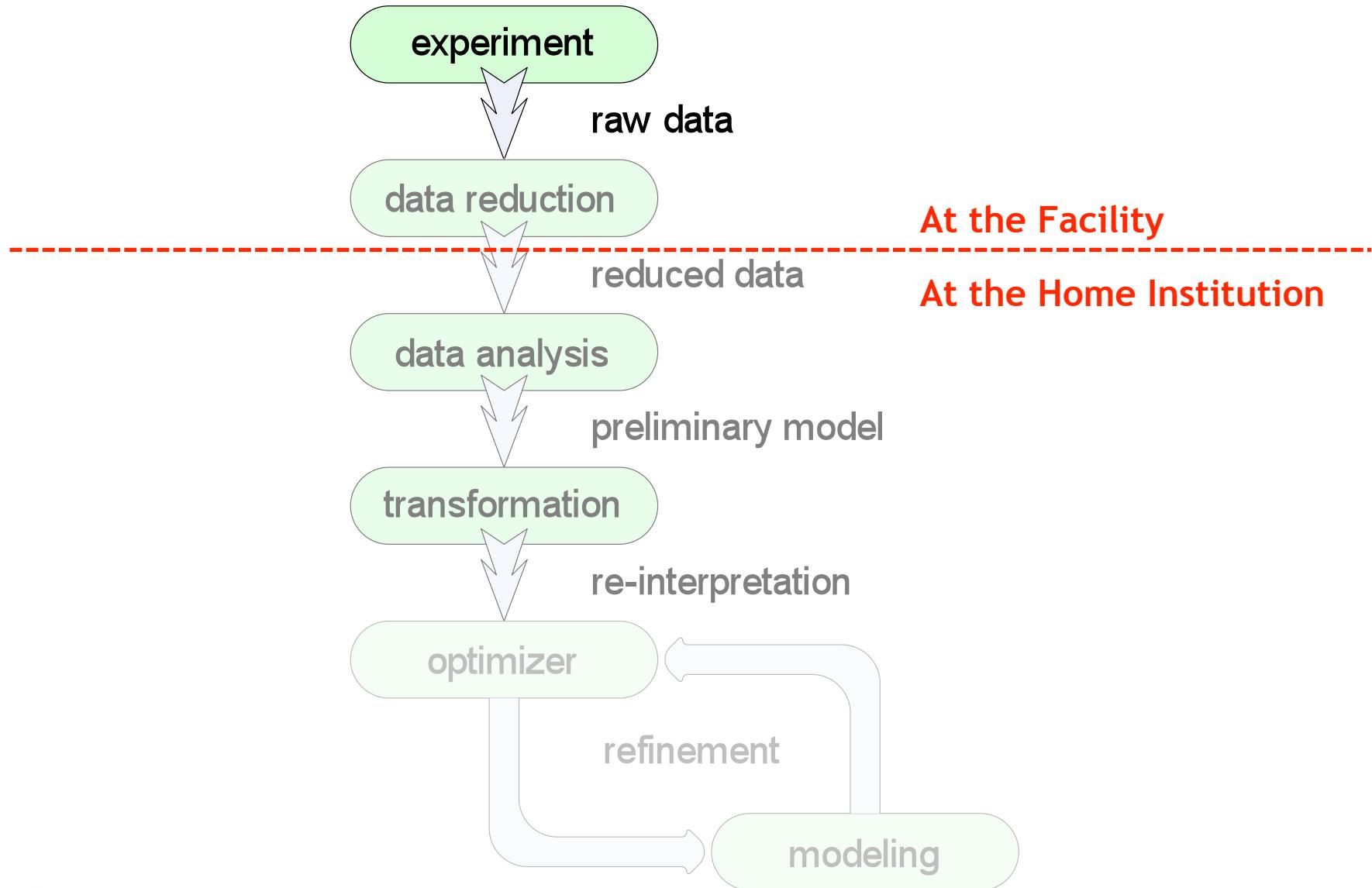
Geopolymers



Highly Explosive Materials
(PBX-9501) Modeling

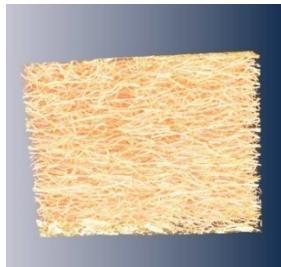


Traditional Operational Workflow

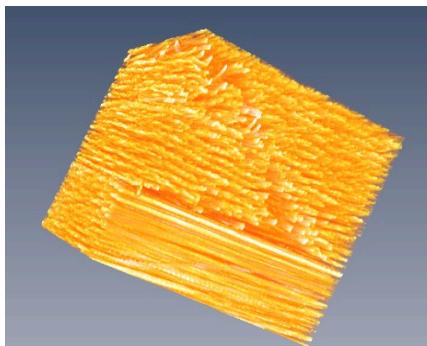


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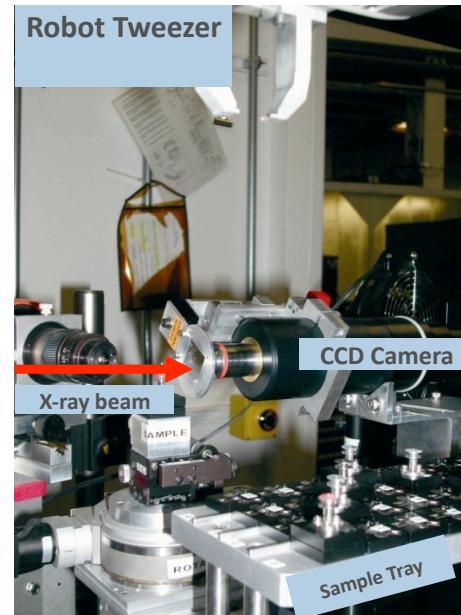
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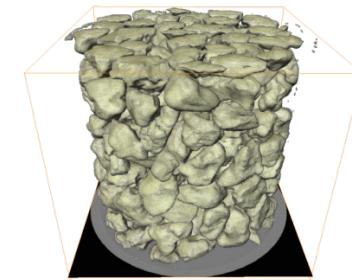


Ceramic coating layers

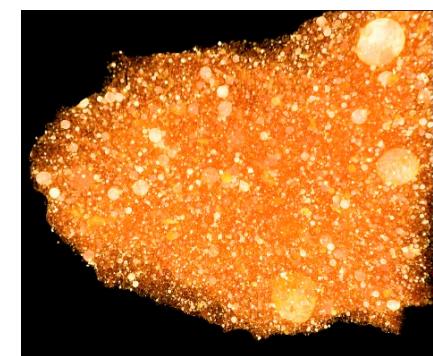


2-BM:

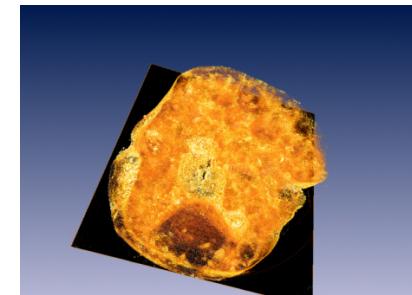
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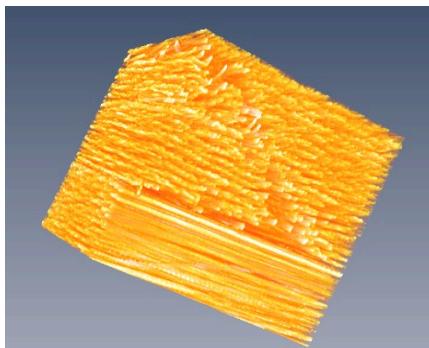


Micro Tomography of Static Samples

High throughput fully automated 1 μm resolution tomography



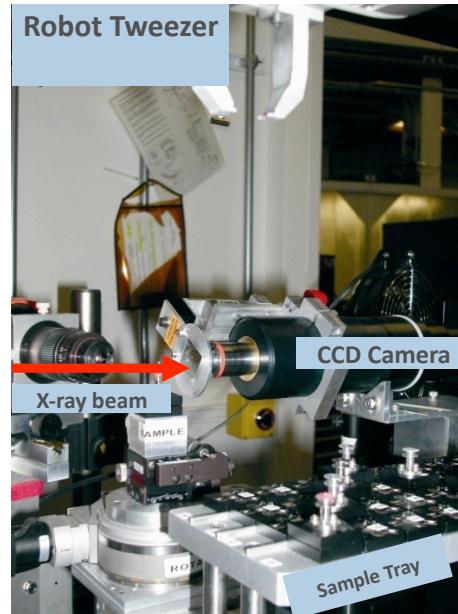
New Reusable Solid Rocket Motors
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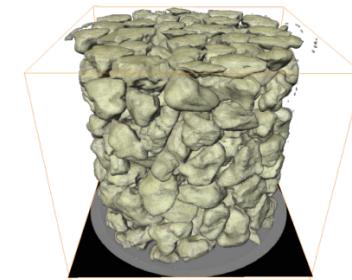


Data handled per sample (every ~ 17 min)

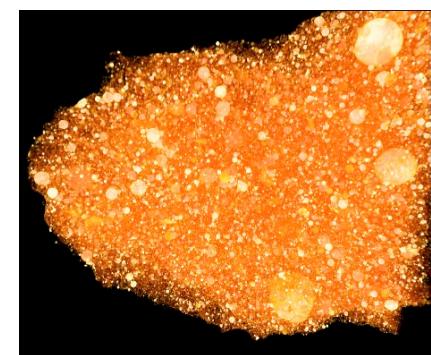
| | Pixels | Size |
|-----------------------|-----------------------|-------------|
| CCD single projection | 2,024 x 2,048 | 8.00 Mbyte |
| Raw data set | 2,024 x 2,048 x 1,440 | 11.25 Gbyte |
| Normalized | 2,024 x 2,048 x 1,440 | 22.50 Gbyte |
| Reconstructed | 2,024 x 2,048 x 2,048 | 32.00 Gbyte |
| | Total | 65.76 Gbyte |

Current CCD technology

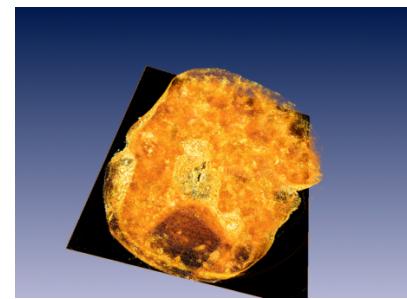
| | | |
|---------------------------|-----|--------|
| Data Processed | 5.4 | TB/day |
| Data distributed to users | 3.6 | TB/day |



Mechanical behavior of sand
under compression



Geopolymers



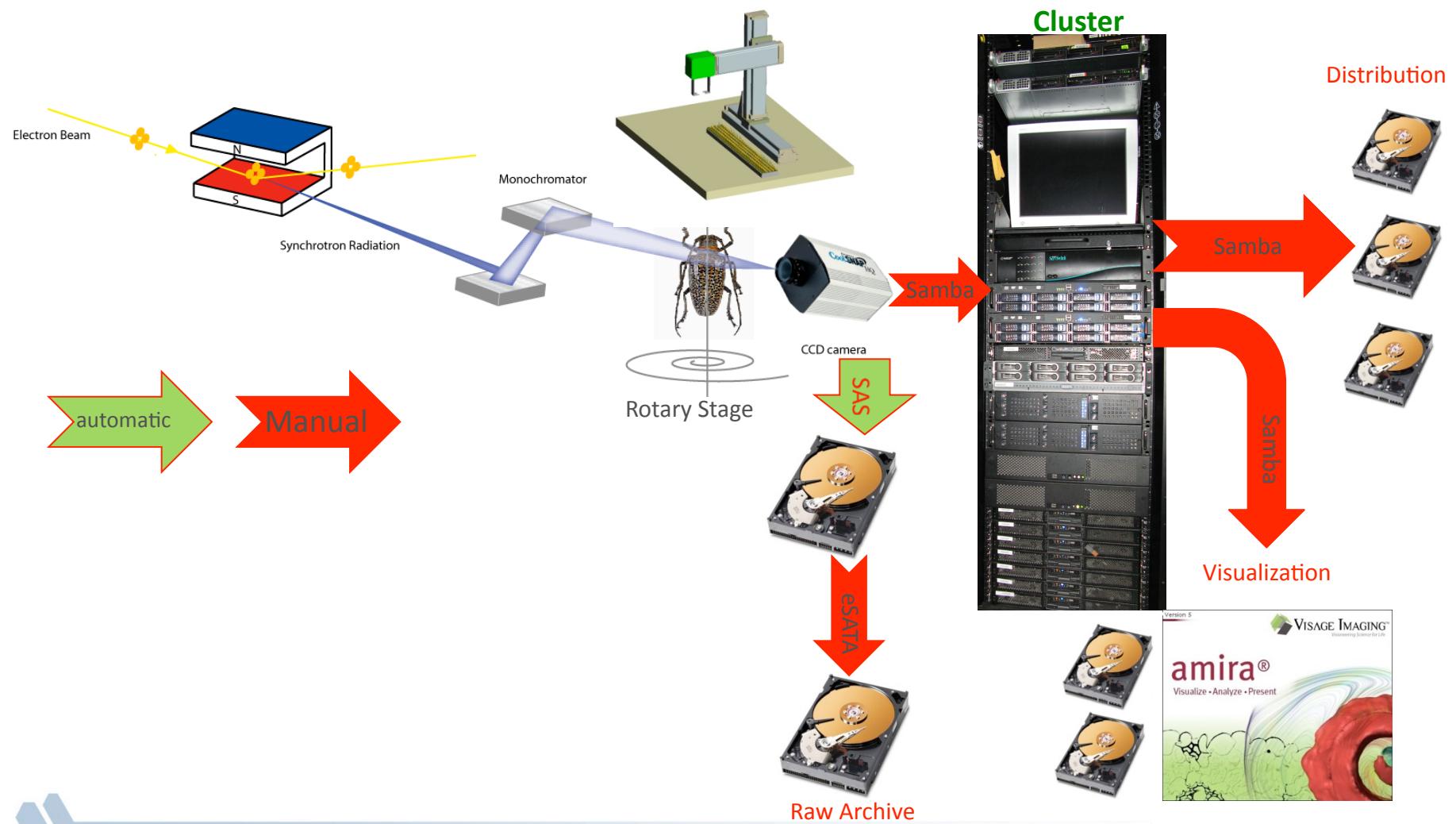
Highly Explosive Materials
(PBX-9501) Modeling



Micro tomography of static samples

Current detectors, controls and data flow

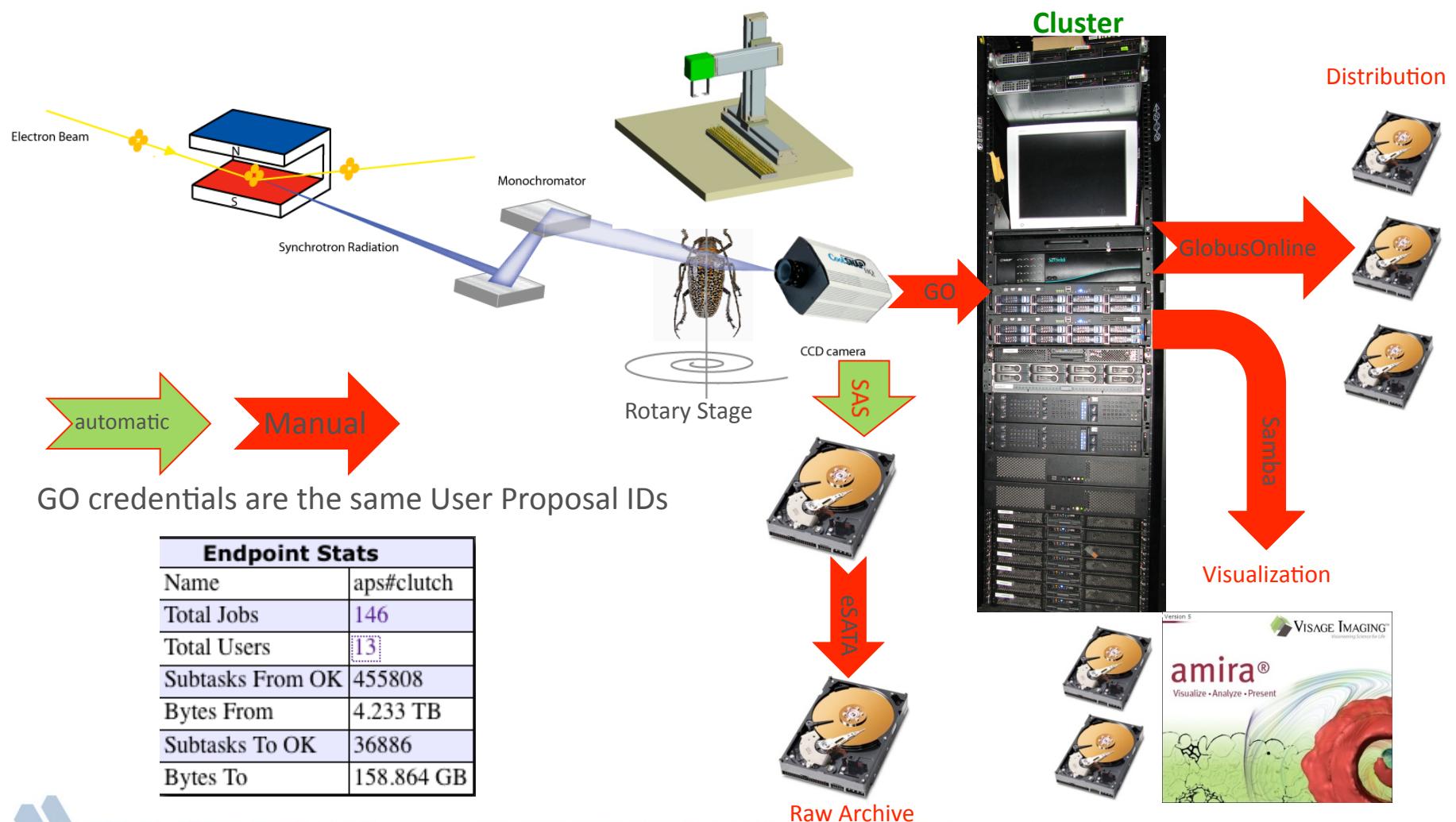
Linux
Windows



Micro tomography of static samples

Current detectors, controls and data flow

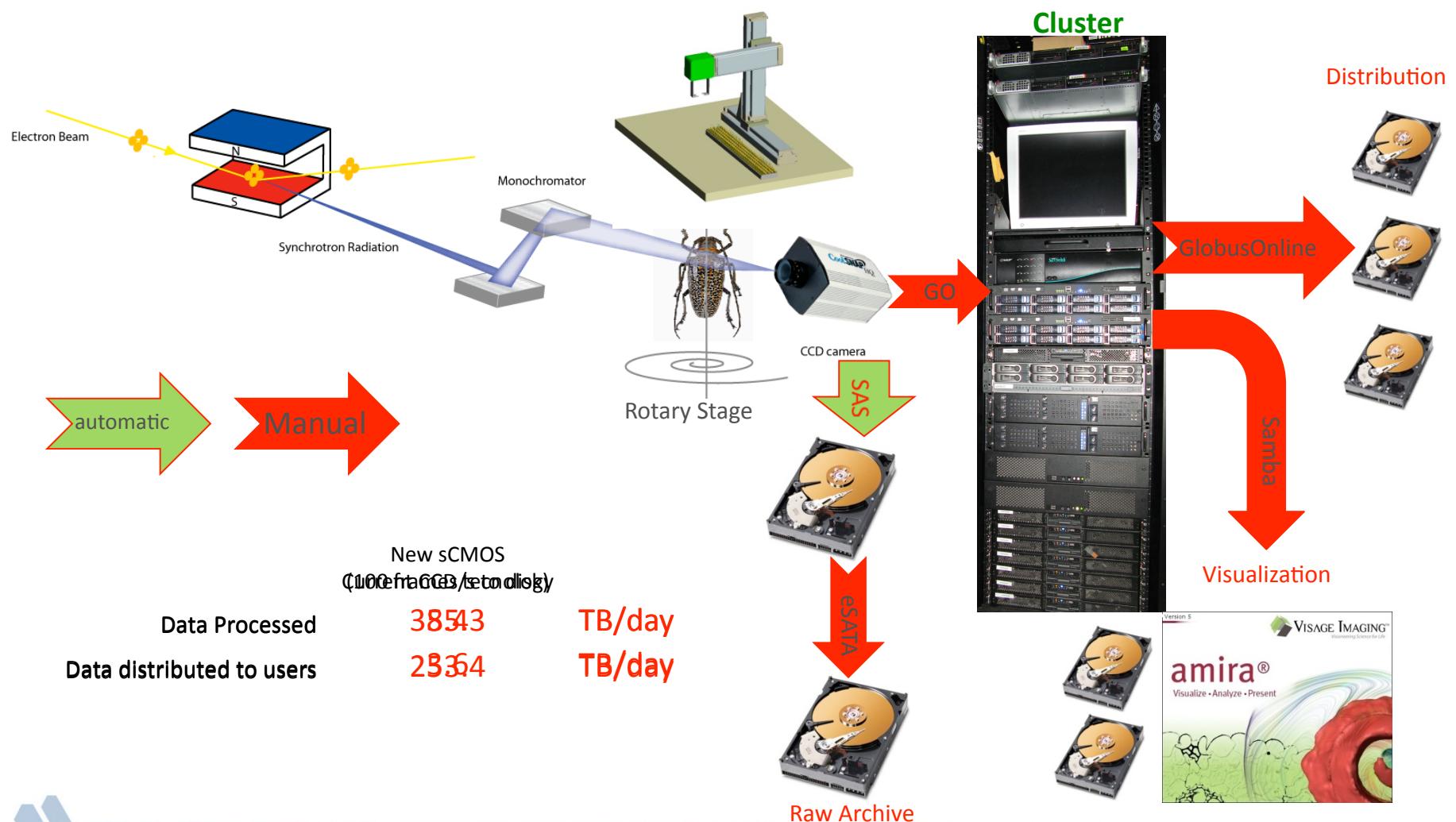
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Windows



Micro tomography of static samples

Current detectors, controls and data flow

Linux
Windows

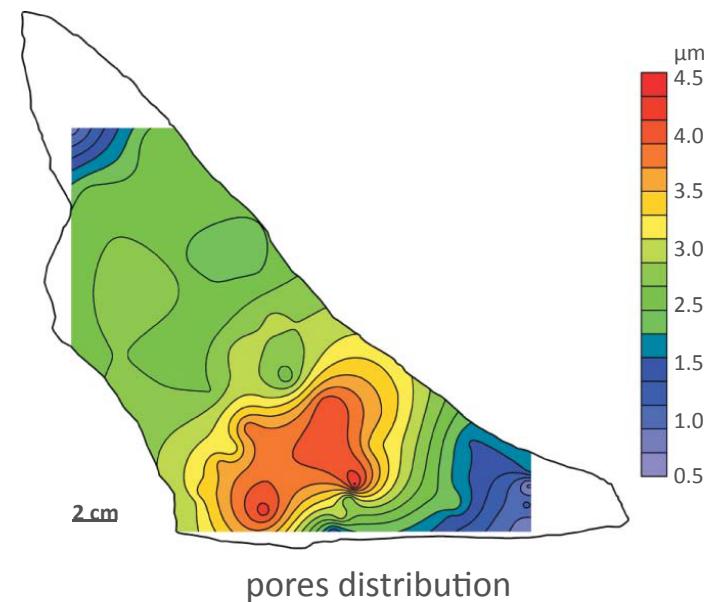
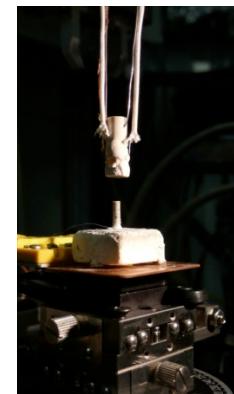
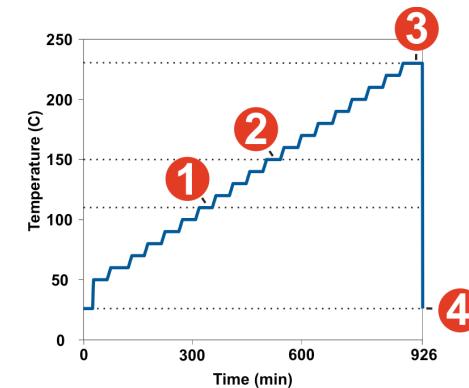
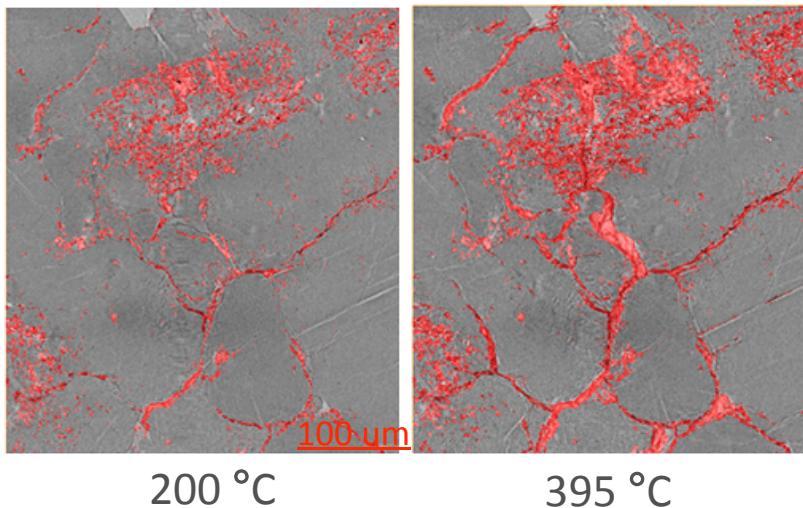


Micro Tomography Science

in-situ studies of real size samples

Thermal expansion cracking in rocks

Carbon sequestration, mine and oil exploration

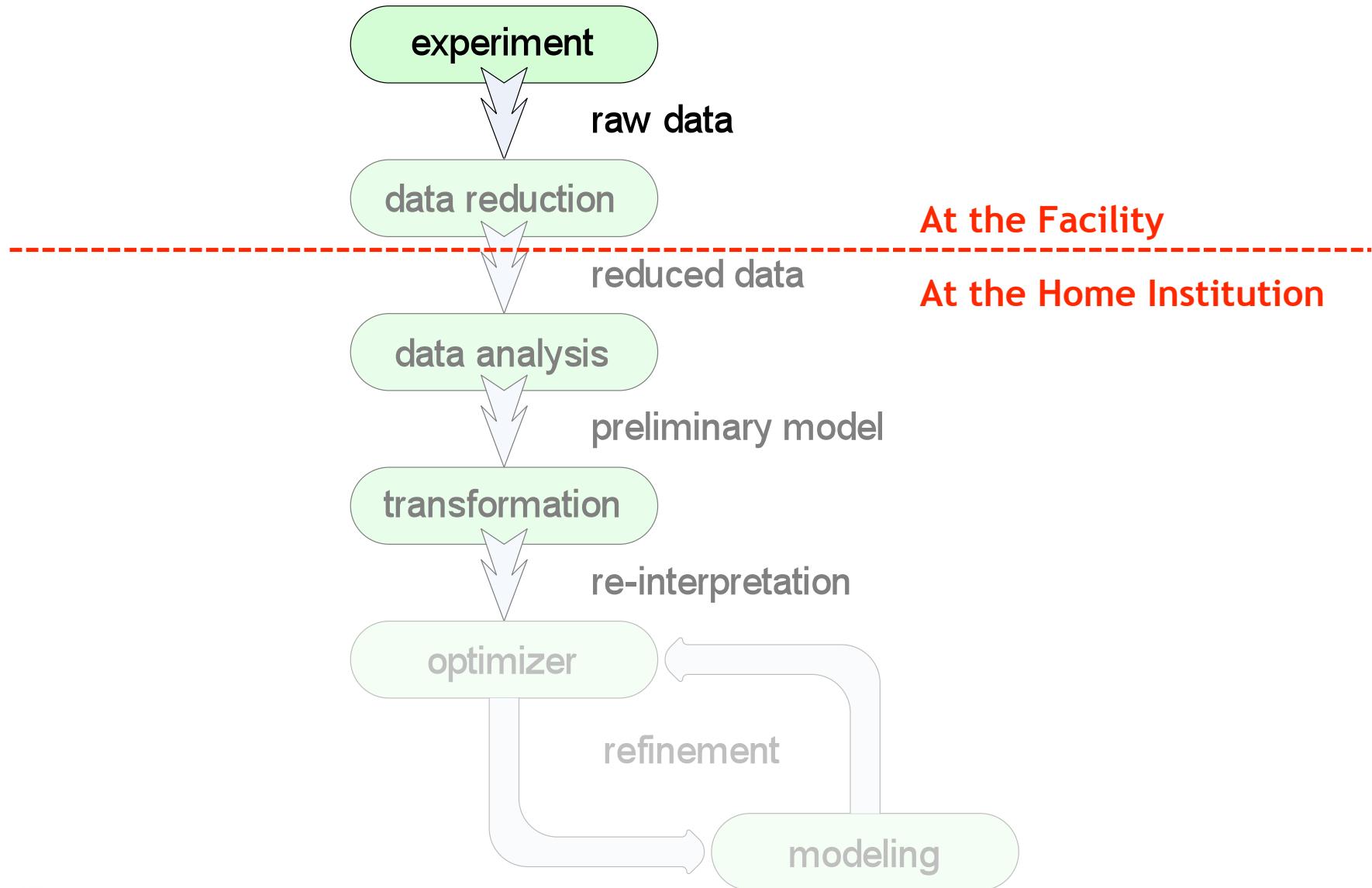


Nature Vol. 459 18 June 2009 doi:10.1038/nature08051

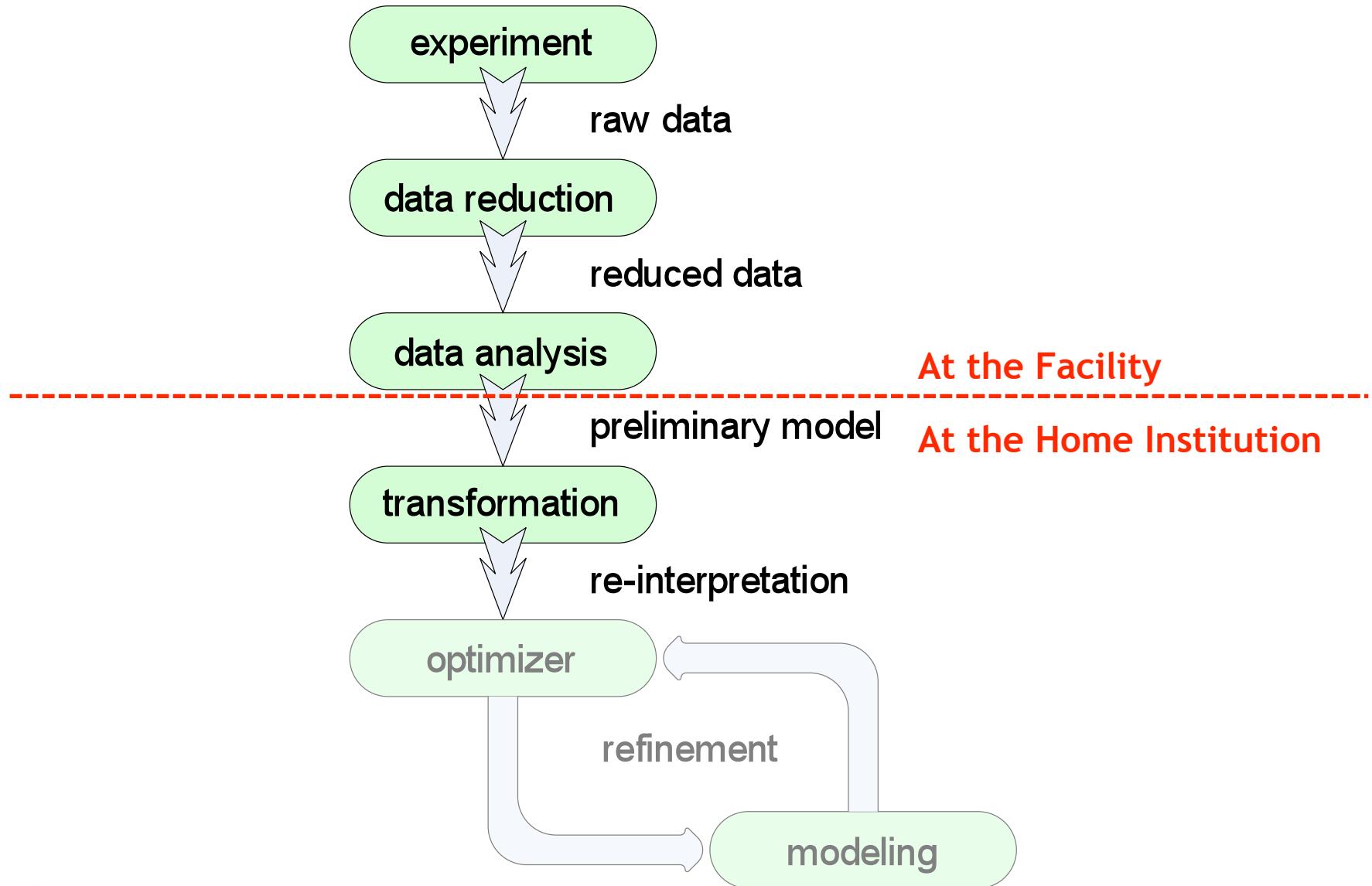
Science 332, 88-91 (2011). DOI: 10.1126/science.1202221



Traditional Operational Workflow



Traditional Operational Workflow

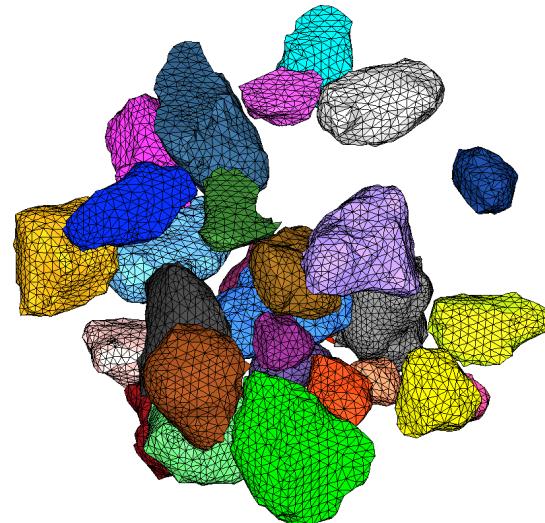
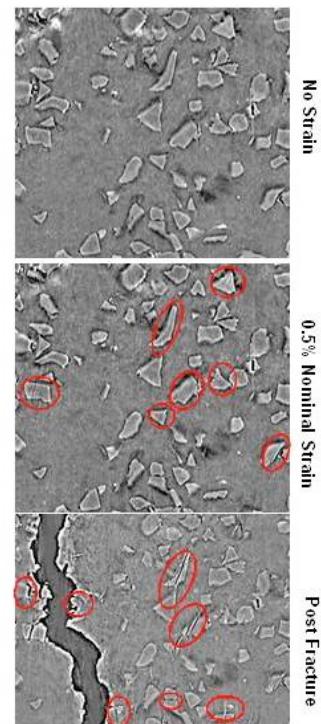
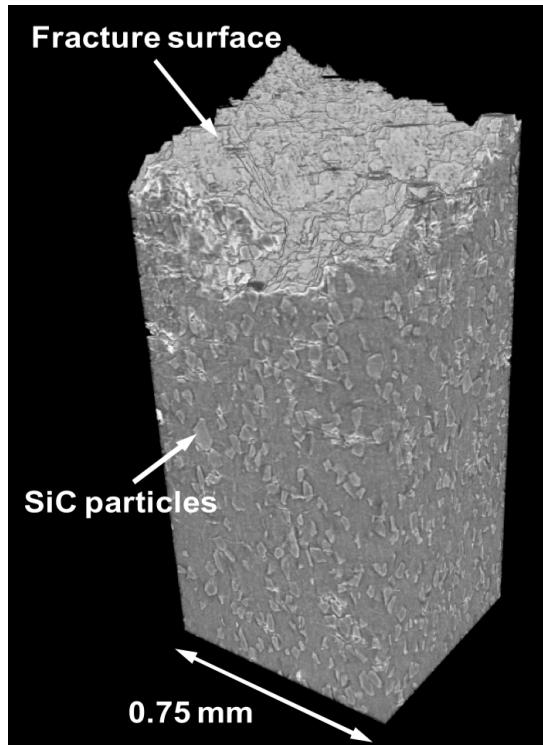


Micro Tomography Science

real size samples in real operational conditions

Mechanical Properties of Metal Matrix Composite Materials

transportation technology, new material, industrial applications



Metal Matrix Composite

N. Chawla J. Williams ASU

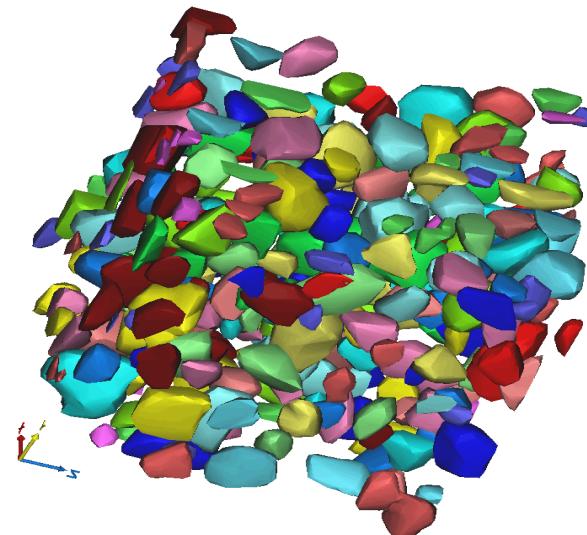
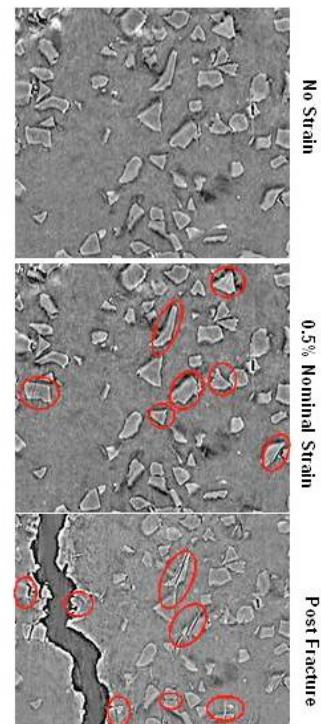
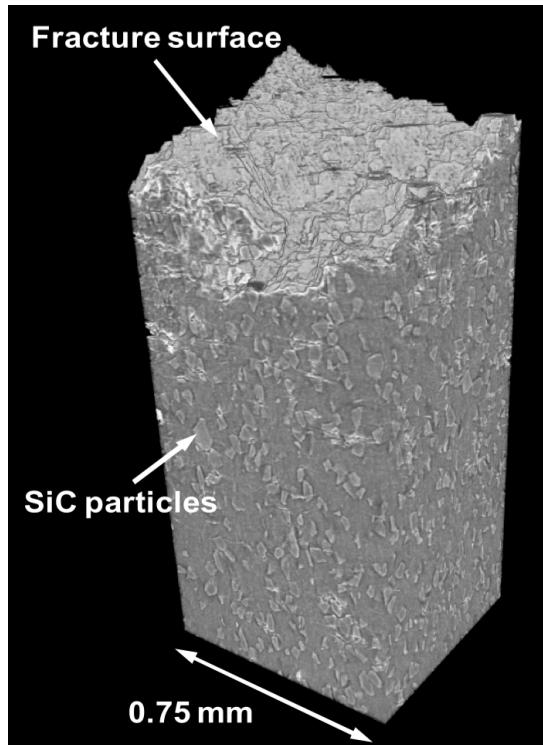


Micro Tomography Science

real size samples in real operational conditions

Mechanical Properties of Metal Matrix Composite Materials

transportation technology, new material, industrial applications



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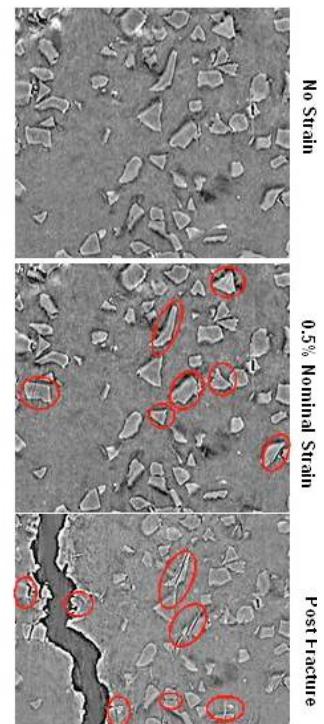
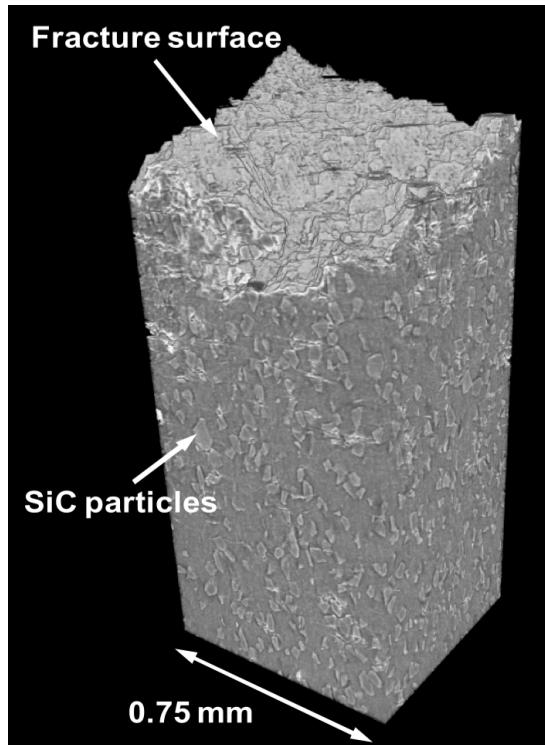


Micro Tomography Science

real size samples in real operational conditions

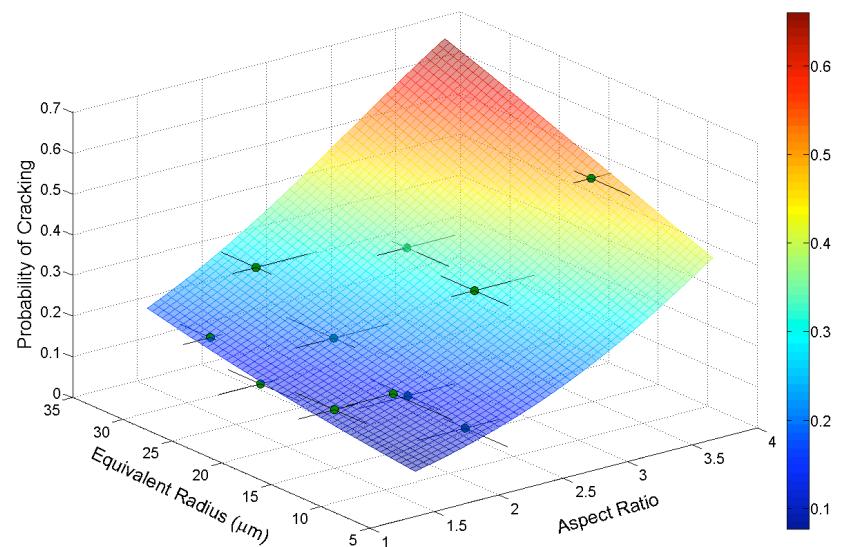
Mechanical Properties of Metal Matrix Composite Materials

transportation technology, new material, industrial applications



N. Chawla J. Williams ASU

Acta Mater. 58 (18), 6194-6205 (2010)

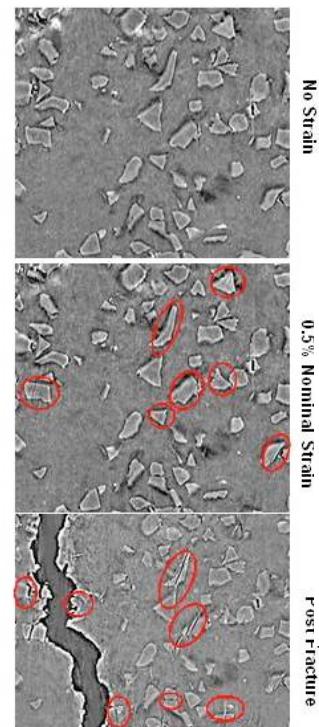
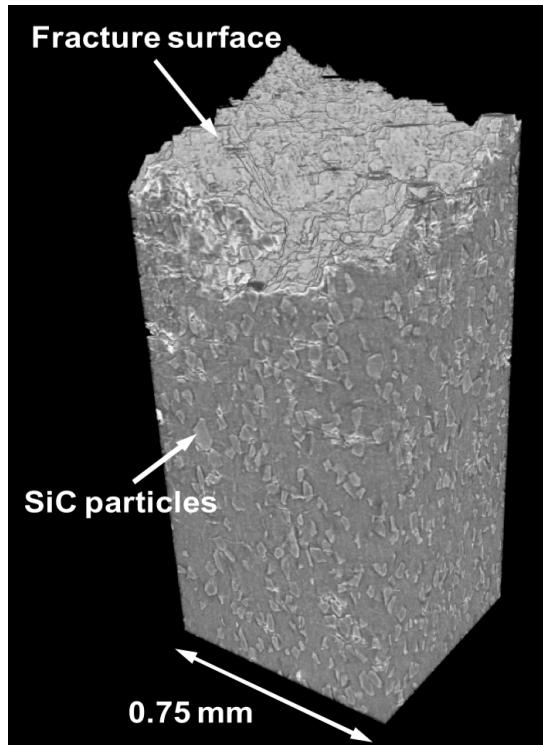


Micro Tomography Science

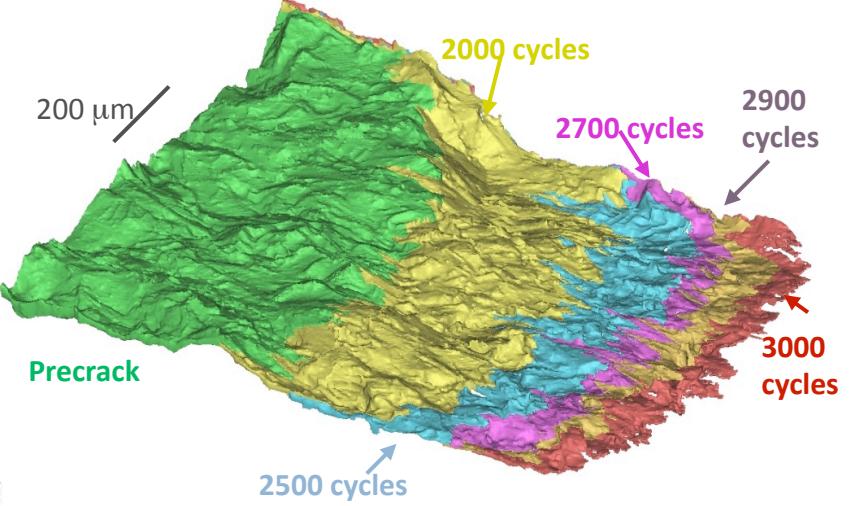
real size samples in real operational conditions

Mechanical Properties of Metal Matrix Composite Materials

transportation technology, new material, industrial applications



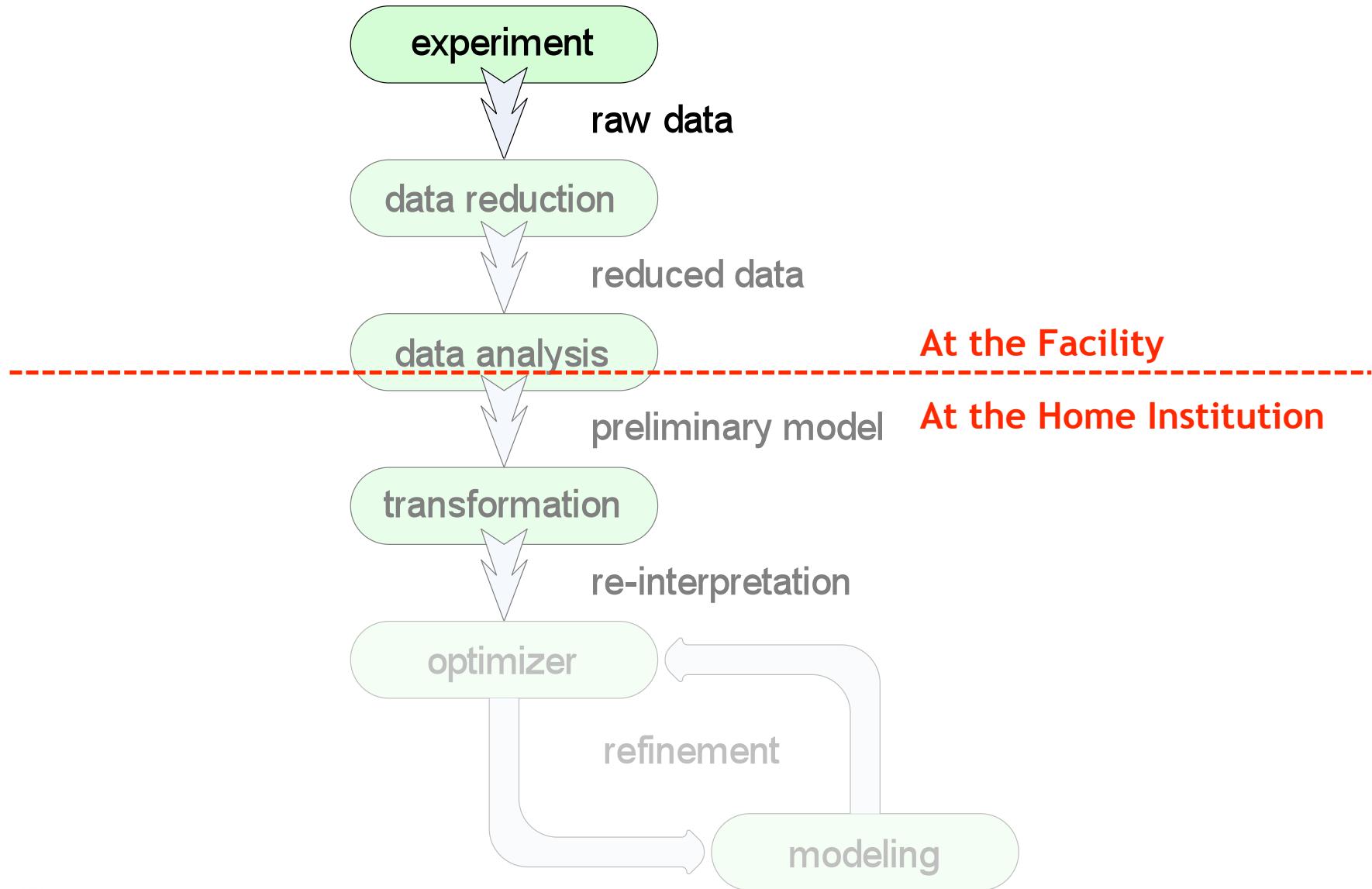
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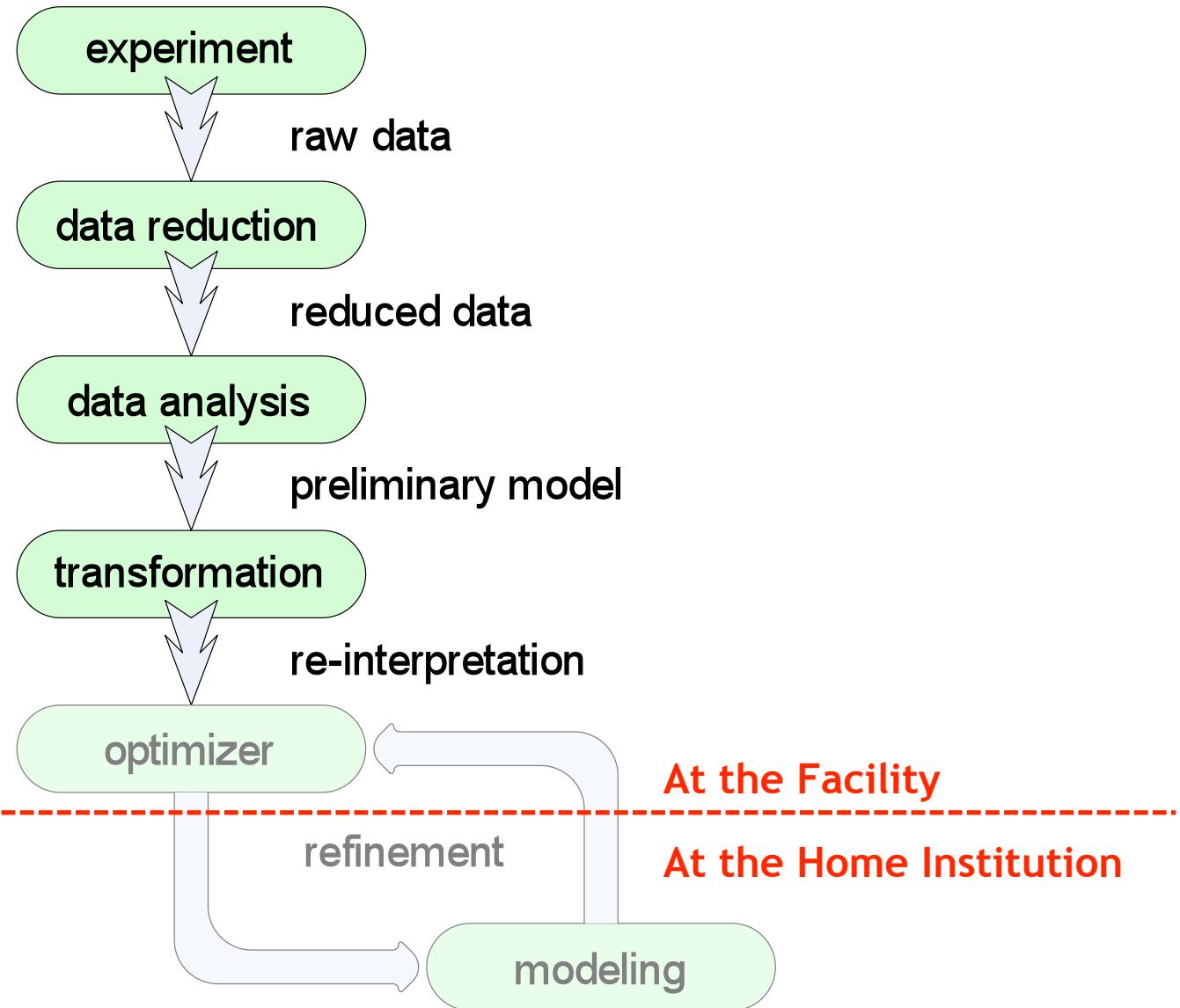
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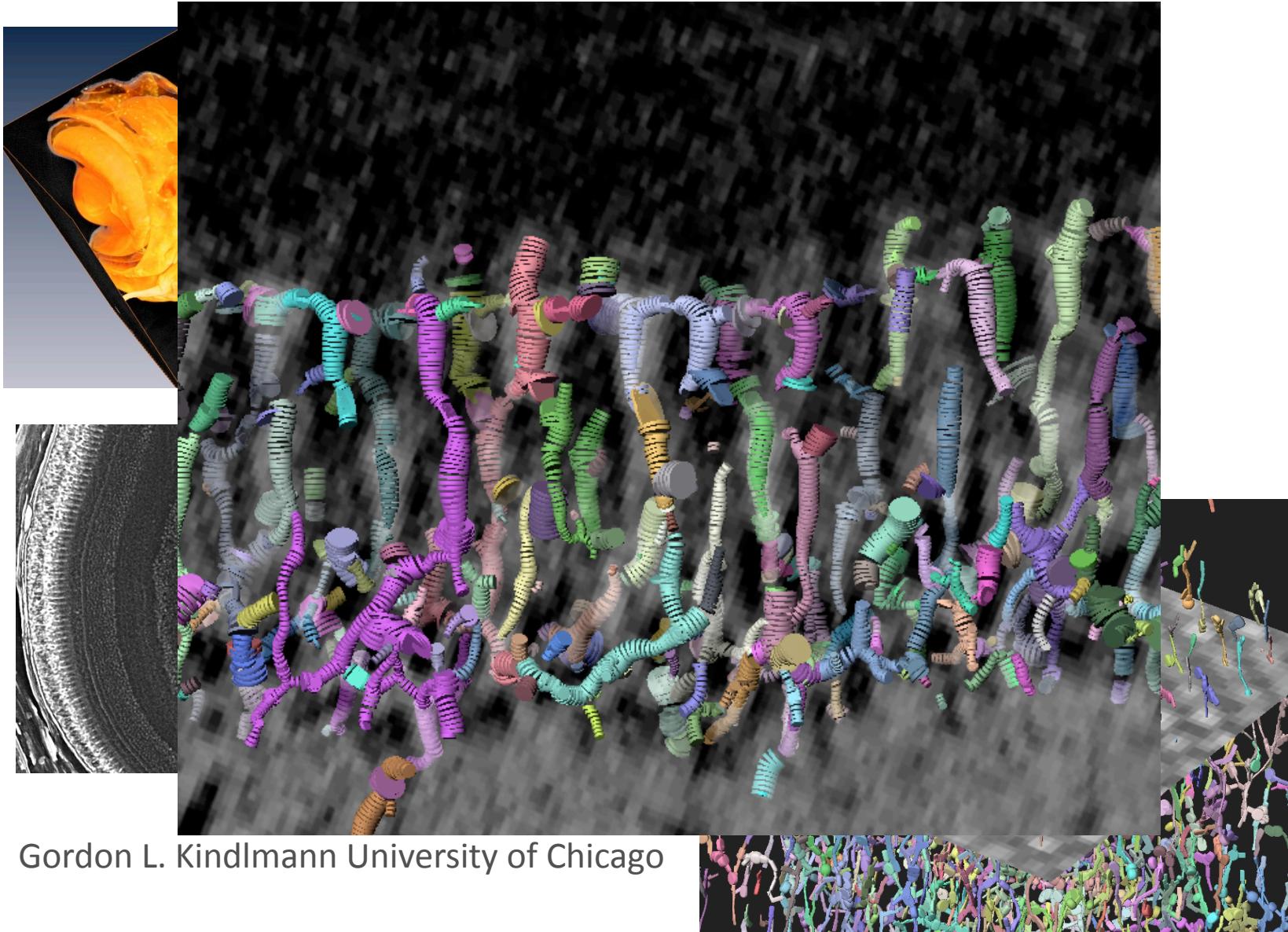
Traditional Operational Workflow



Traditional Operational Workflow



Challenges in data modeling and data mining 2D/3D of Juvenile Zebra Fish Retina



Gordon L. Kindlmann University of Chicago

SPIE, (2010), 78040M. DOI: 10.1117/12.860783



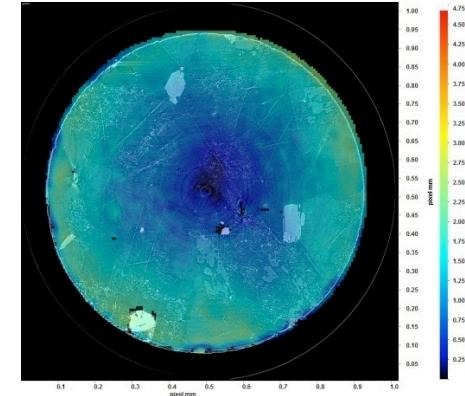
Computing Challenges

Very large data volumes

- Data mining

Image registration of dynamic system

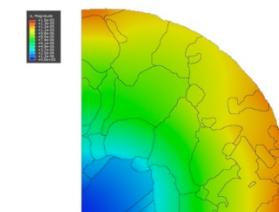
- 3D registration of sections
- Feature detection (e.g., synapses)
- Network analysis



Modeling

Multi scale data integration

- Stitching and alignment of overlapping tiles
- Visualization



Thermal Expansion Displacement in rocks

Integration of data from different instrument

- Micro and nano tomography
- Tomography and fluorescence
- Tomography and diffraction



Data Exchange for Scientific Data and Metadata

Scientific Metadata

- Tomography Reconstruction
 - Iterative, analytical, interpolation type, etc.
- Instrument
 - Pixel size, orientation, etc.
- Sample
 - Temperature, pressure, etc.
- Data
 - 3D density map

All definition manual, code examples etc. in less than
20 pages !

Infrastructure Metadata

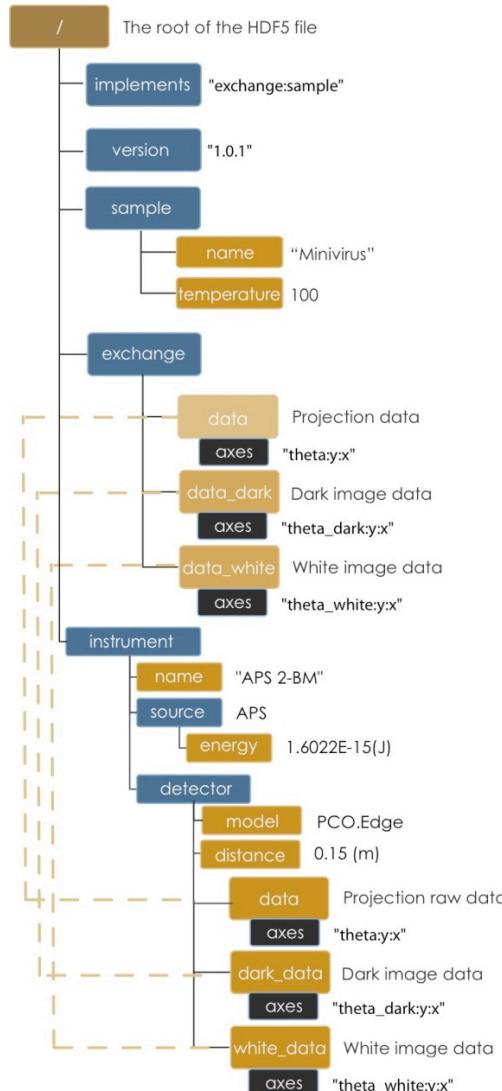
- Data transfer Status
 - End-points, progress, etc.
- Processing Status
 - Data ingestion date
- Cluster Queue status

Provenance Layout

/provenance
 /next “process_n”
 /process_n
 /status
 /ref
 /message
 /infrastructure_n



Data Exchange for Scientific Data and Metadata



6.1 Top level (root)

This node represents the top level of the HDF5 file and holds some general information about the file.

Table 2: 2FXi top level entries

| Member | Type | Example |
|----------------|----------------------|---|
| implements | string | "exchange:instrument:sample:provenance" |
| version | string | "1.0.1" |
| exchange_N | Exchange class | |
| instrument | Instrument class | |
| sample | Sample class | |
| provenance | Provenance class | |
| reconstruction | Reconstruction class | |

implements - A colon separated list that shows which components are present in the file. The only *mandatory* component is "exchange" but a more general 2FXi file will also contain sample and instrument information, if so these will be declared in implements as "exchange:sample:instrument"

version - 2FXi format version.

exchange_N - The measurements recorded in this file.

instrument - The instrument used to collect this data.

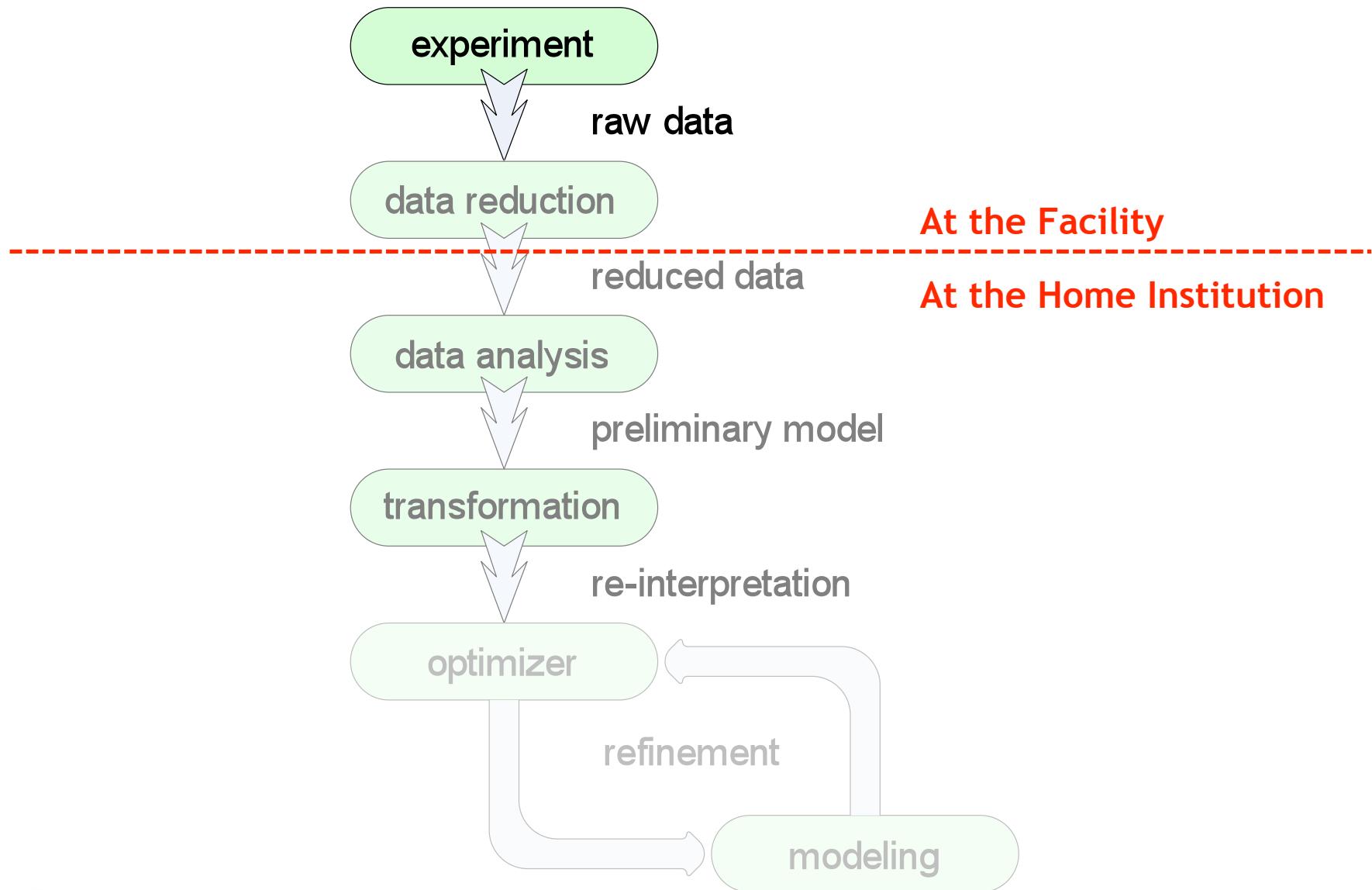
sample - The sample measured.

provenance - The Provenance class describes all process steps that have been applied to the data.

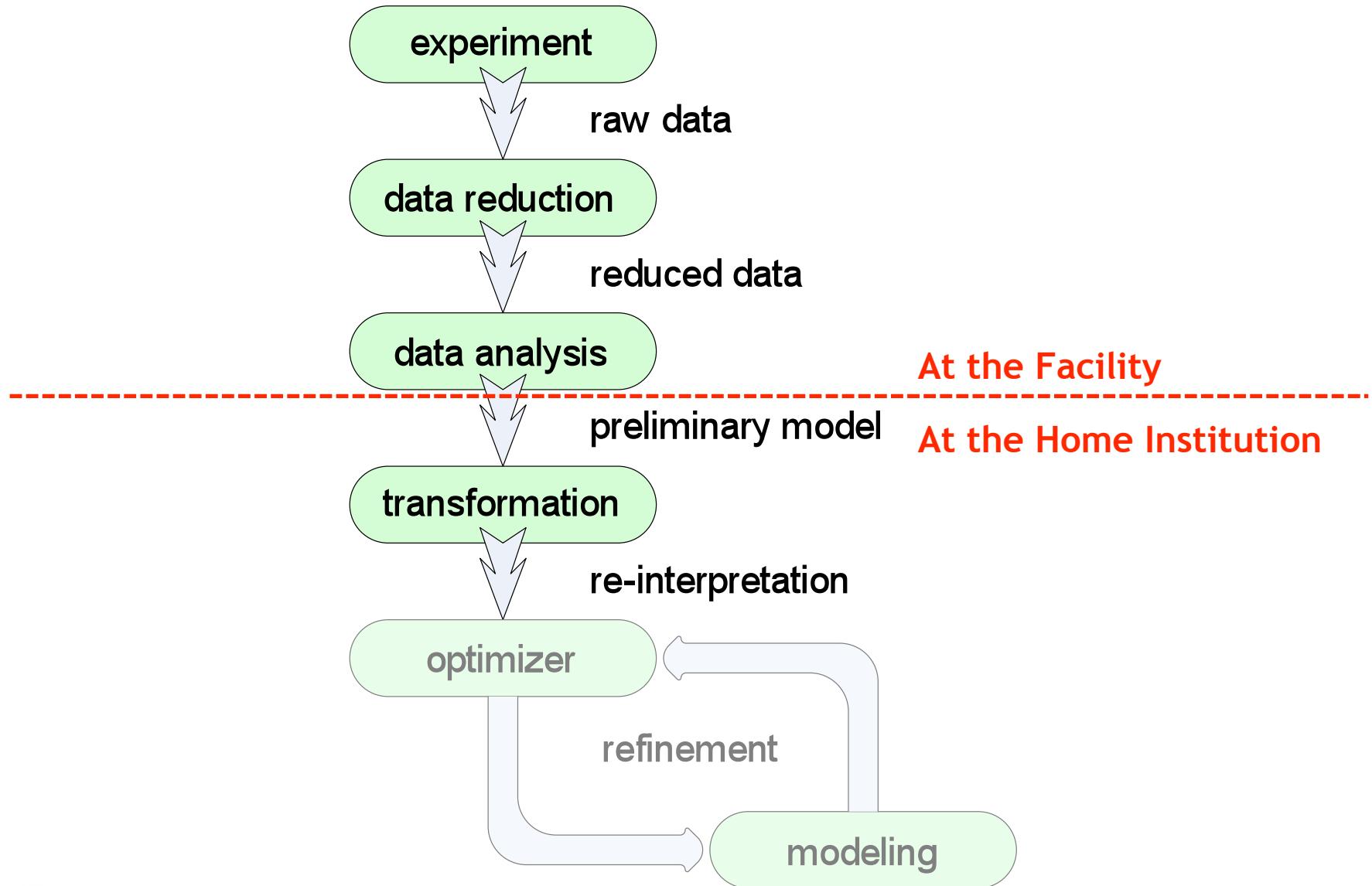
reconstruction - The Reconstruction class contains all information and parameters required to run a tomography reconstruction.



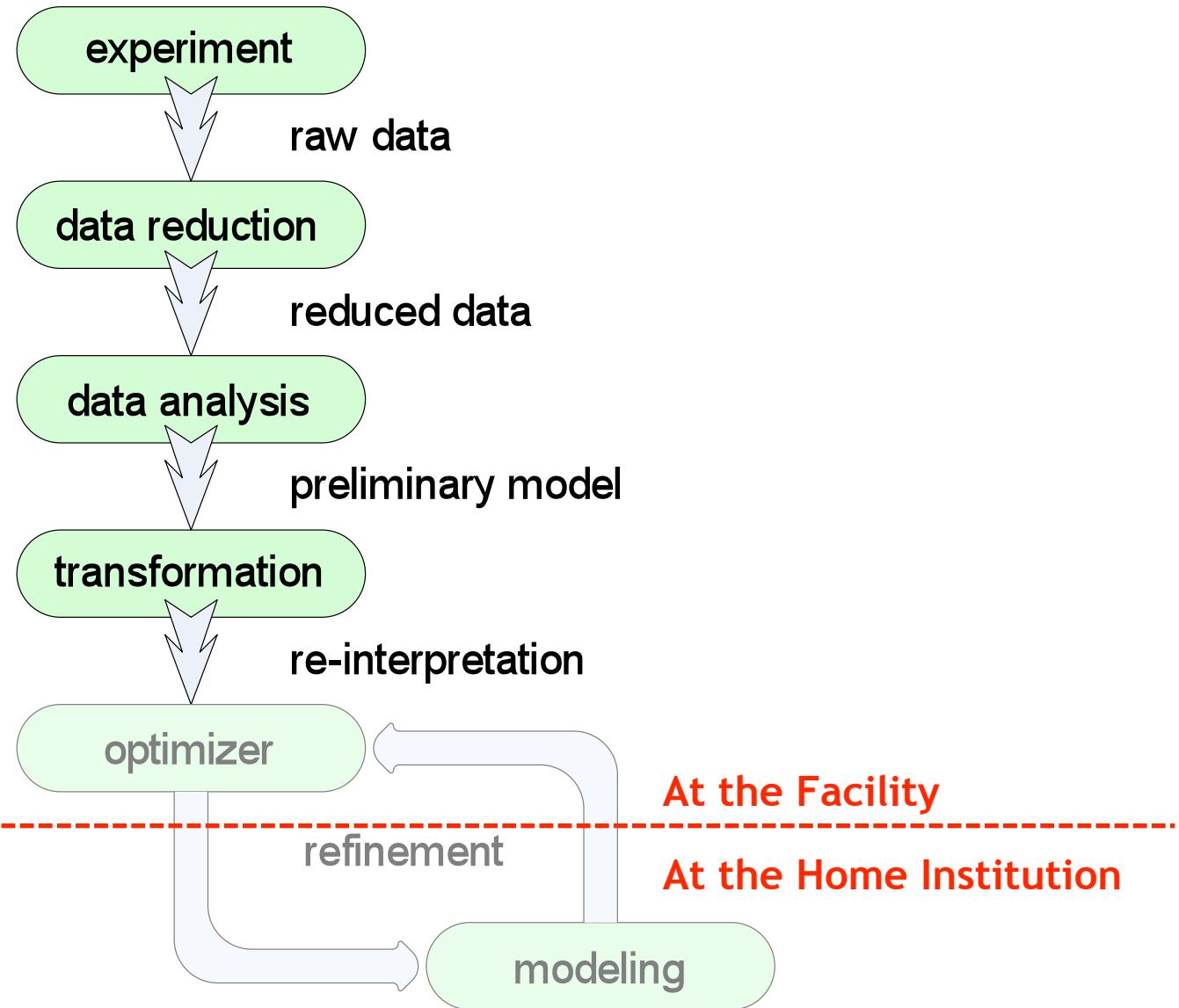
Traditional Operational Workflow



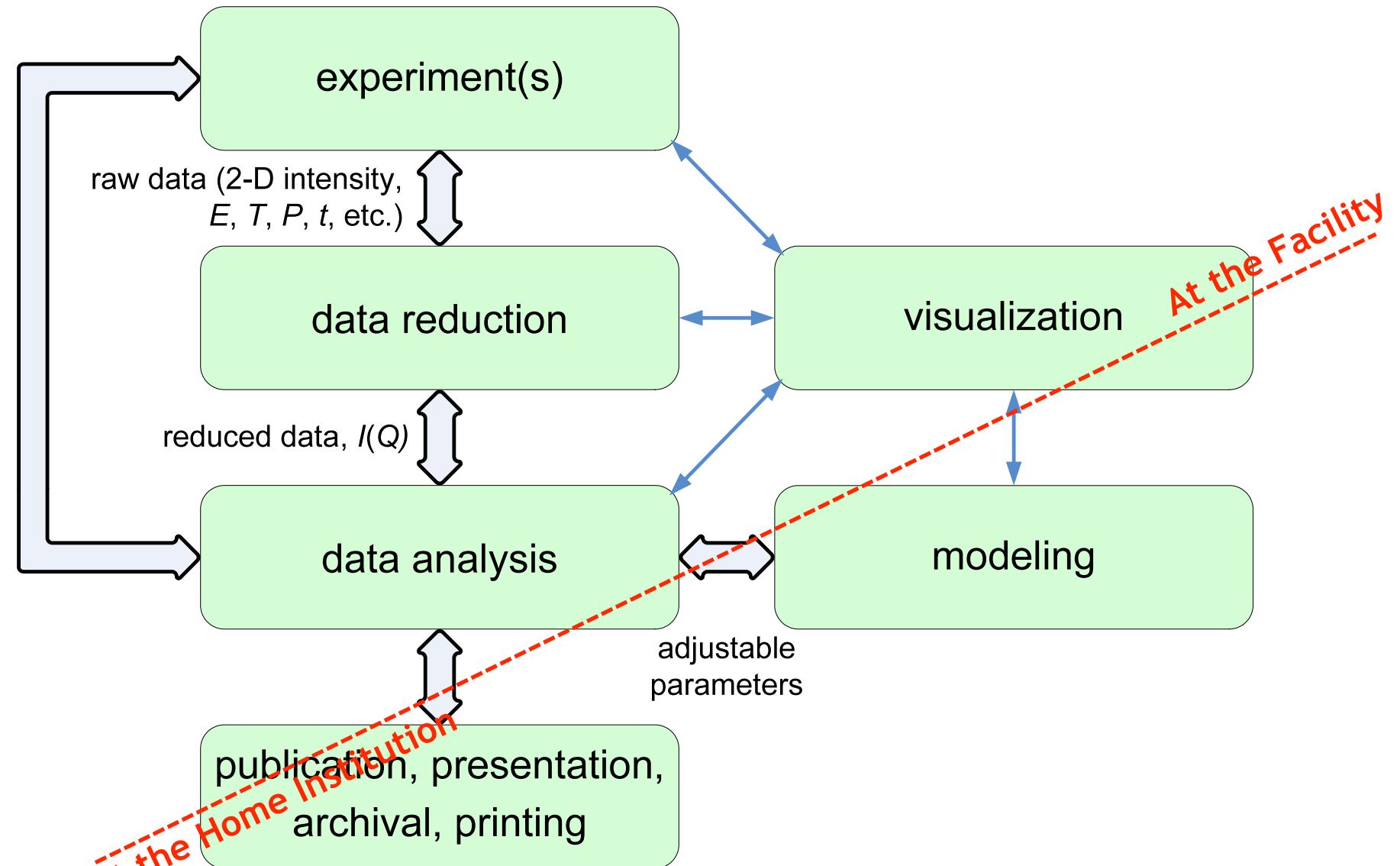
Traditional Operational Workflow



Traditional Operational Workflow



Preferred Operational Workflow



Conclusions

From 3D static to 3D dynamics => computing challenges

Gridftp provided a powerful tools for data distribution

- The Globus On line user friendly version made the real break through

Data integration in an essential tool for

- Software sharing
- Multiscale and multi technique data integration





Thank you

IMG staff: Kamel Fezzaa, Steve Wang, Wah-Keat Lee, Xianghui Xiao, Yongsheng Pany, Joan Vila, Alex Deriy, Pavel Shevchenko, Joe Arko and Francesco De Carlo

IMG users: Nik Chawla, Florian Fusseis, Keith Cheng, C. Powel, Wilson Chiu, Jung Ho Je, Jake Socha, Wen-lu Zhu

