PRISMS

The Materials Commons

A Novel Information Repository and Collaboration Platform for the Materials Community

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The University of Michigan

U.S. DEPARTMENT OF ENERGY | Office of Science

UNIVERSITY OF MICHIGAN

PRISMS

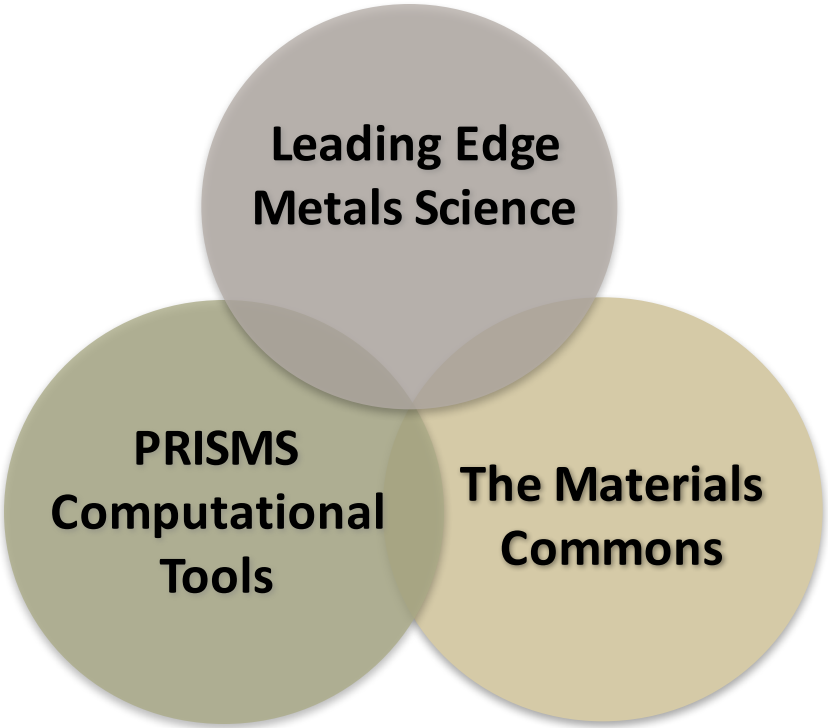
DOE Software Innovation Center

- A 5-year grant **to accelerate the development of predictive materials science**

- Involves:
  - 11 faculty
  - 5 staff scientists
  - 16 students & postdocs

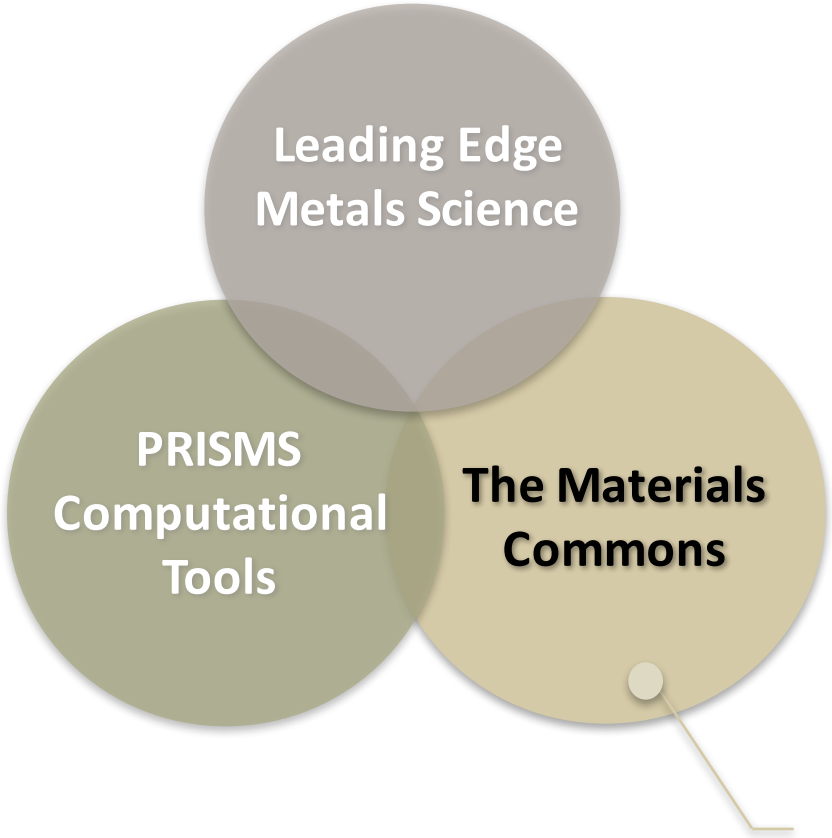
- DOE resources leveraged by significant UM cost share

Center for PRedictive Integrated Structural Materials Science (PRISMS)



PRISMS Overarching Vision

Enable accelerated predictive materials science.



- Collaboration
- Experimental & Simulation Information
- Seamless, Continuous Workflow
- Provenance Tracking
- Accelerate model building and validation

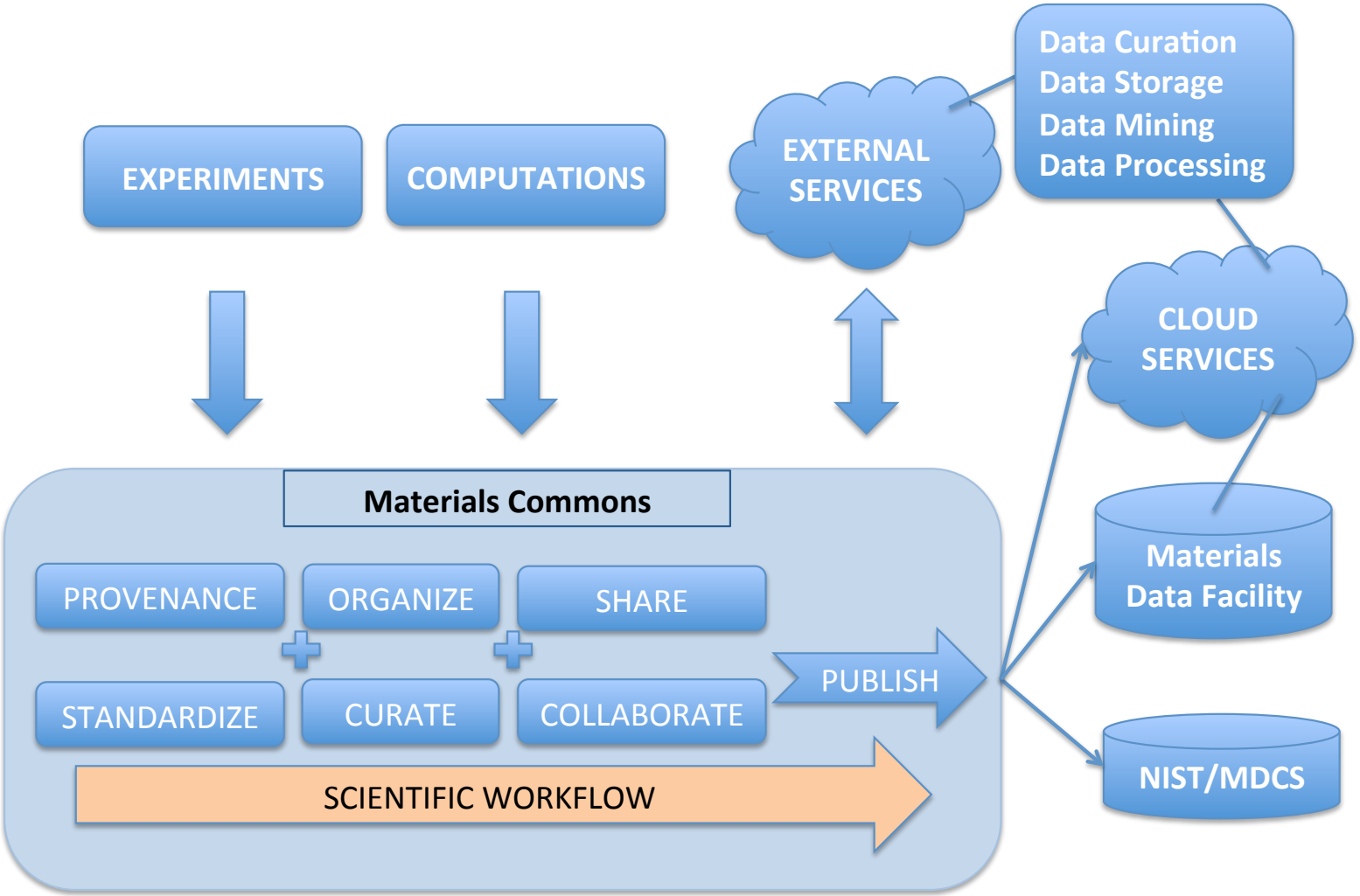
The Materials Commons

The Materials Commons consists of:

- 2 full time professional staff
- >25 PRISMS faculty and grad students as users.
- A 390 TB Isilon storage cluster data repository
- A website for uploading and downloading data, adding provenance, sharing and searching for data
- An application installed on your computer for uploading and downloading data
- A REST based API to access and extend the capabilities of the repository

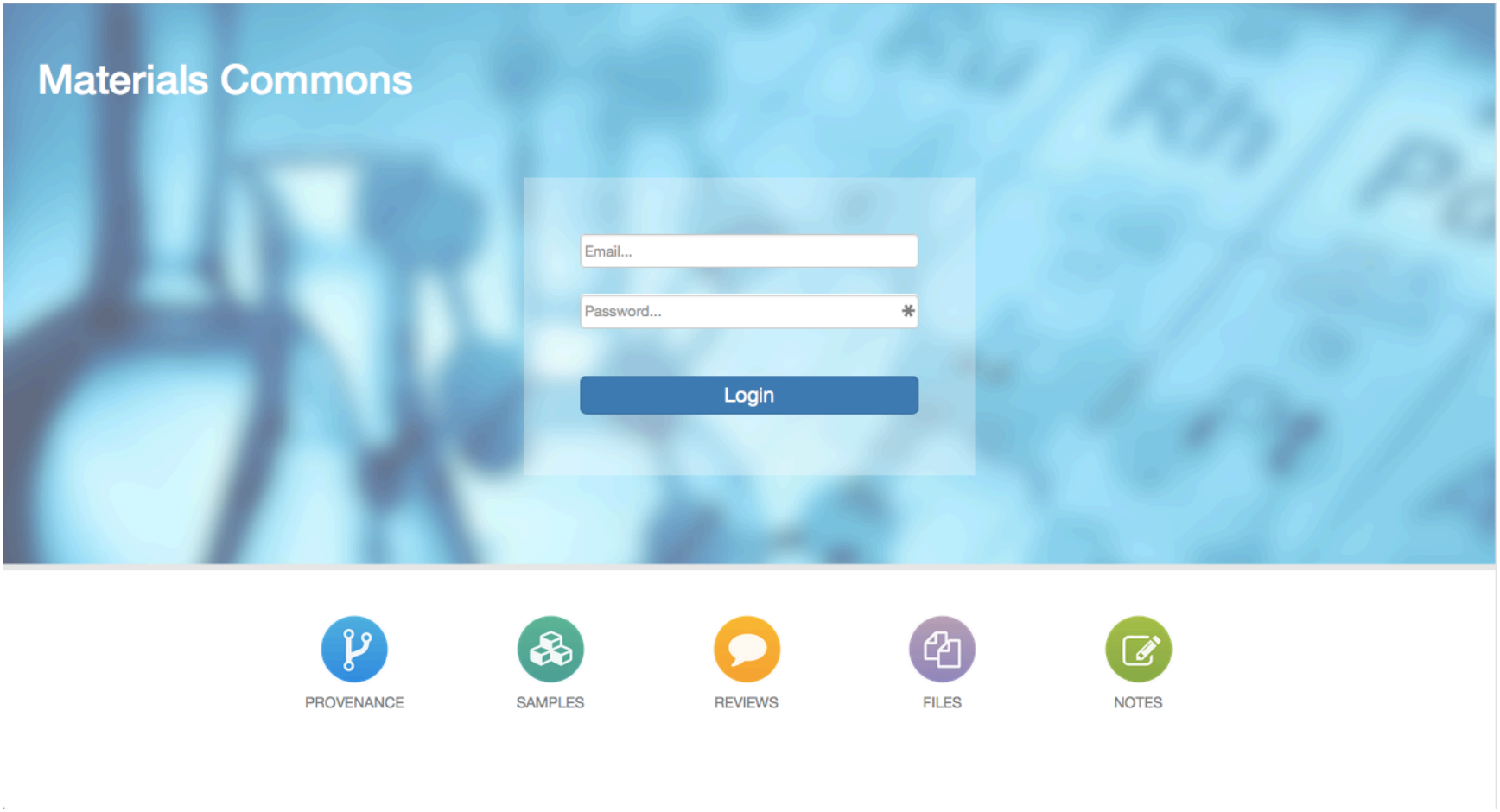
- Interacting with NIST, ICE, CHiMaD etal, (and you?) to share best practices, schemas, etc.

The Materials Commons - Workflow

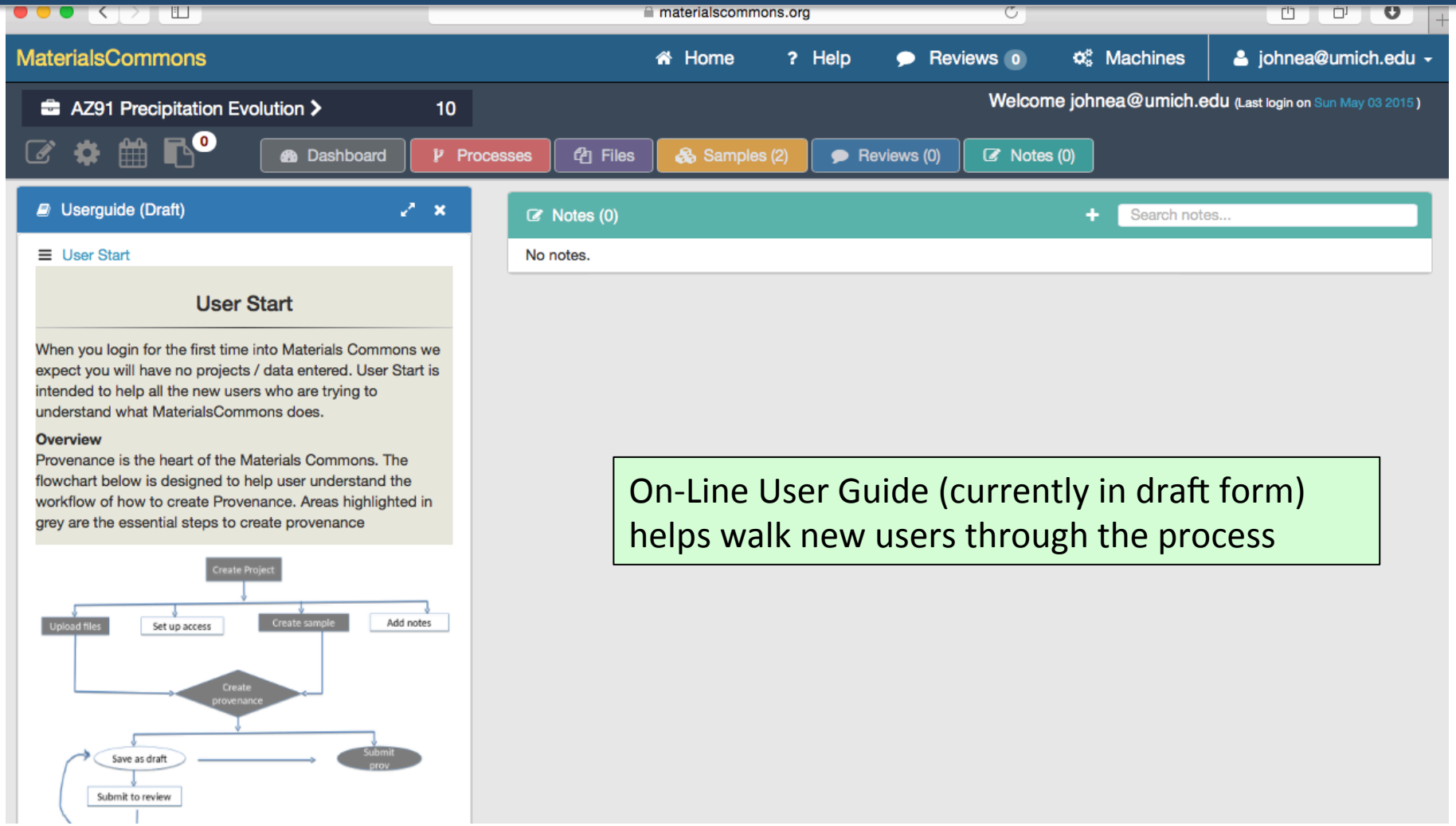


The Materials Commons:

https://materialscommons.org



The Materials Commons - Interface



On-Line User Guide (currently in draft form) helps walk new users through the process

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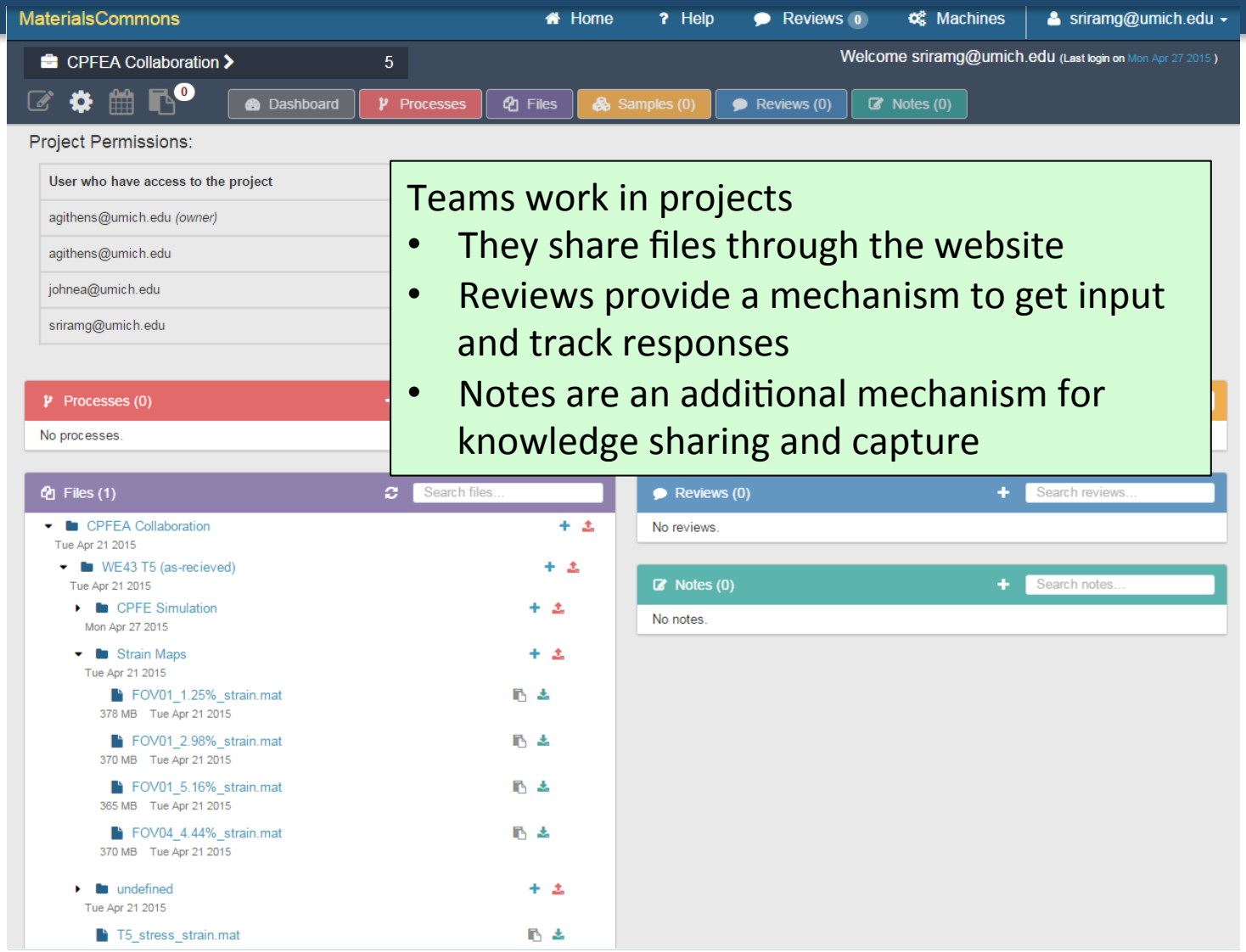
The Materials Commons - Collaboration



Teams work in projects

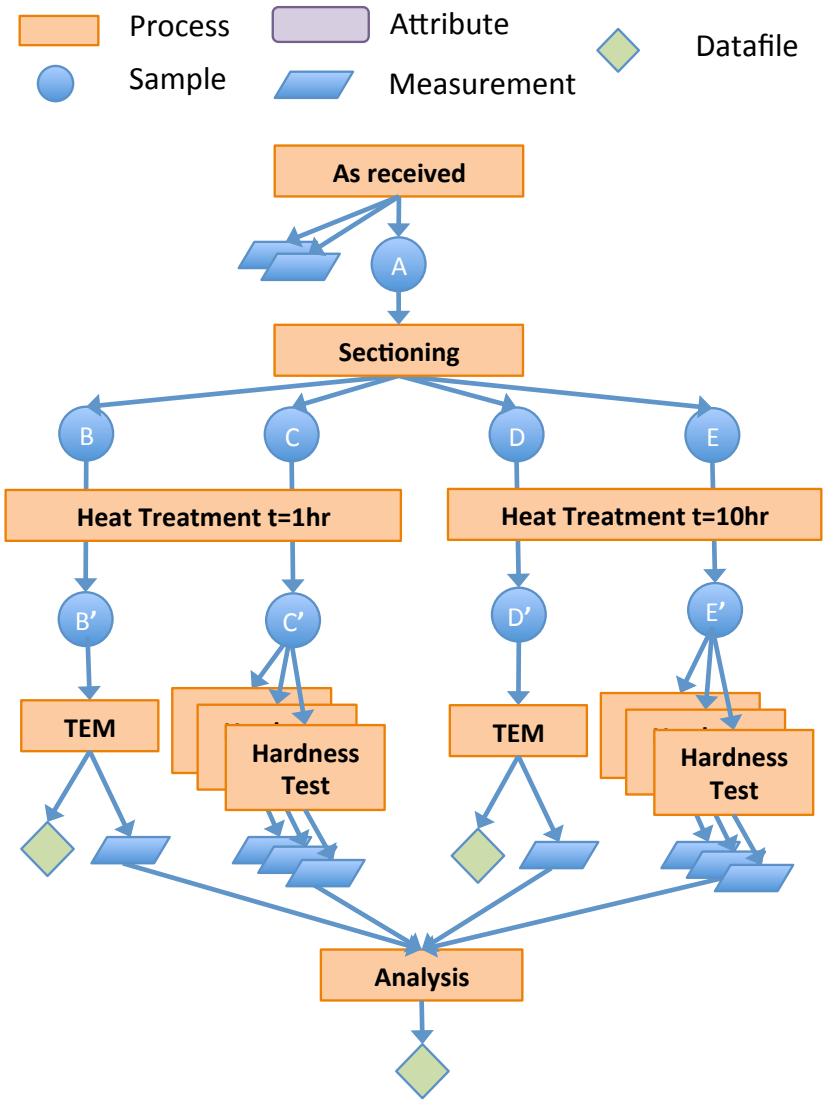
- They share files through the website
- Reviews provide a mechanism to get input and track responses
- Notes are an additional mechanism for knowledge sharing and capture

PRISMS

Materials Commons Data Model

- *Sample:* Representations of real or virtual things
  - materials, experimental or virtual specimens, etc.
- *Sample Attributes:* Measured attributes of a sample
  - grain size, weight, modulus, concentration, diffusivity, etc.
- *Measurements:* A measured value of a sample attribute.
  - may be one or many per sample attribute
- *Process:* Representations of actions
  - APT, SEM, Fatigue Test, Monte Carlo Calculation, Continuum Plasticity Calculation, etc.
  - specifices if a process transforms a sample attribute
  - templates specify what provenance information must / should / can be given

Materials Commons Data Model

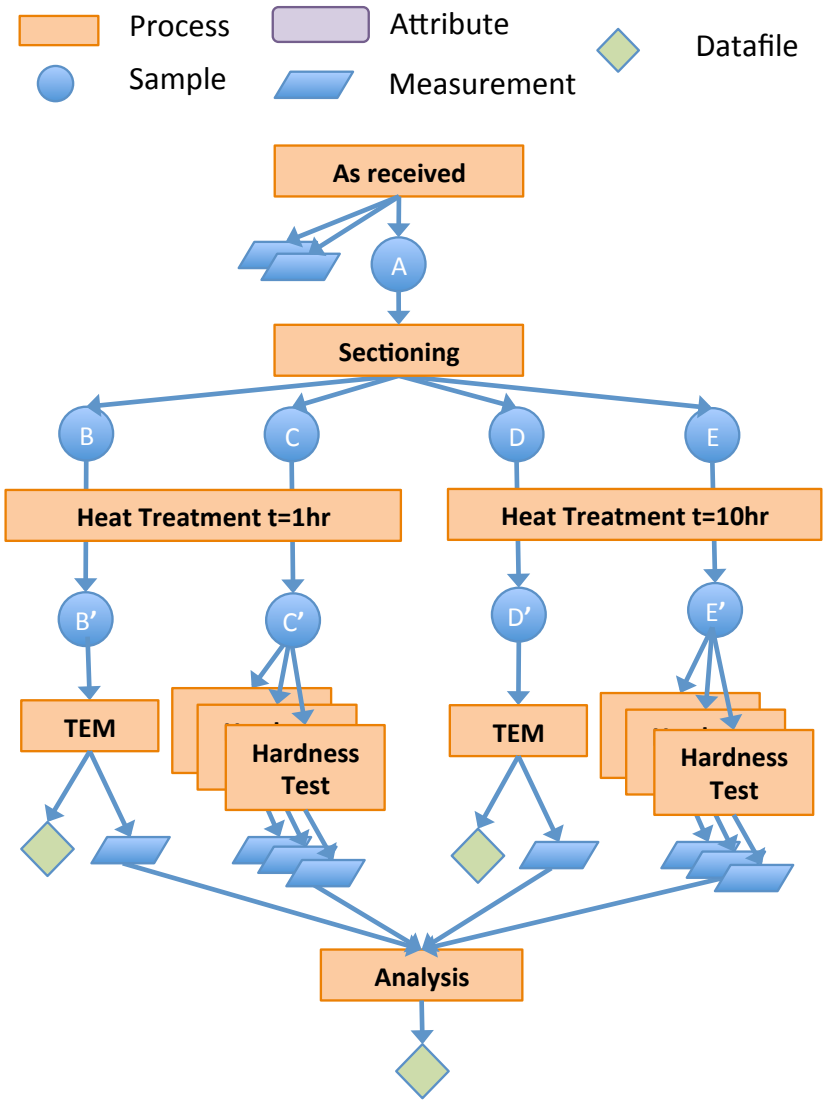


Example experiment:

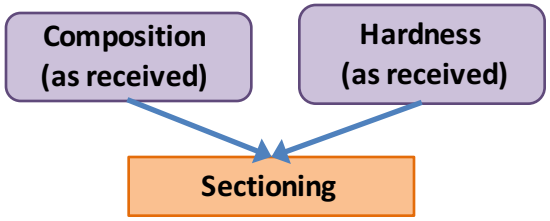
Ppt. size & hardness = f(heat treatment)

- Recieve material
- Section into specimens
- Measure ppt. size by TEM
- Measure hardness by indentation tests
- Analyze the results, fit them to a model, and create plots.

Materials Commons Data Model

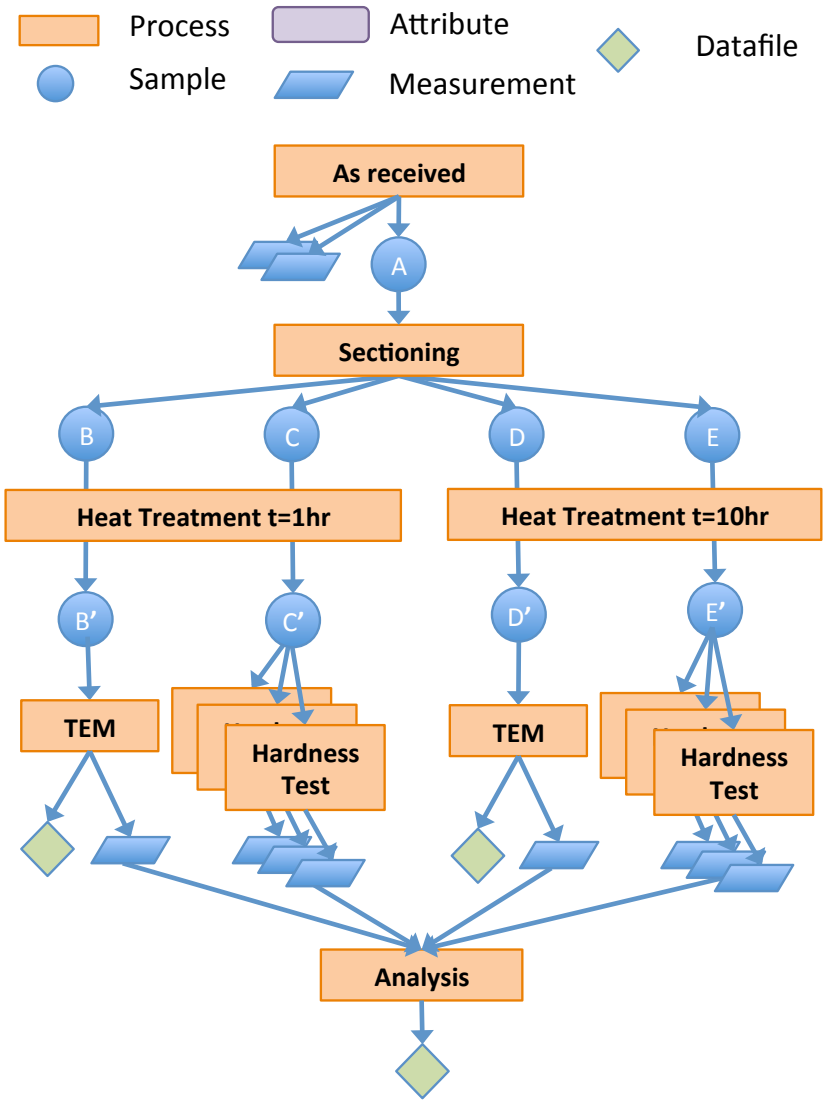


Scientific knowledge is encoded in the process data:



- Sectioning creates new samples, but the created samples have the same composition and hardness.
- Measurements on one sample (A, B, C, D, or E) can be applied to all samples.

Materials Commons Data Model



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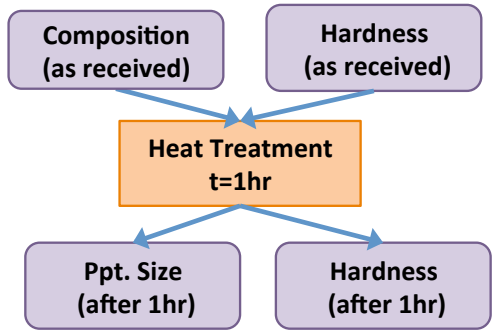
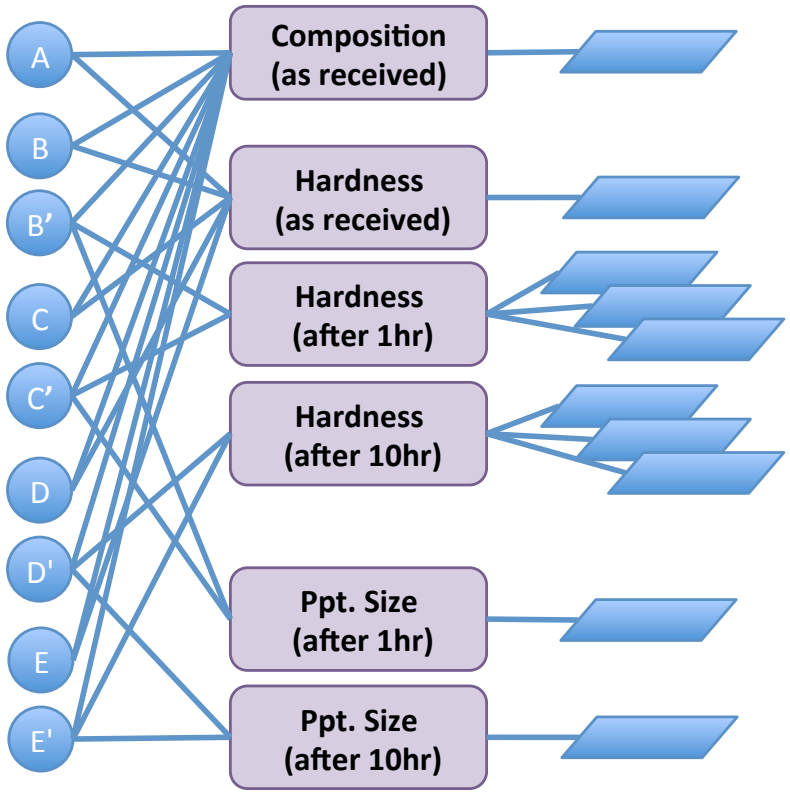


- Heat treatment (ex. B -> B') does not transform the composition, but it does transform the hardness and ppt. size.

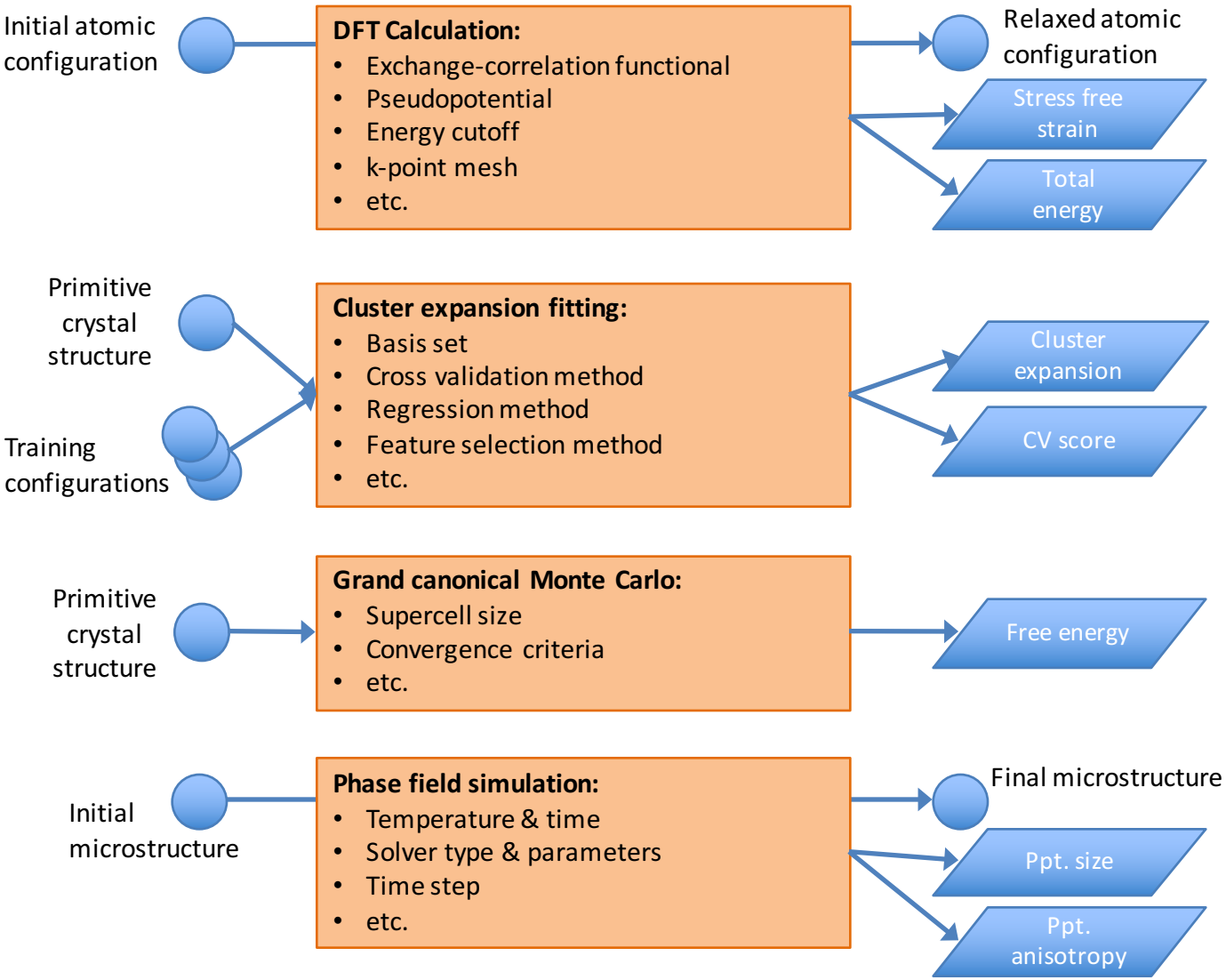
Materials Commons Data Model



Attributes may be shared across samples, so measurements are immediately applied to all relevant samples.

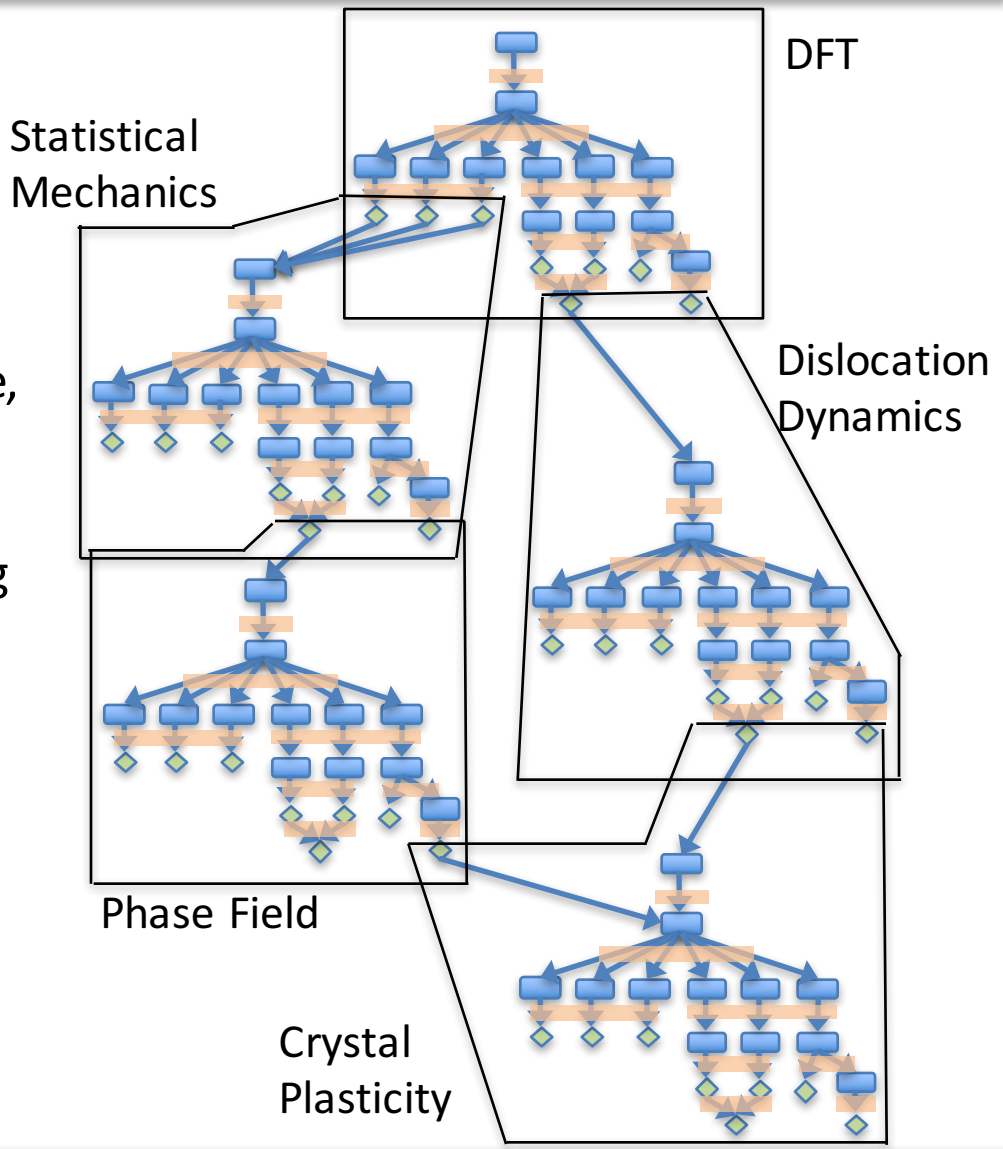
- Composition:
  - shared by all samples
- Hardness (as received)
  - shared by {A, B, C, D, E}
- Hardness and Ppt. size (after 1hr):
  - shared by {B', C'}
- Hardness and Ppt. size (after 10hr):
  - shared by {D', E'}

Provenance for Multi-scale Modeling



Share provenance

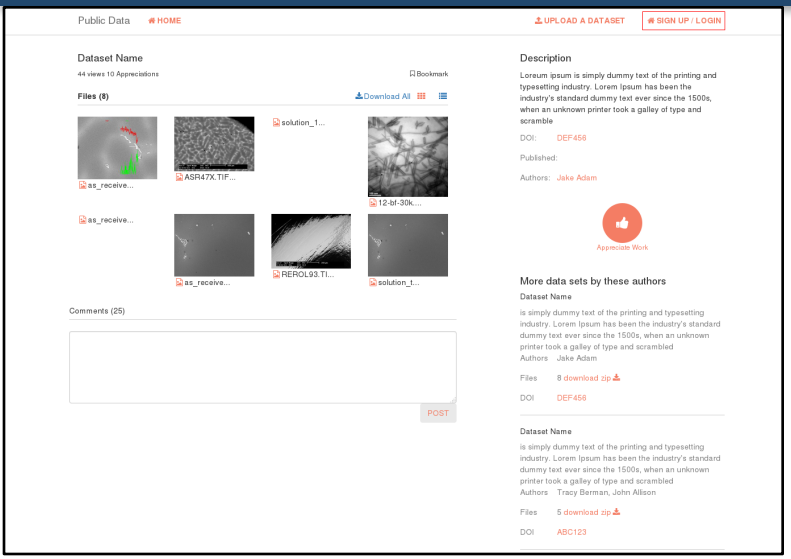
- Once a project or dataset is shared with you, you may include it's sample, processes, etc. in another project.
- Data may be re-used while maintaing provenance



Use Data

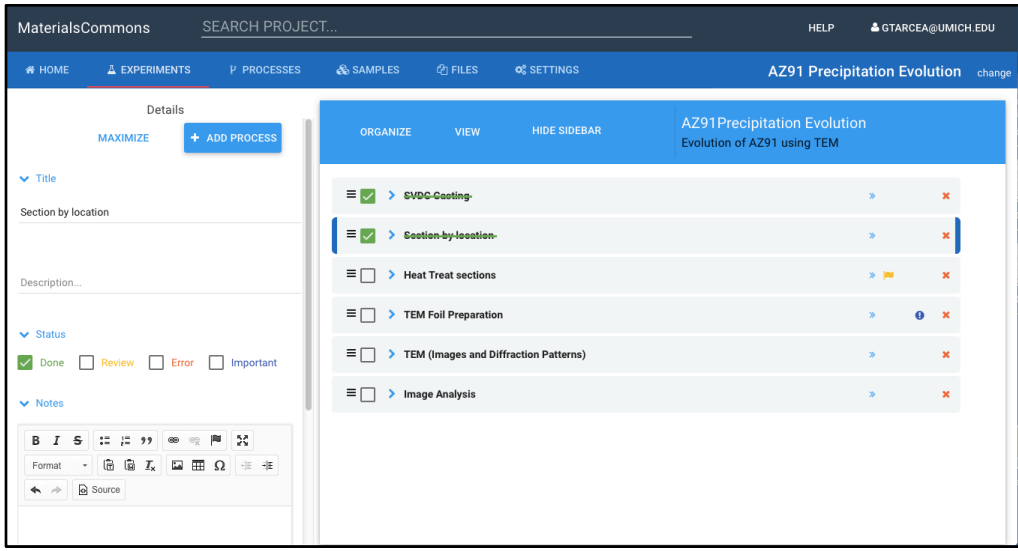
- Flexibly visualize and analyze
- Fit constitutive models
- Fit process models
- Provenance graph -> workflow -> optimization:
  - Multi-scale integration
  - Material design
  - Model reduction
  - Optimal design of experiments and computations

The Materials Commons
Upcoming Features



- Make public datasets:
  - Persistent identifiers
  - Search and browse for datasets
  - Give / get feedback, usage stats
  - Download formatted data
  - Re-use data in new projects, maintaining provenance

- New "Experiments" inteface:
  - Organize 'task' or 'todo' list
  - Document as you go
  - Provenance graph is built for you
  - Ready to make public when finished
- Python API
  - Write scripts to upload & download data and provenance



PRISMS

Conclusions

- The Materials Commons is a novel information repository and collaboration platform for the materials community
  - Focus on PRISMS technical emphasis areas
- Aim to be a seamless part of the scientific workflow
  - Structured data storage, with provenance
  - Collaborative
- Enables data use for science and engineering

Materials Commons Technologies

- API/REST Services are all JSON based
- Data Sync is moving to MsgPak, Curve, and ZeroMQ
- Website uses Socket.IO for real time updates, REST/JSON for service access
  - Just started integrating this in
- JSON Document store on backend (RethinkDB)
- Website written using AngularJS
- Backend is a mix of Python and Go
- Some Erlang mixed in
- RabbitMQ used for pipeline processing

Architecture Block Diagram