

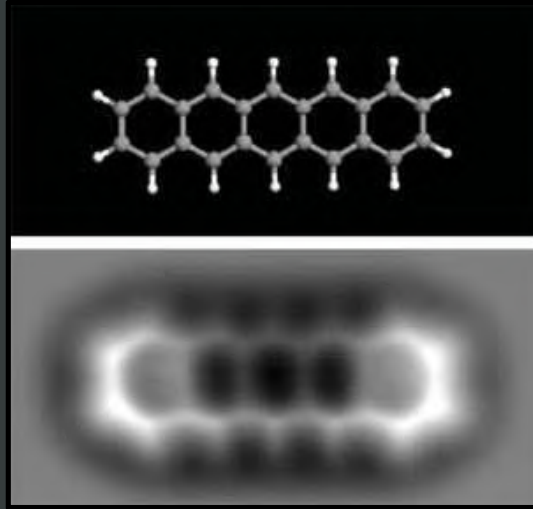


Cassandra Taxonomy

NANOLAYERS RESEARCH COMPUTING UK LTD.

Domain : Scanning Probe Microscopy

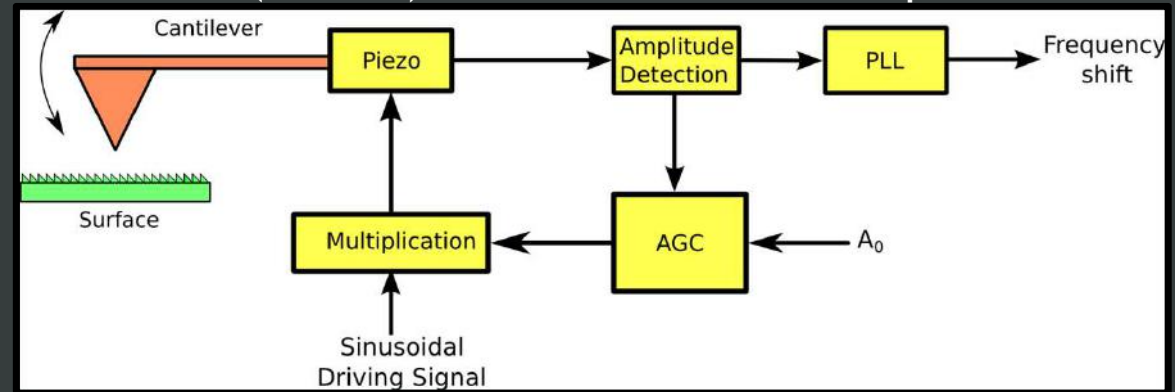
Incredible Resolution on Surfaces



Nature Methods (2009) 792

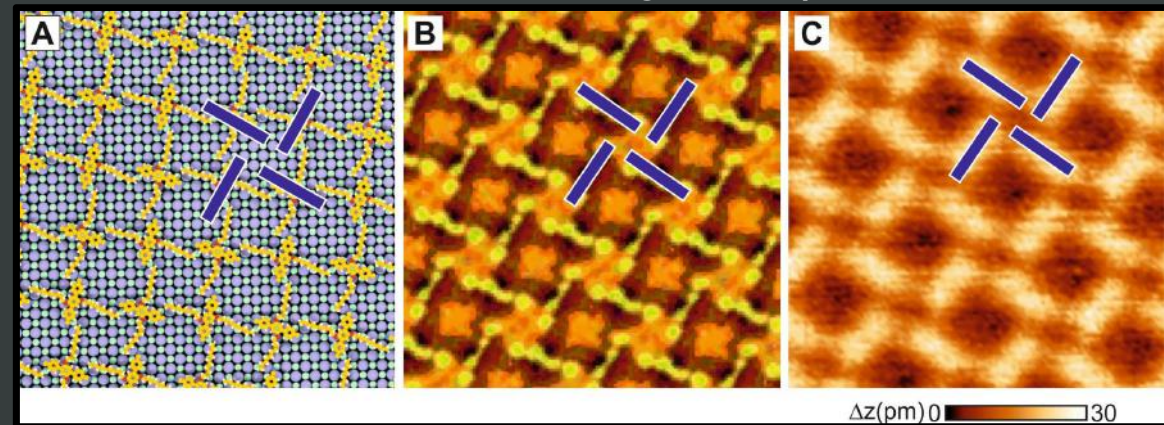
- Complex Experiments and Systems
- Images Need Post-Processing
- Requires Detailed Knowledge to understand image contrast
- High Speed Measurements generate too much data to process manually

(Virtual) Atomic Force Microscope



Computer Physics Communications (2015) 429-438

Direct Atomistic Image Interpretation



Advanced Materials Interfaces (2014) 1400414.

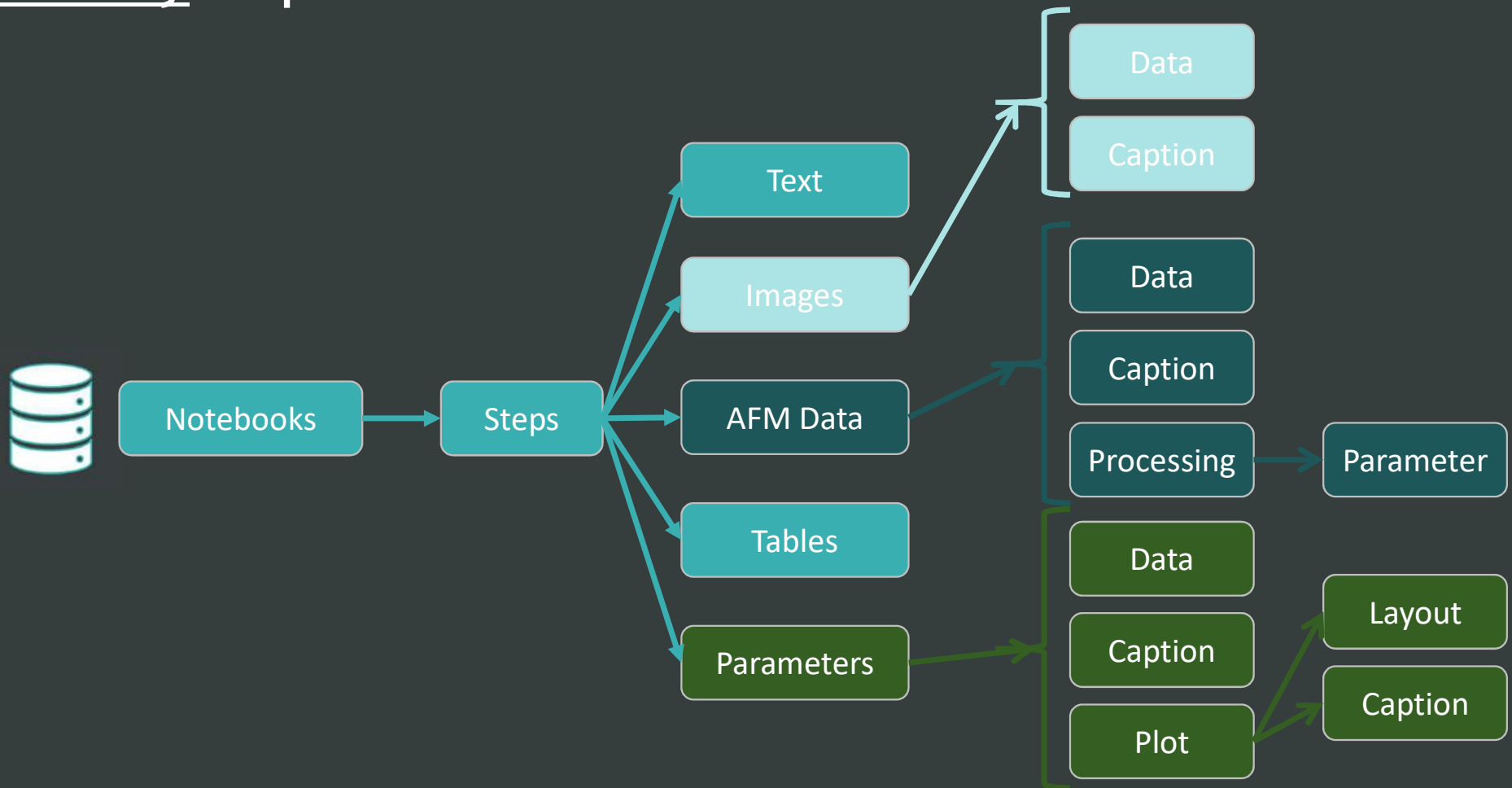
Purpose

- The Cassandra taxonomy aims to label atomic force microscopy (and scanning probe in general) experiments
- Documentation of atomic force experiments. Labelling and storage of microscopy images



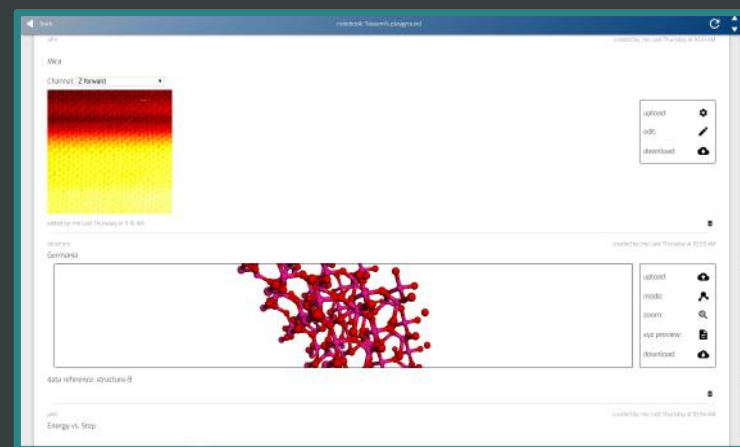
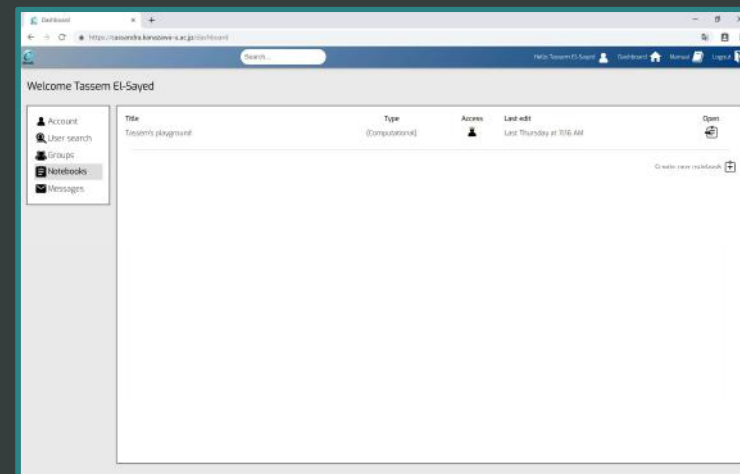
- Facilitates [thorough metadata capture](#) in order to enable virtual AFM simulations
- Enables the application of machine learning techniques to [automate post processing](#)

Taxonomy Representation



Example Use Cases

- **Automated labelling** of experimental data
 - Capture parameters directly from the instrument
- Record of images and how they were **processed**
 - Post processing is an often ignored step in publications
 - Skill dependent, Researcher Dependent
 - Difficult to Reproduce!
- **Rapid sharing** of data and collaboration
 - Share raw data from AFM experiments within lab groups
 - Facilitate theory-experiment collaboration
- **FUTURE: Insights into processing images** from the data processed by experts
 - Automated teaching tool to pass on image processing knowledge
 - AI post-processing of previously inaccessible old image libraries



Overlaps

Other **Microscopy** Techniques

- TEM, STM, combined STM/AFM, KPFM
- Natural extensions that benefit from many of the same capabilities

General **Experimental Metadata Challenge**

- Developing Taxonomy and Ontology for Experiments is Challenging
 - Running a simulation requires you to input all relevant steps and parameters
 - Experiments can easily be run without recording many of the necessary details
 - LabCore / Cassandra facilitates the capture of all such details by digitizing lab notebooks