An Integrated Collaborative Environment for Materials Research

ICE INTEGRATED COLLABORATIVE ENVIRONMENT

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Integrity ★ Service ★ Excellence

Presentation Roadmap

- Introduce ICE
- Review integration case
- Present a vision for the future of ICE and like systems

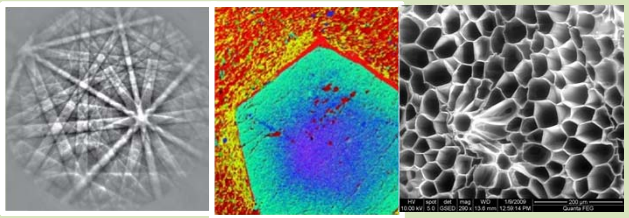
Acknowledgements

- Dr. Charles Ward
- Bryon Foster
- The rest of the team

Materials and Manufacturing
Research Infrastructure

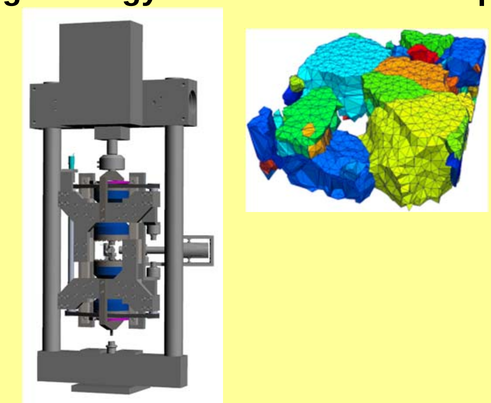
- **700+ scientists and engineers**
- **108,000 sq ft lab space, 200 lab modules**
- **750+ computers associated with research equipment**
- **1000+ computers on desks: 2 separate networks**
- **80+ scientific and engineering software packages**
- **Local computational clusters & remote HPC**

Materials Characterization Facility



DSRC Lightning

High Energy Diffraction Microscopy



And no supporting collaborative research environment

An Integrated Collaborative Environment

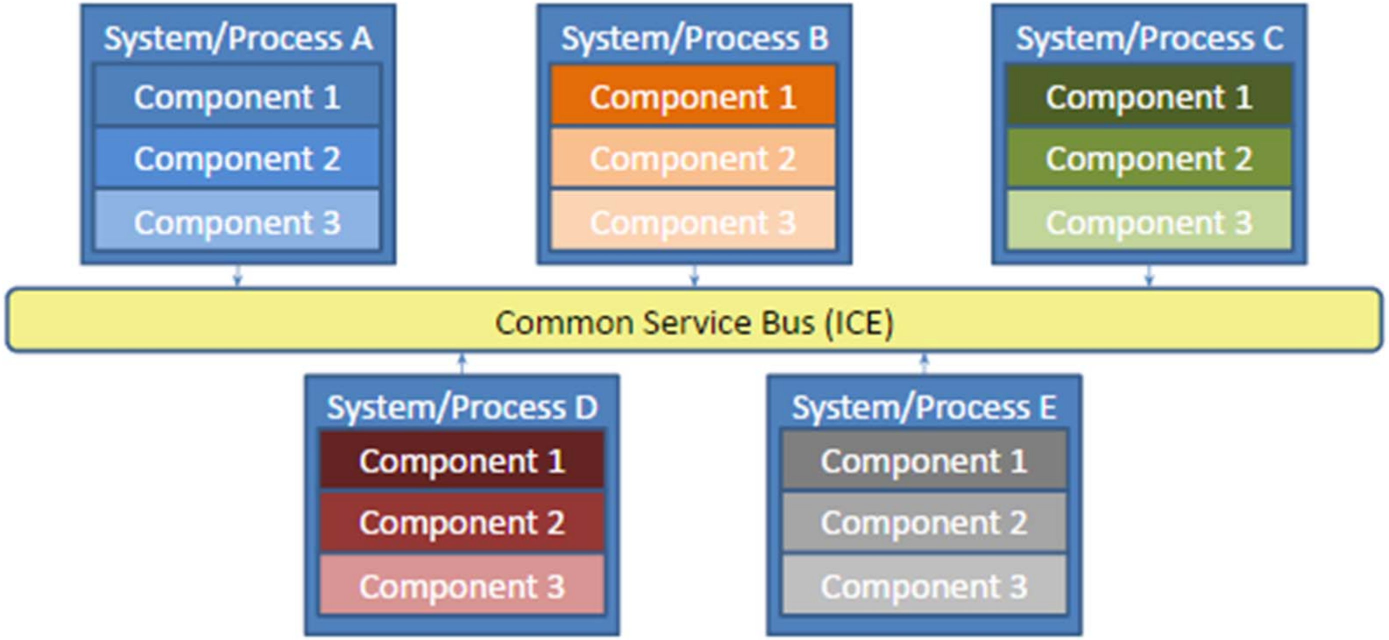
- The Materials Genome Initiative (MGI) calls for a Materials Innovation Infrastructure, in agreement with the goals of ICMSE
- ICE is a highly tailored, federated infrastructure built for the R&D community
- ICE represents a joint effort between software and materials engineers to deliver game-changing functionality

ICE-Enabled Capabilities

- The coordination and management of research activities
- The collection of research data (structured and unstructured)
- Complete traceability of material evolution
- Legacy data sources to continue to exist in many cases, but with connections to ICE API
- Growth of the RX ICMSE culture

Federated Concept

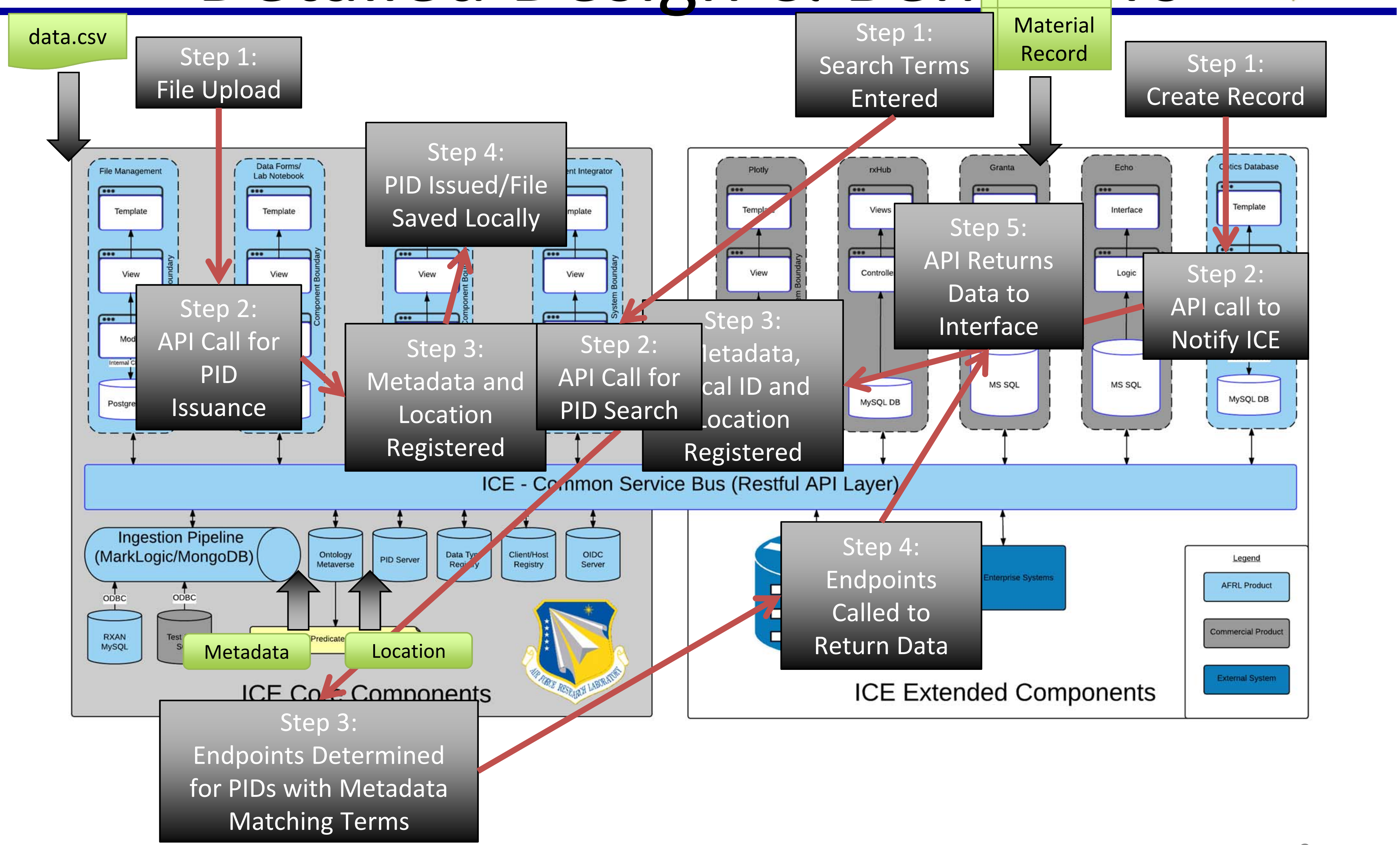
- The Federated Architecture allows for self-governance of connected systems
- Systems may be COTS tools, in-house developed applications, or any hybrid thereof
- Systems do not talk directly to each other - ICE “brokers” all transactions between connected systems



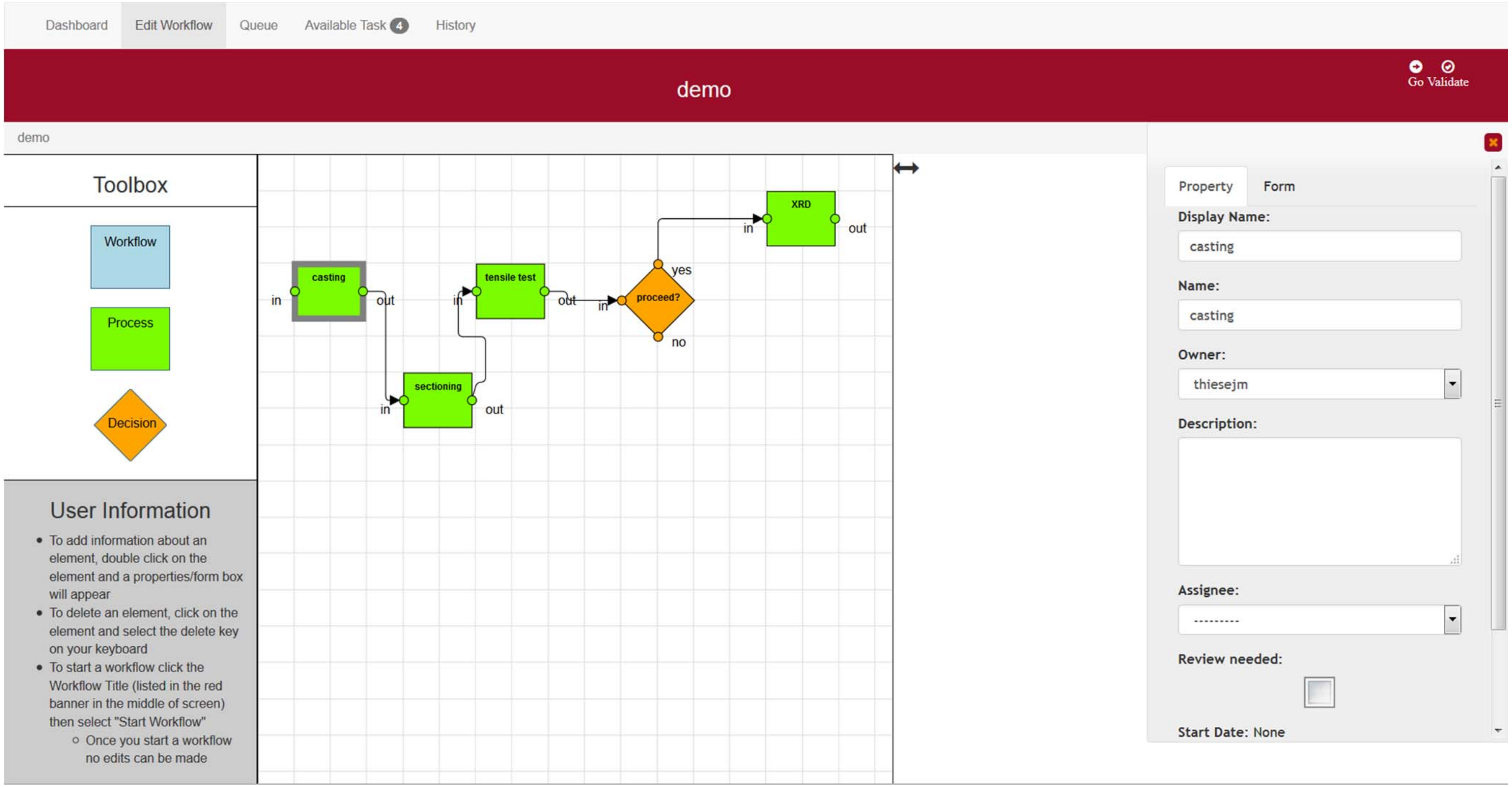
Architectural Solution

- ICE Core - Collaboration platform (Hub), Common Service Bus and Apps(Django), advanced visualization (Plotly)
- ICE Extended - Material properties database (Granta), MTS Echo, Dream.3D
- Persistent identification, triple-based metadata, data type registration and SSO
- Graphical workflow design tools, item management, file management, advanced search tools

Case 1: PID Store | Case 3: Searching/Querying Data | PID Linked to Local ID



Data Creation via Workflow



Data Retrieval via Search

Search

718

Search

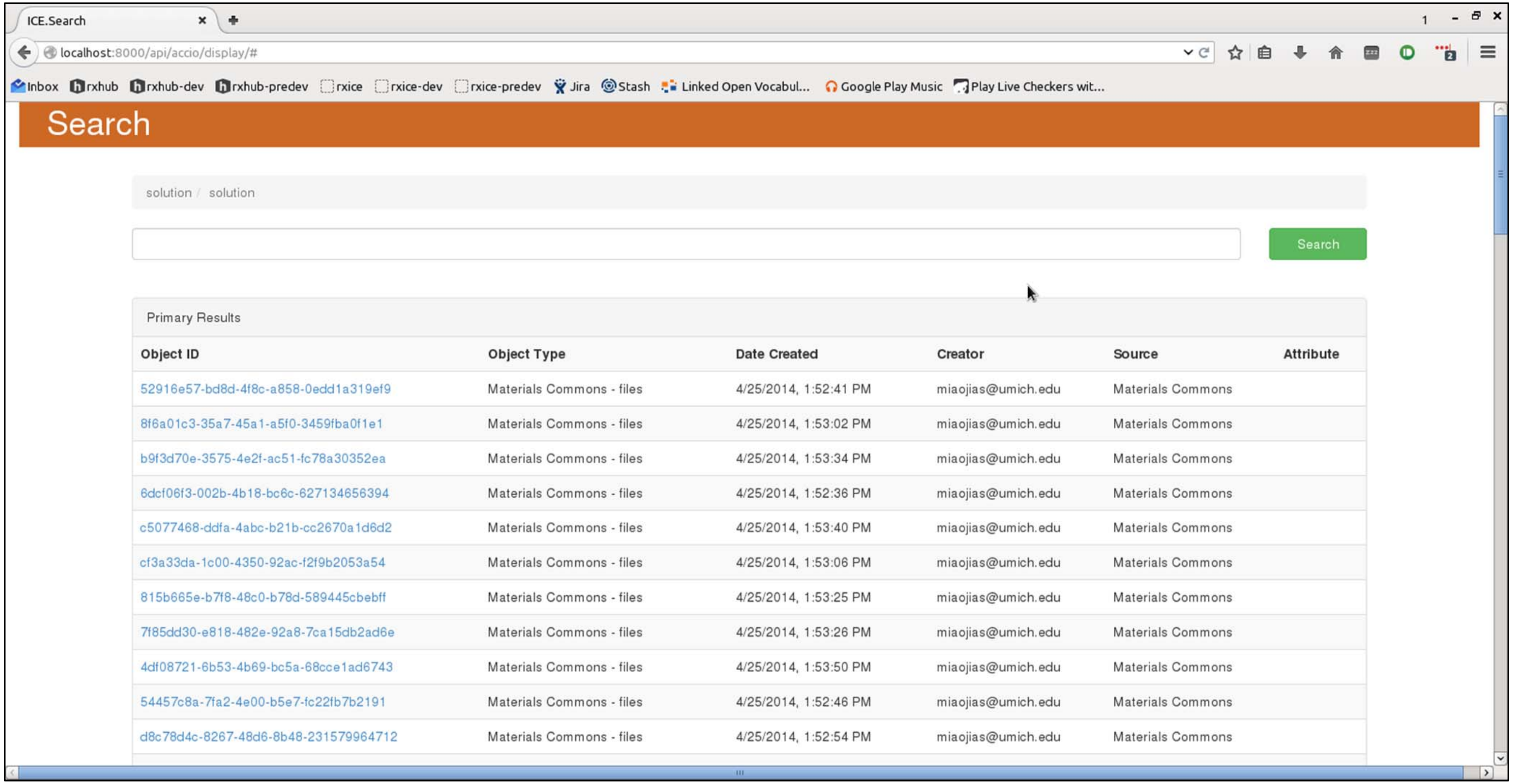
Primary Results

Object ID	Object Type	Date Created	Creator	Source	Attribute
78	Casting	11/18/2015, 5:25:05 PM	Workflow	ICE.forms	
82	Casting	11/19/2015, 8:31:48 AM	Workflow	ICE.forms	
57	XRD	11/20/2015, 3:16:54 PM	Workflow	ICE.forms	
61	Sectioning	11/24/2015, 10:18:02 AM	Workflow	ICE.forms	
46	TensileTest	11/24/2015, 11:46:22 AM	Workflow	ICE.forms	
65	TensileTest	12/4/2015, 11:49:32 AM	Workflow	ICE.forms	
4	CastingThermocouples	12/10/2015, 9:21:15 AM	Workflow	ICE.forms	
139	Casting	1/8/2016, 9:14:36 AM	Workflow	ICE.forms	
88	TensileTest	1/8/2016, 9:14:38 AM	Workflow	ICE.forms	
18	CastingAttributes	1/8/2016, 12:47:24 PM	Workflow	ICE.forms	
13202	GRANTA	Invalid Date	unknown	GRANTA	
13201	GRANTA	Invalid Date	unknown	GRANTA	
26678	GRANTA	Invalid Date	unknown	GRANTA	
16221	GRANTA	Invalid Date	unknown	GRANTA	
26403	GRANTA	Invalid Date	unknown	GRANTA	
26693	GRANTA	Invalid Date	unknown	GRANTA	
26694	GRANTA	Invalid Date	unknown	GRANTA	
12249	GRANTA	Invalid Date	unknown	GRANTA	
12250	GRANTA	Invalid Date	unknown	GRANTA	

System Connection

- Test case – U of M's Materials Commons
- Add Materials Commons API to ICE.Search
  - ICE delegates search mechanism to Materials Commons
  - Materials Commons relies on Elasticsearch (full text) vs object search (ICE.Search)
- Connection established after 4 hours of collaboration
  - RESTful call with authentication token and search string
  - JSON returned, shaped into search result format

Search Extended to Materials Commons



Object ID	Object Type	Date Created	Creator	Source	Attribute
52916e57-bd8d-4f8c-a858-0edd1a319ef9	Materials Commons - files	4/25/2014, 1:52:41 PM	miaojias@umich.edu	Materials Commons	
8f6a01c3-35a7-45a1-a5f0-3459fba0f1e1	Materials Commons - files	4/25/2014, 1:53:02 PM	miaojias@umich.edu	Materials Commons	
b9f3d70e-3575-4e2f-ac51-fc78a30352ea	Materials Commons - files	4/25/2014, 1:53:34 PM	miaojias@umich.edu	Materials Commons	
6dcf06f3-002b-4b18-bc6c-627134656394	Materials Commons - files	4/25/2014, 1:52:36 PM	miaojias@umich.edu	Materials Commons	
c5077468-ddfa-4abc-b21b-cc2670a1d6d2	Materials Commons - files	4/25/2014, 1:53:40 PM	miaojias@umich.edu	Materials Commons	
cf3a33da-1c00-4350-92ac-f2f9b2053a54	Materials Commons - files	4/25/2014, 1:53:06 PM	miaojias@umich.edu	Materials Commons	
815b665e-b7f8-48c0-b78d-589445cbebff	Materials Commons - files	4/25/2014, 1:53:25 PM	miaojias@umich.edu	Materials Commons	
7f85dd30-e818-482e-92a8-7ca15db2ad6e	Materials Commons - files	4/25/2014, 1:53:26 PM	miaojias@umich.edu	Materials Commons	
4df08721-6b53-4b69-bc5a-68cce1ad6743	Materials Commons - files	4/25/2014, 1:53:50 PM	miaojias@umich.edu	Materials Commons	
54457c8a-7fa2-4e00-b5e7-fc22fb7b2191	Materials Commons - files	4/25/2014, 1:52:46 PM	miaojias@umich.edu	Materials Commons	
d8c78d4c-8267-48d6-8b48-231579964712	Materials Commons - files	4/25/2014, 1:52:54 PM	miaojias@umich.edu	Materials Commons	

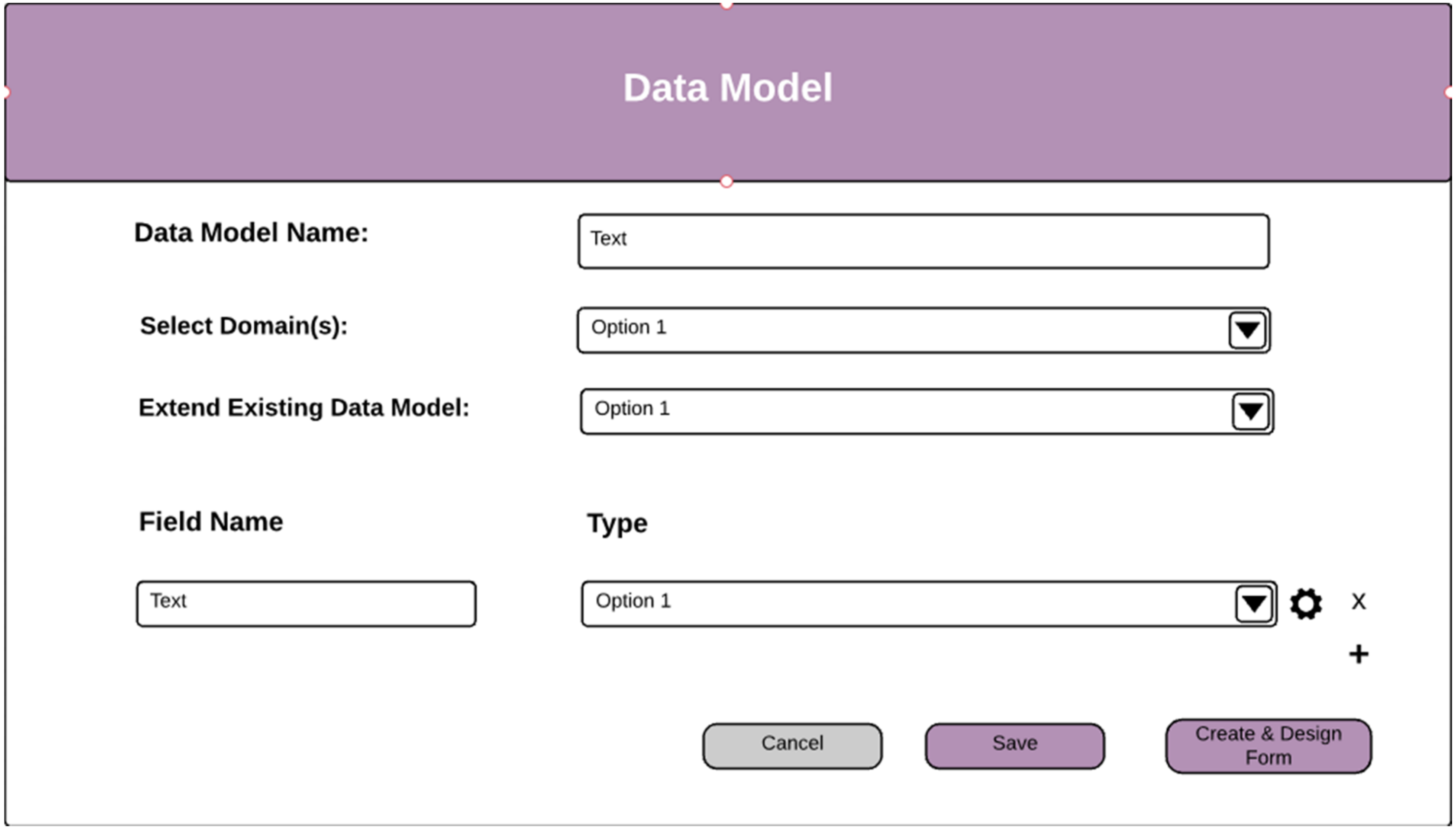
Object Instantiation

- Persistent Problem – how to treat workflow processes, participants, and items (physical and digital) as first class objects?
- Begin to register various data types – object "classes"
- Ex. Tension test, titanium specimen, etc.
- Invoke registered data types wherever possible
- Index all metadata assignments based on object type

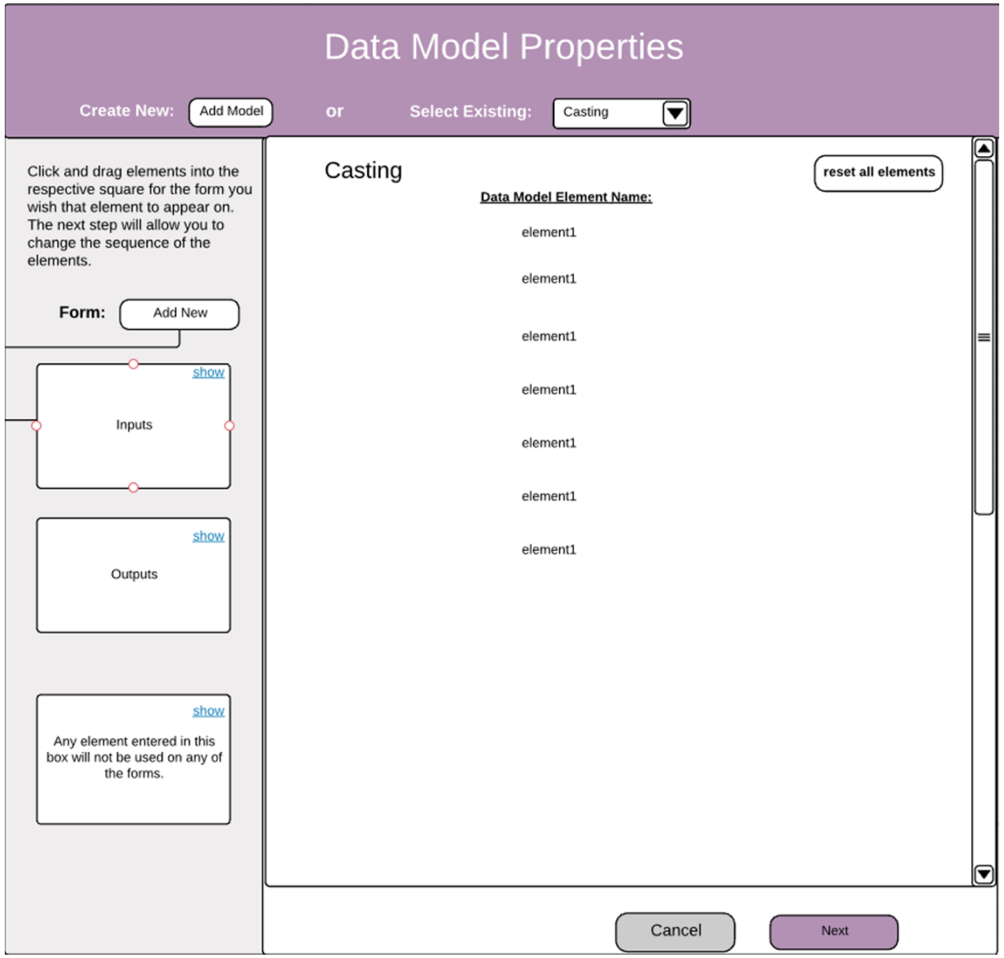
New Functionality

- Data Model Builder – open up the DTR to certain users
- Graphical interface for defining data models and linkages/nesting
- DTR is implemented with OO principles of inheritance
- Use a NoSQL structure to define “parent” classes (casting) and child classes (investment casting)
- Restrict instantiation of new objects (even metadata) to those entries in the DTR.

Example 1 – Data Model Builder



Example 2 – Form Builder



An Improvement, but…

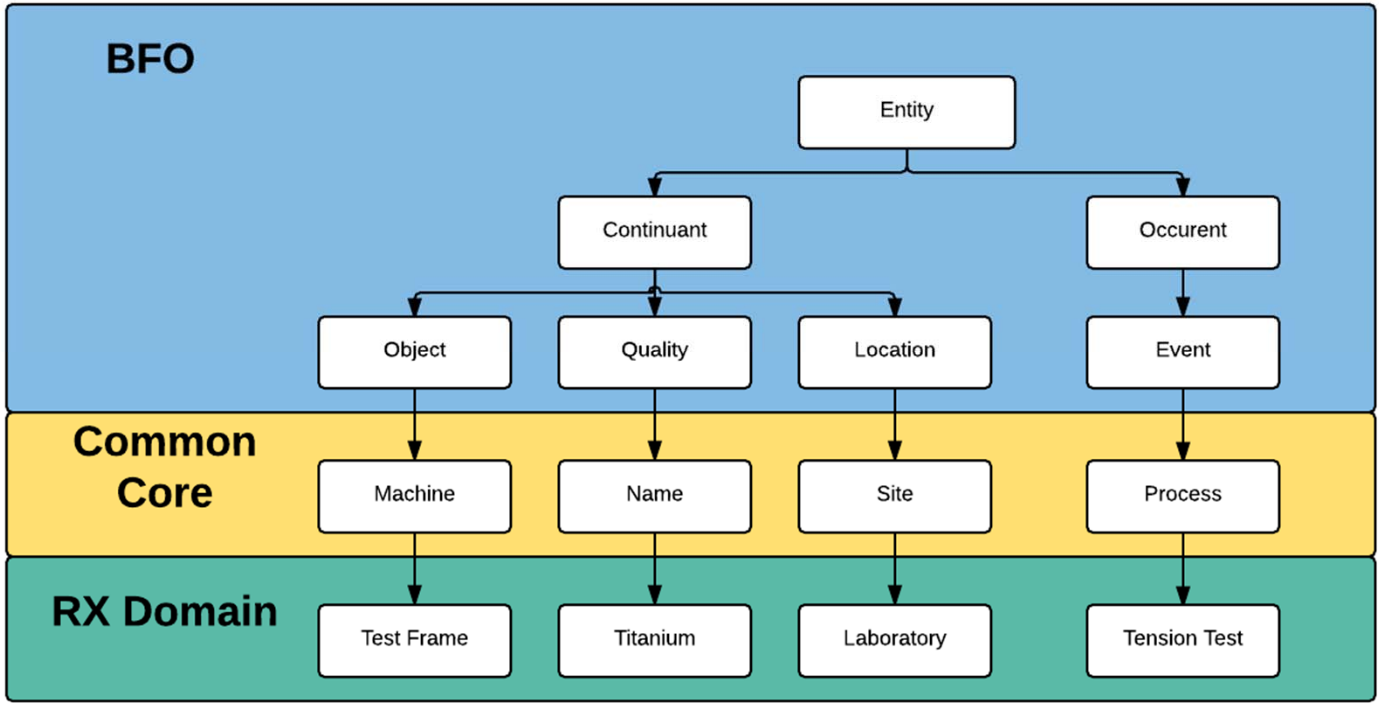
- Still not “semantic” – how do we relate our classes?
- We need a simple way (baby steps) to start building vocabularies, taxonomies, and domain-specific ontologies
- Our users are overwhelmed at the utterance of “ontology”
- Enter the Basic Formal Ontology

Basic Formal Ontology

- Created by Dr. Barry Smith and others circa 2000
- Establishes a high level framework for building out domain ontologies
- Successfully used in biomedicine, human genome project, Army, etc.
- Extended by “common core” ontologies, and further in domain specific ontologies

BFO High Level

- Try to abstract objects from processes (test frame from the test for example) and use “occurents” only as needed
- Most things can and should be described as continuants
- Separate objects from qualities/properties

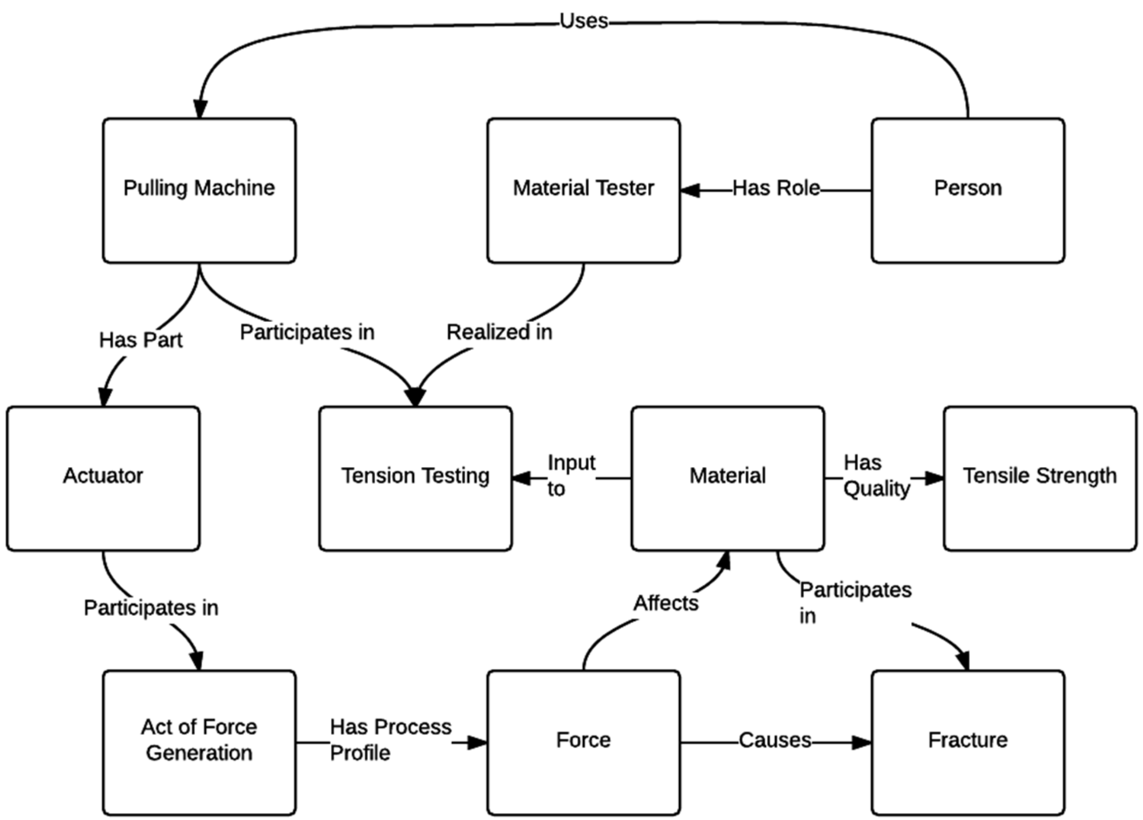


Approach

- Whiteboard a concept
- Build a taxonomy
- Define relationships
- Construct domain ontology from taxonomy and relational elements
- Continuously refine the ontology
- Propagate into other domains

Example – Tension Test

- First stab – not perfect, but gives plenty of elements to start fitting into a taxonomy
- Key point – the SME must be involved and be comfortable with the flow



Taxonomy and Relationships

- Materials
  - Metals
    - Stainless Steel
  - Non-Metals
  - …..
- Quality
  - Porosity
  - Density
  - Transmittance
  - ….
- Relationships
  - Participates in
  - Contains

- Systems like Granta do this pretty well already
- Downside is that the qualities are dependent

- Object instances pull from all tiers:

-Ex: Sample of Stainless Steel has qualities X, Y, Z, and was part of Test A

- Qualities are only invoked in the instance, not the class

Value Proposition

- System integration is greatly enhanced by using common schema/vocabulary/ontology
- Eases total ecosystem burden with standard models/classes
- Existing schema/ontology momentum in many S&T communities

Next steps

- Engage SMEs and flesh out the mechanical test domain
- Build into BFO domain ontology in Protégé
- Flatten out the taxonomy and ontology
- Build an inferencing engine for determining identities based solely on qualities, similar to a graph-based templating search
- Implement common domain elements in partnering systems

- **We need to collaborate!!**

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