# A Multi-Modality Integration Framework for Chemical Imaging

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## Purpose

Enable user-driven integrated analysis of experimental results across a wide spectrum of chemical imaging techniques, allowing users to integrate, synthesize, and correlate results with confidence without necessarily in-depth knowledge of these techniques. This will facilitate accelerated knowledge creation and exploitation.

## Expected Outcomes

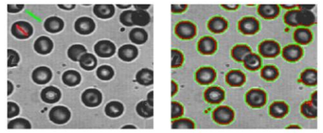
A strong, open, multimodal integration framework for analytical and knowledge capturing tech-nologies in chemical imaging that allow the fast and precise analysis, comparison, and integration of experimental results from many different imaging technologies.

## Computational Challenges

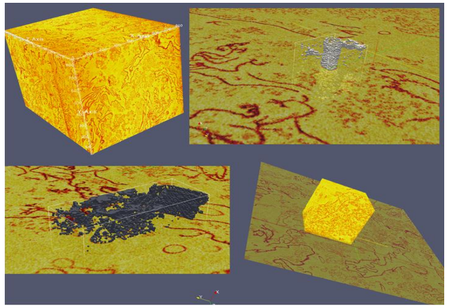
### Selected Use Case -- Project 1.1

Challenge: Timely image reconstruction &feature identification

Serial 2D images of *Shewanella* collected at high resolution form a 3D dataset containing tubular and curtain-like structures



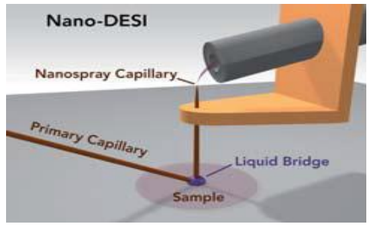
Assignment of background (green) and foreground (red) seeds for automatic segmentation



Visualization and segmentation in Paraview of large 3D image datasets reveals tubular and curtain structures

### Selected Use Case -- Project 2.2

Challenge: Processing raw data due to high data volumes.

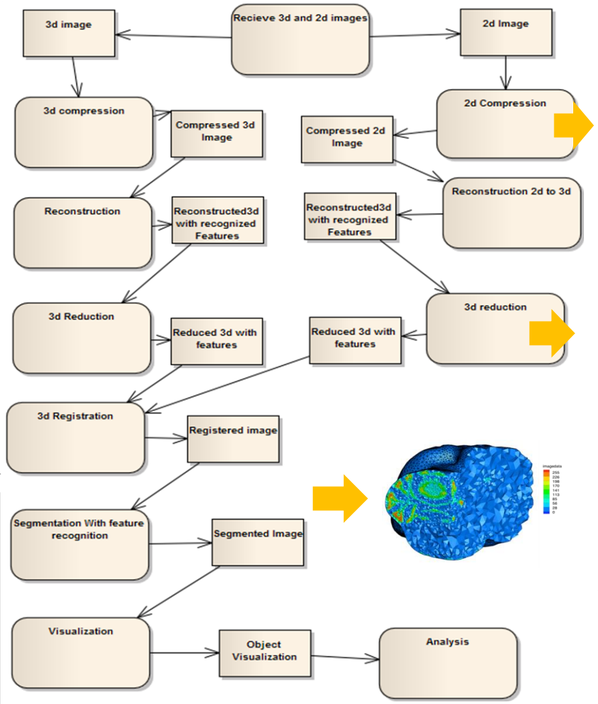



NanoDESI was developed for high-resolution spectrometry.

Efficient visualization is data intensive – a scan of 1cm*1cm sample size, with spatial resolution at 5µm and mass resolution at 700 can generate a data file over 4GB.

- Current MS data analysis products have difficulty in reading and analyzing generated data.
- Long processing time (over hours) and frequent crash impedes discovery.

## Integrated Workflows




## Scientific Outreach

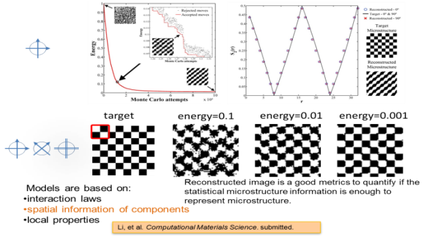
*J. Microscopy,* IEEE Engineering in Medicine and Biology Society Proceed., *Computational Materials Science* (submitted); presented at NOBUGS, XFEL, EMSL workshop, etc.; joined W3C

## Solutions and Achievements

Initial results: 30% reduction in lossless and 80% in lossy compression

Evaluate image reconstruction accuracy, efficiency, and uncertainty

Develop hybrid algorithm

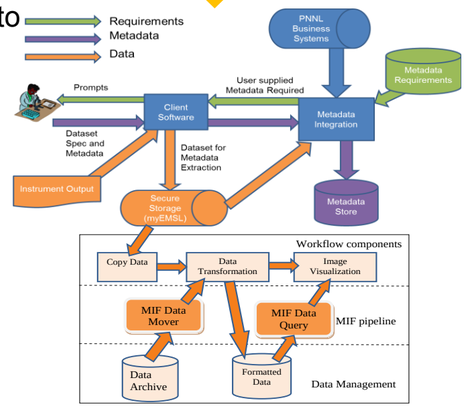



Develop efficient mapping of image 'fields' to arbitrary unstructured grids

Develop tool suite for feature recognition and segmentation

Compose workflows

Develop semantic framework.

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