Graphical Materials Histories – Making the Invisible Visible

David Elbert: elbert@jhu.edu

CDO PARADIM Materials Innovation Platform (MIP) (2DLIM/Quantum Materials)
ARL HTMDEC Extreme Data (ceramics and alloys)
NASA IMQCAM STRI (additive metals digital twin)
NSF DMREF (streaming data alloys and recycled polymers)
DOE-BES Catalysis (zeolite scaling)

Scope: Data Production and Use

MaRDA (Materials Research Data Alliance)
MaRCN FAIROS-RCN

Scope: Community – People are Infrastructure, Too

Co-Conspirators!

Maggie Eminizer (JHU)
Ali Rachidi (JHU)
Matt Turk (UIUC)
Kacper Kowalik (NCSA/UIUC)
Craig Willis (UIUC)





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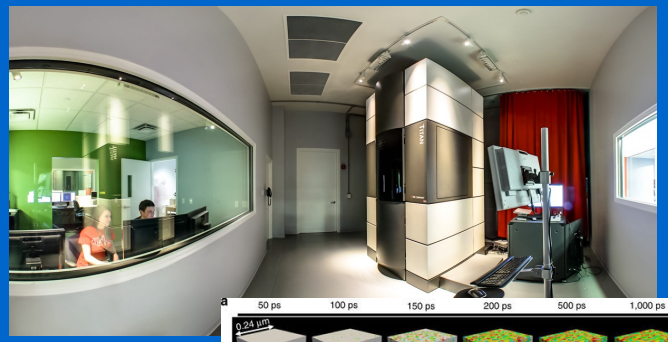
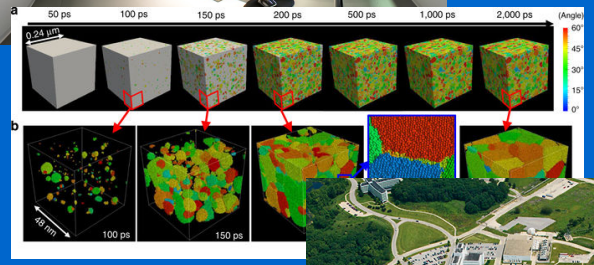
Challenges





- Materials Data is Vast and Diverse
- Materials Research is Widely Distributed
  - Place/Time/Kind
- Workflows are Numerous/Diverse/Changing
- AI/ML is Powerful yet Nascent
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- *First-Mile Problem – Model Instantiation Tools and Automation*
  - OpenMSI Streaming and Modeling
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  - PID samples/instruments/anything linked or shared – Simplify the Simple
- Intellectual Interoperability
  - Incentivized to have solved the problem
  - "Do it my way"

Scientists are the worst judges of the reuse of their own data

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Why? (don't forget about why! Use cases change but why often stays the same.)

Fundamental Materials Problems – How do you Discover a Novel Material?

- Understand how a material works
- Reveal structure-property-synthesis relationships
- Provide path to make designed materials
  - If you can't make it, it doesn't exist
- Expand knowledge of parameter and design space

Can AI/ML Address Fundamental Problems?

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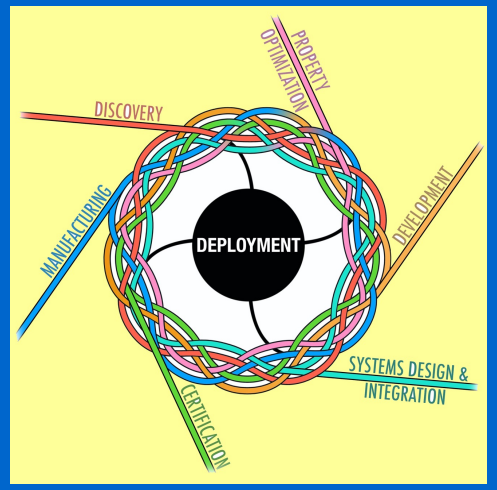
Material Histories Are Fundamental

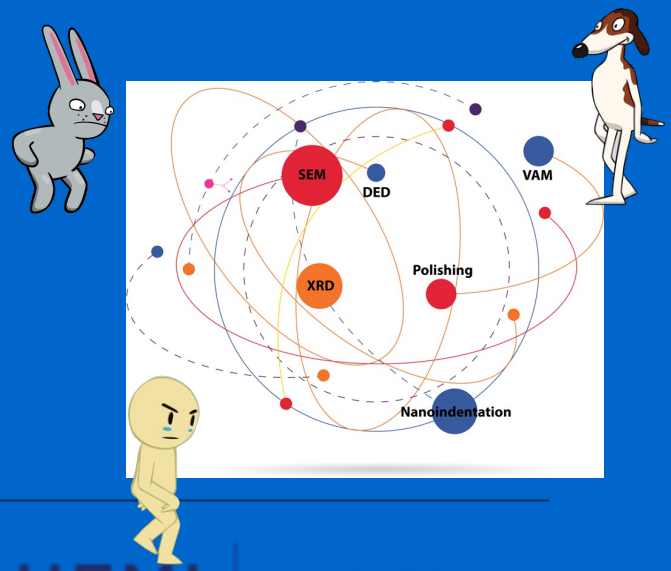
Data alone is not enough

- History is directed
- Graphs underlie research
- Graphs underlie production

Histories are Connected Data



MGI Strategic Plan https://mgi.gov



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Autonomy Revolution: *A Secret Superpower*

- Automating Everything
- High Throughput
- Automation + Decisions = Autonomy
- Data Infrastructure
  - Enables automation
  - Deploys decisions

Review Article | Published: 30 January 2023

The rise of self-driving labs in chemical and materials sciences

Milad Abolhasani & Eugenia Kumacheva

Nature Synthesis **2**, 483–492 (2023) | Cite this article

14k Accesses | **9** Citations | **23** Altmetric | Metrics

The high-throughput highway to computational materials design

Stefano Curtarolo, Gus L. W. Hart, Marco Buongiorno Nardelli, Natalio Mingo, Stefano Sanvito & Ohad Levy

Nature Materials **12**, 191–201 (2013) | Cite this article

43k Accesses | **1357** Citations | **34** Altmetric | Metrics

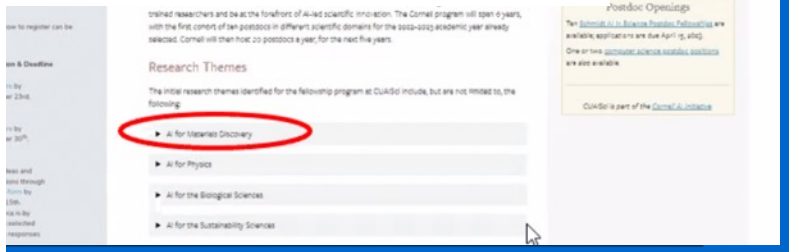
Review Article | Published: 09 March 2023

Combinatorial synthesis for AI-driven materials discovery

John M. Gregoire, Lan Zhou & Joel A. Haber

Nature Synthesis **2**, 493–504 (2023) | Cite this article

1258 Accesses | **5** Altmetric | Metrics



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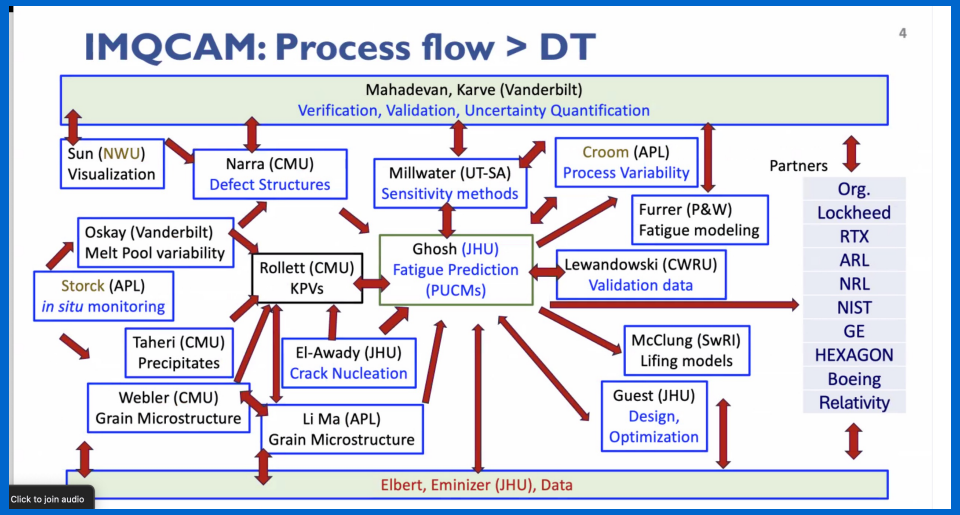
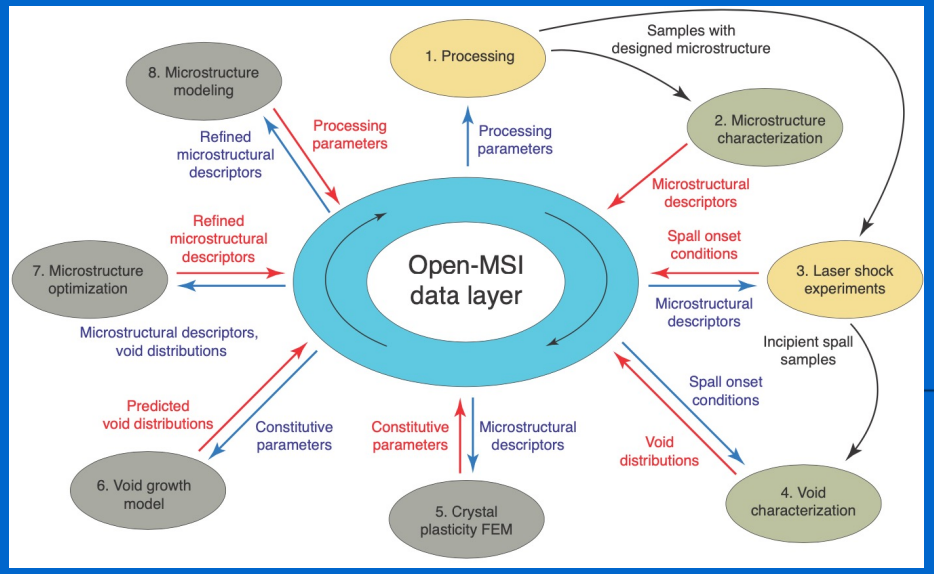
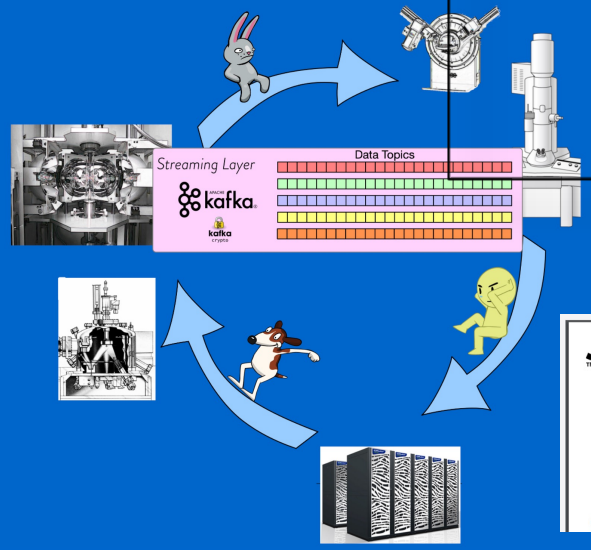
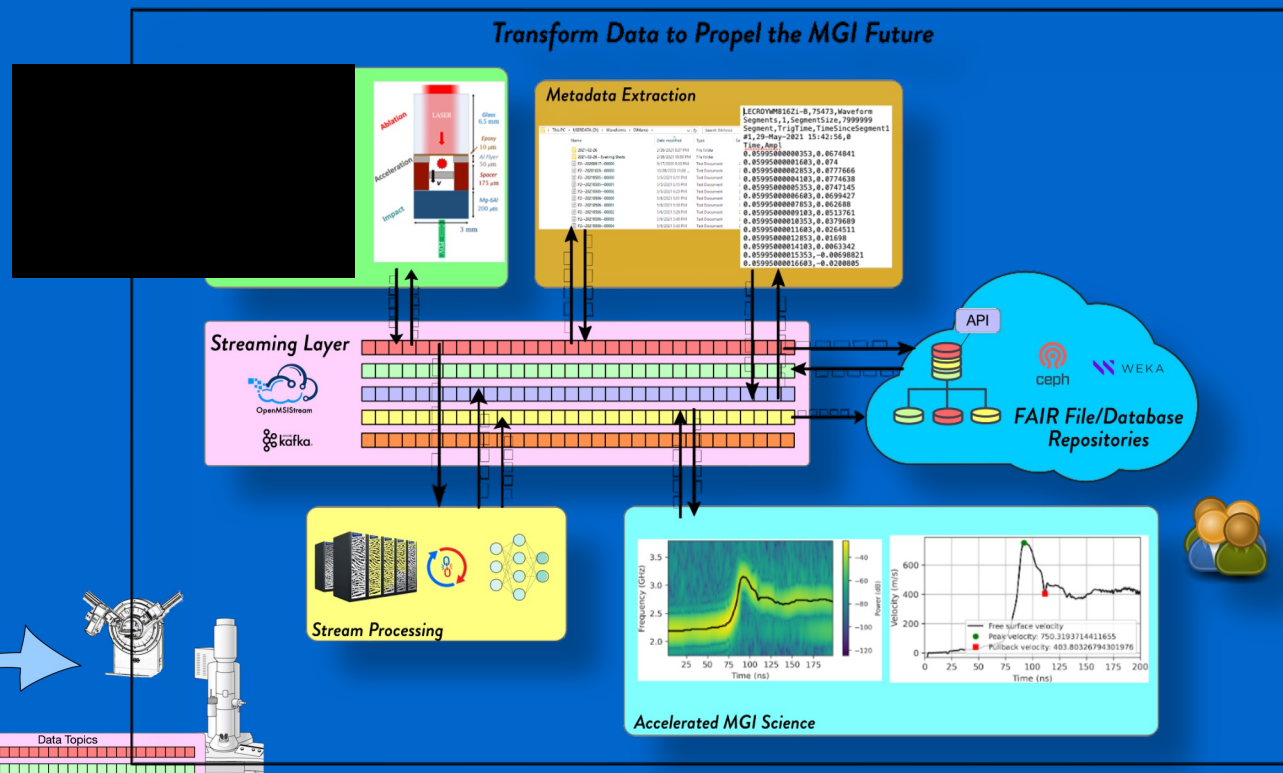
Workflows Connect to Workflows

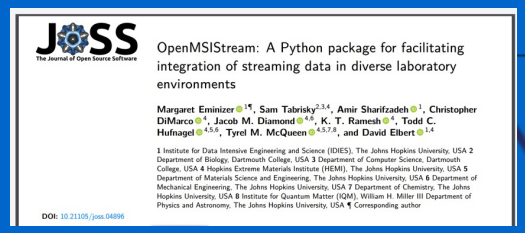
Data aggregation across complex, changing scientific workflows











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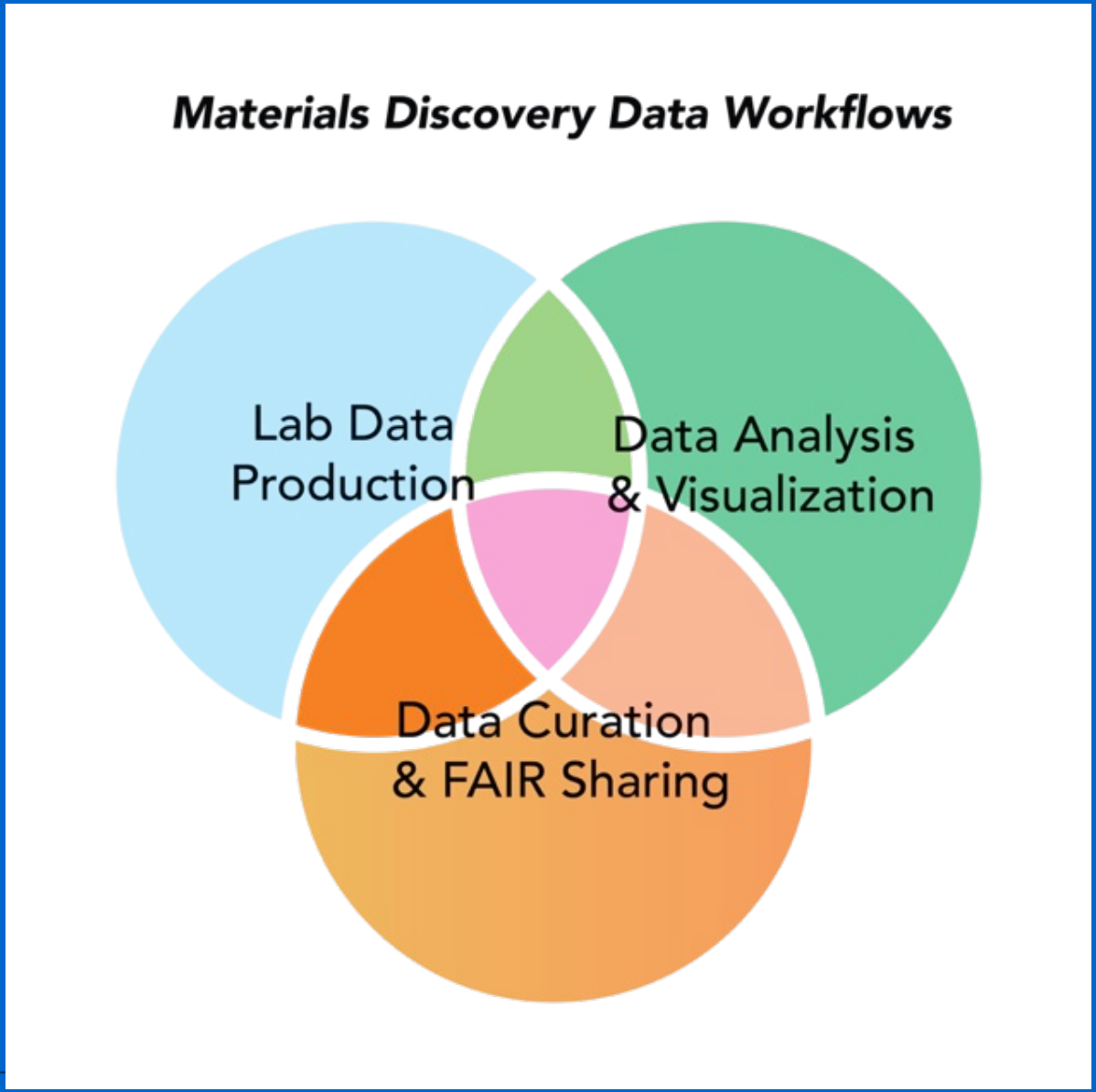
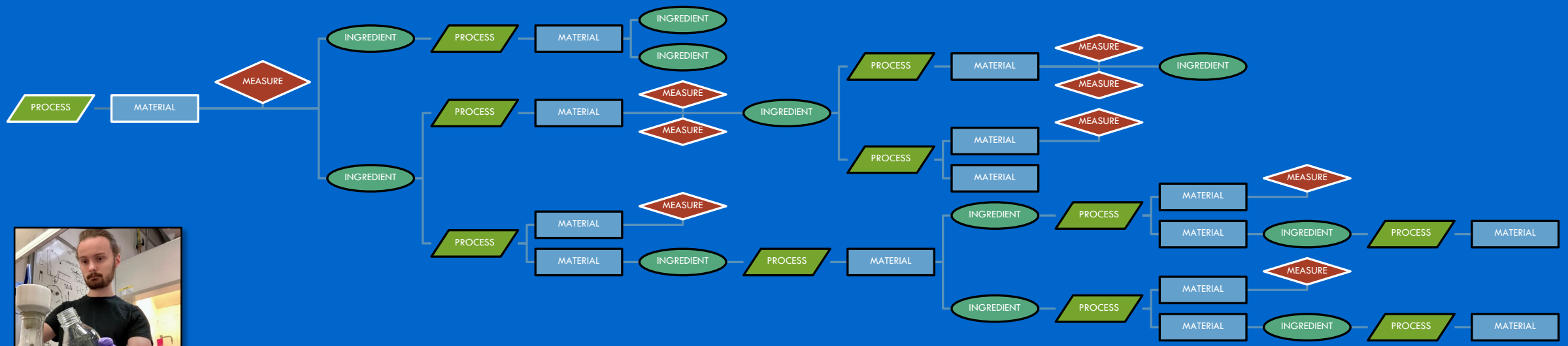
Workflows Unlock Everything

- Three Types:
  - Lab Data Production
  - Data Analysis and Visualization
  - Data Curation/Sharing
- Explicitly Describe Workflows
  - Prescribed or Captured
  - Directed Acyclic Graphs
  - Transparent/Repeatable/Connectable
  - Automated/Runnable



Material History Data Model (GEMD https://citrineinformatics.github.io/gemd-docs)

Work the way materials scientists work!



Gannon Murray, rising junior
Earlham College

https://github.com/paradimdata/YVO4_project

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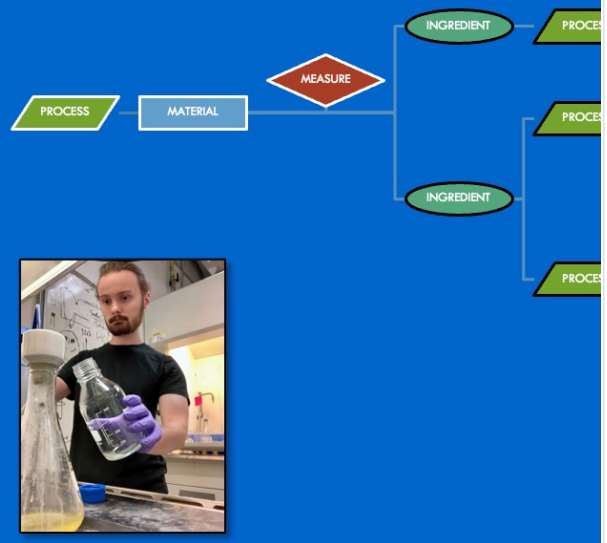
Coding the History

Details that never make it to the the literature



gb-murray Fixed GBM1005

Preview | Code | Blame 414 lines (414 loc) · 20.6 KB

Crucible Growth of YVO_4 from V_2O_5 and Y_2O_3 in Air

YVO4 was grown in an alumina crucible from Y and V oxides using a furnace.

The purpose of the experiment was to test the effects of vanadium deficiency on phase formation.

Performed 2023-06-09 @ ML by GBM

In [9]:

```
### Imports ###

from tools.attr_utils import *
from tools.block.Block import Block
from tools.utilities import *

from utils.block_builders import *
from utils.base_builders import *
from utils.provenance import Provenance

from gemd import FileLink
from gemd.json import GEMDJson
import gemd

import os
```

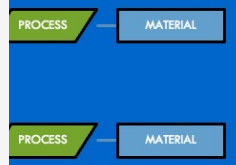
In [10]:

```
### Provenance ###

prv = Provenance(
    name='Gannon Murray',
    email='gmurra12@jh.edu',
    tag='GBM',
    page='1003',
    title='Crucible Growth of YVO4',
    date='2023-06-09'
)
```

In [11]:

```
### Workflow ###

GBM1003 = {}
```

Screenshot



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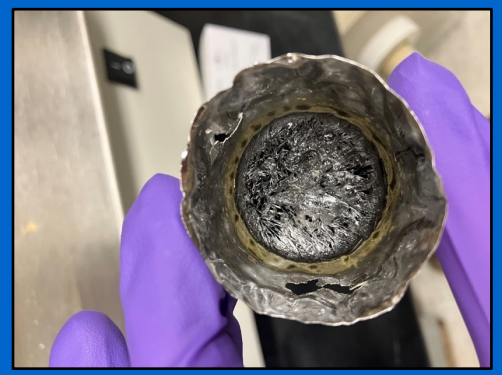
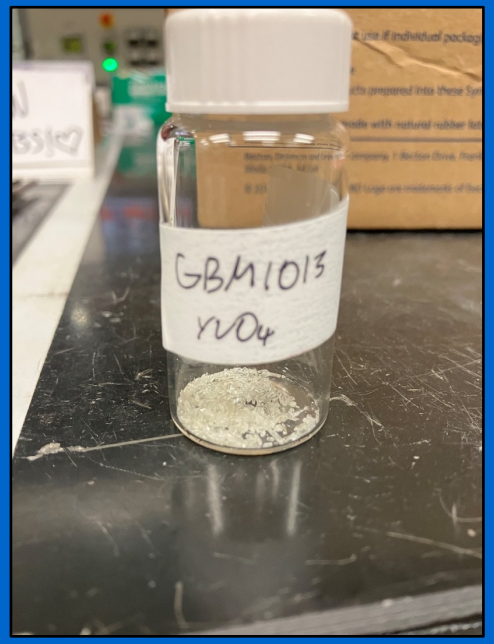
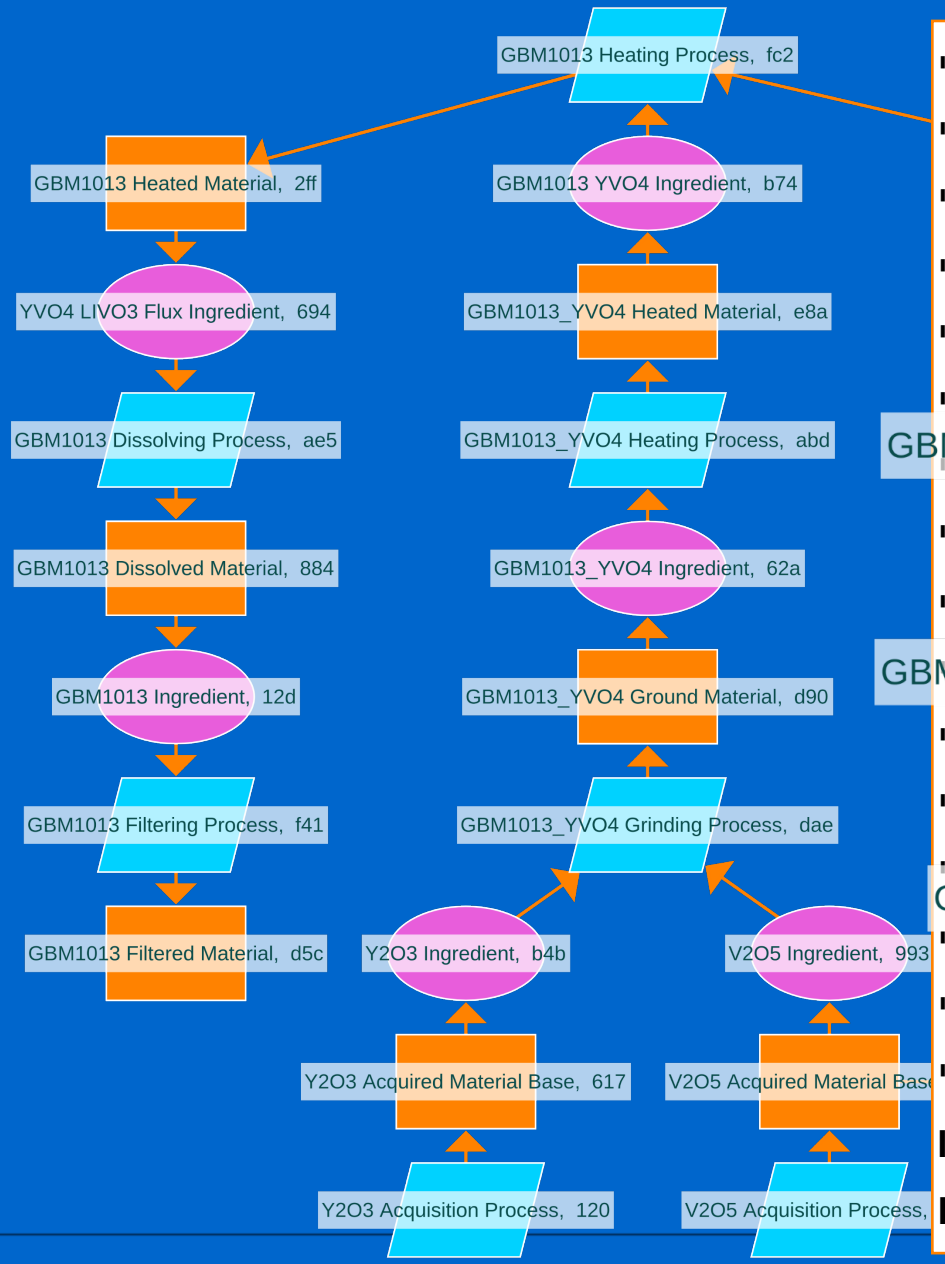
https://github.com/paradimdata/YVO4_project







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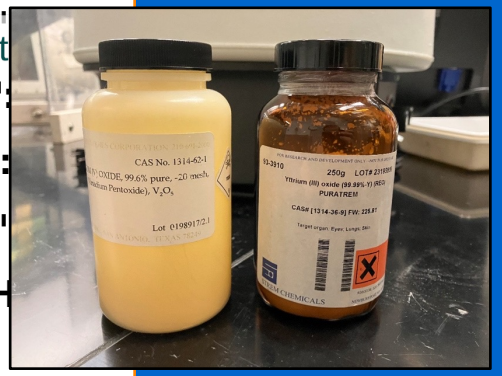
"Step 1, {'quantities': {'Duration': 0.0, 'Temp': 0.0, 'Type': 'Init'}, 'type': 'nominal_composition'}":"False"
"Step 2, {'quantities': {'Duration': 9.0, 'Temp': 900 ... mp'}, 'type': 'nominal_c ... False"
"Step 3, {'quantities': {'Duration': 1.0, 'Temp': 900.0 ... d'}, 'type': 'nominal_c ... False"
"Step 4, {'q ... uration': 9.0, 'Temp': 0.0, 'Type': 'Ramp'}, 'type': 'nominal_c ... False"
"Step 5, {'qu ... uration': 'Temp': 0.0, 'Type': 'End'}, 'type': 'nominal_composition'}":"False"
label:"GBM1013_Flux_Medium H ... Process, 5e1"



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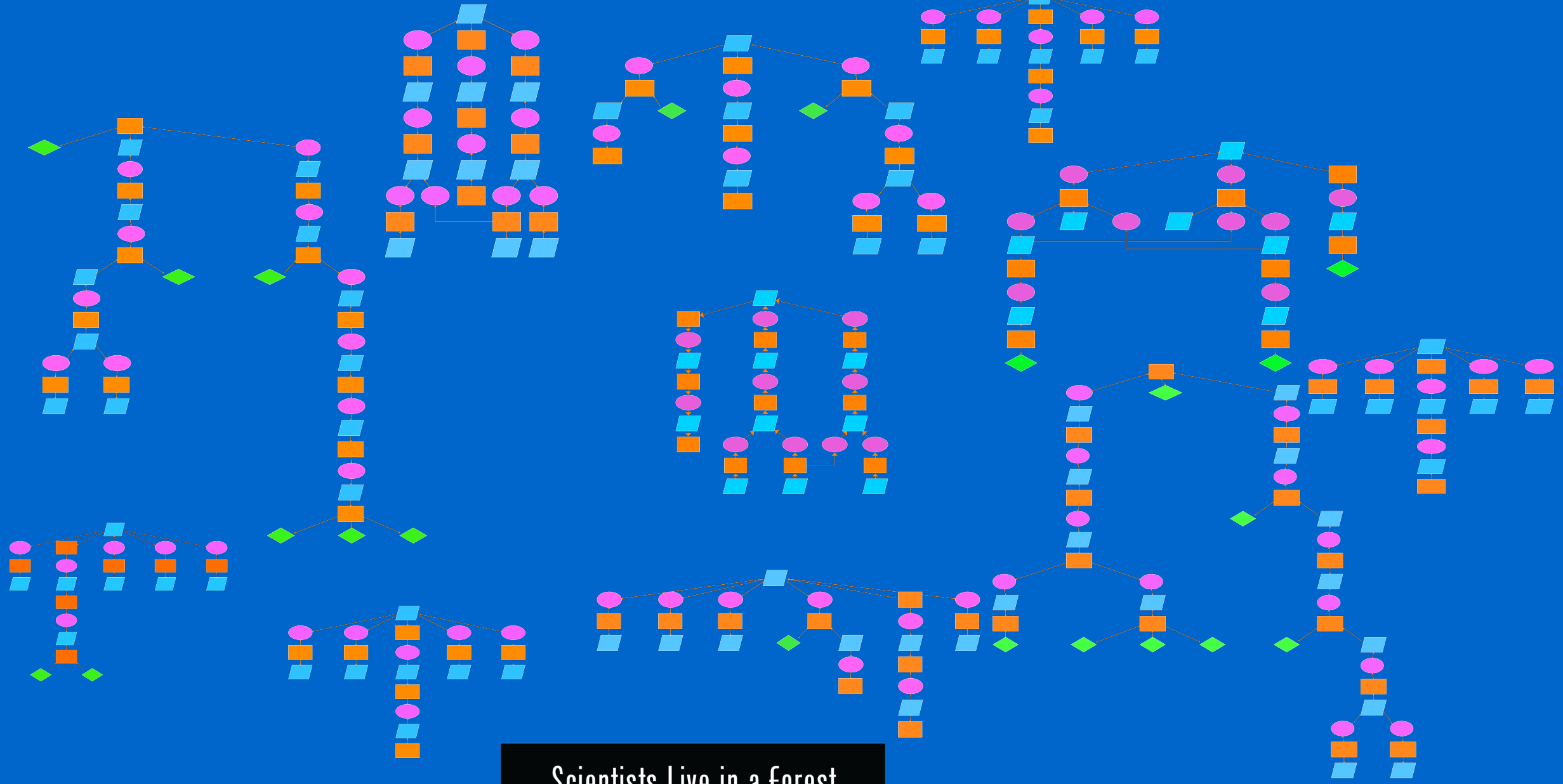

Scientists Live in a Forest
They've Never Seen

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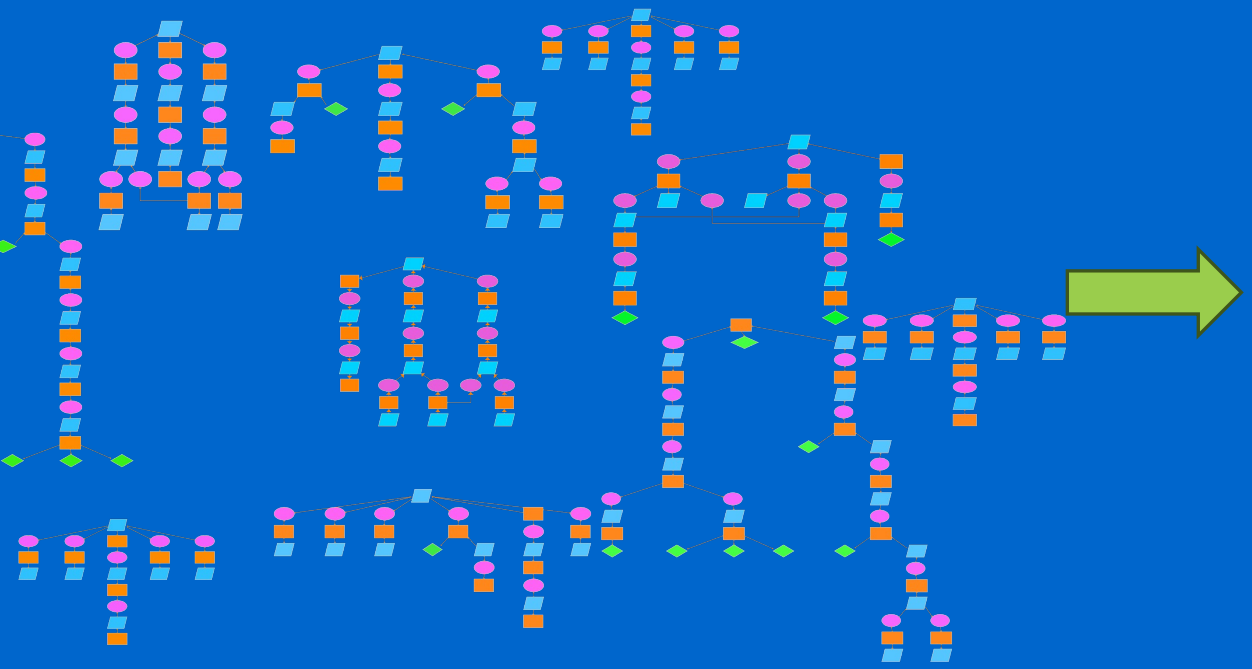
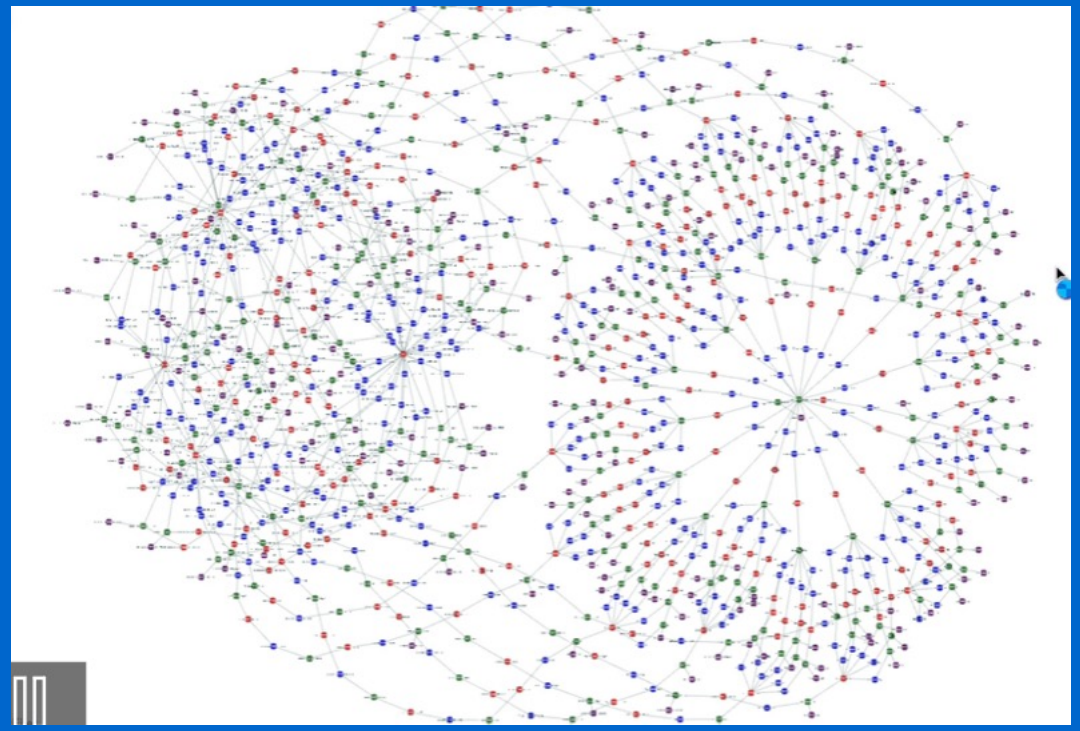
What if you could see the real structure of your research?

Concepts → HTMDEC Data





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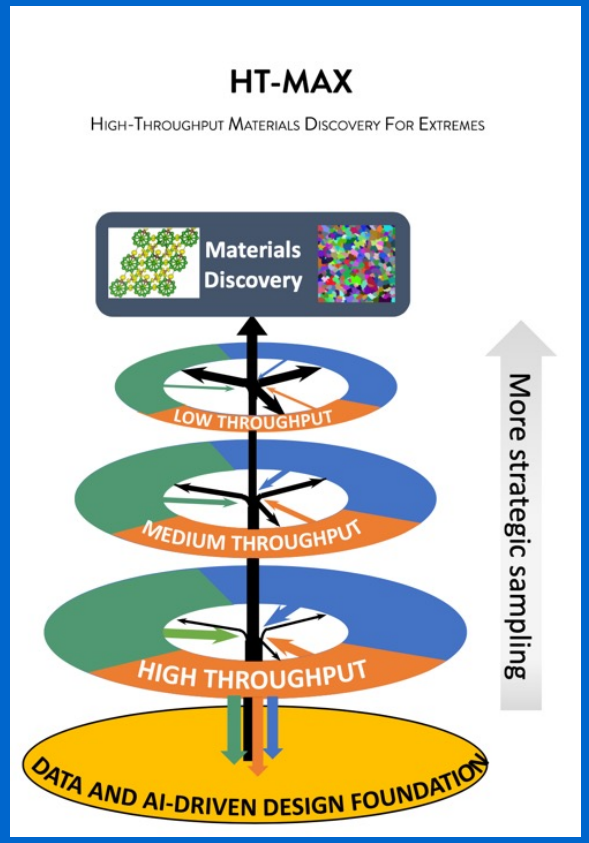
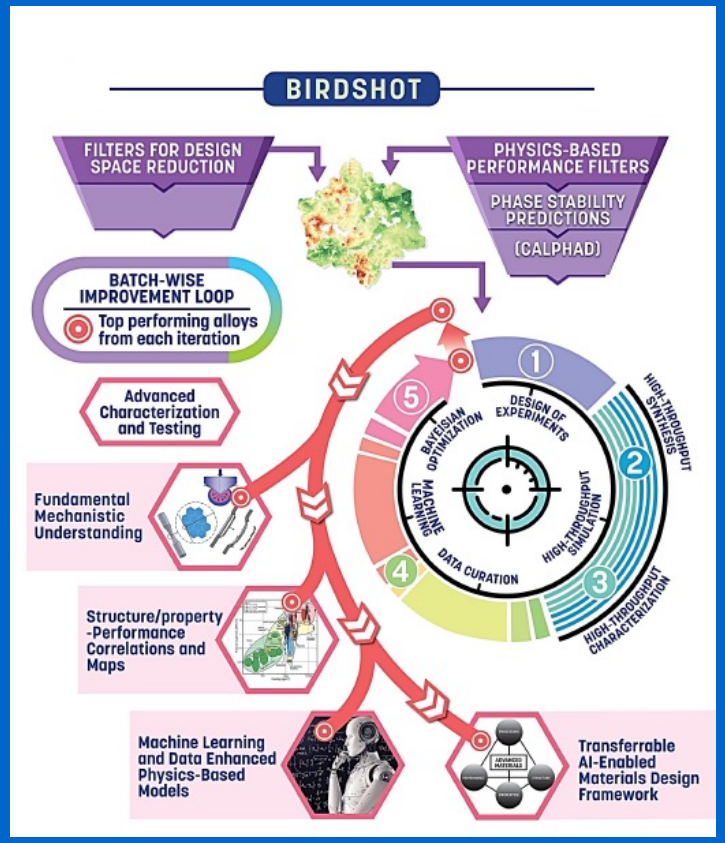
HTMDEC Centers

Technical Thrusts:

- Data Driven Materials Design
- High-Throughput Synthesis and Processing
- High-Throughput Characterization
- ML- Augmented Physics Based Models





Scientists are the worst judges of the reuse of their own data

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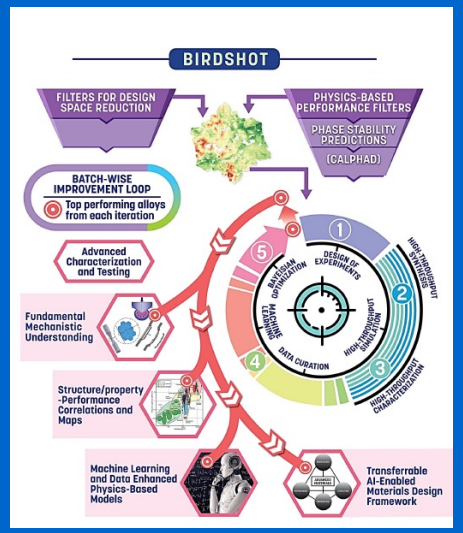
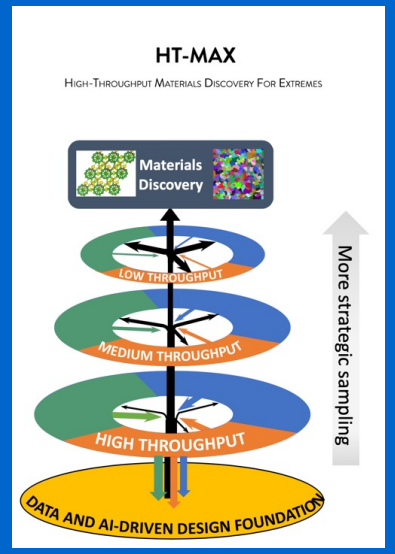
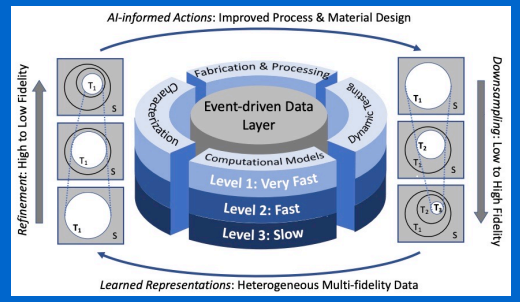
HTMDEC Different Philosophies, Same Goal: High Throughput

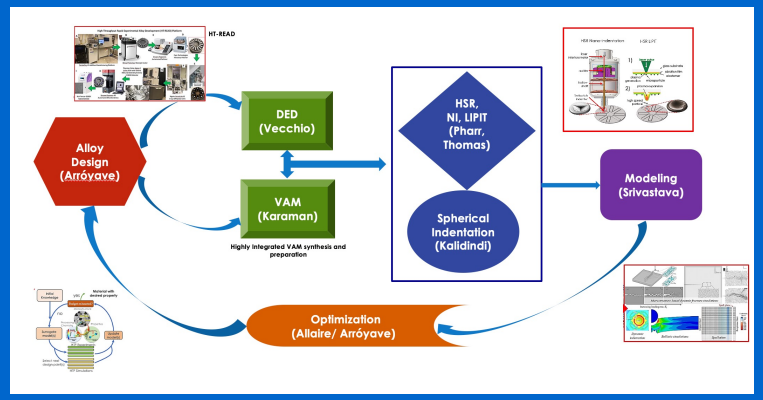


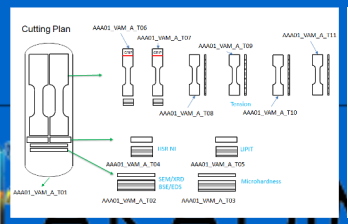
- Manual
- Structured

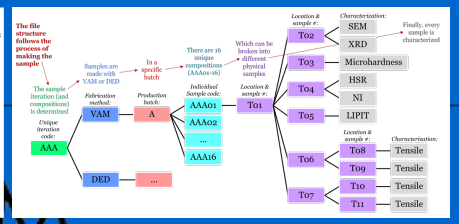


- Robotic Automation
- Variable
- Event Driven









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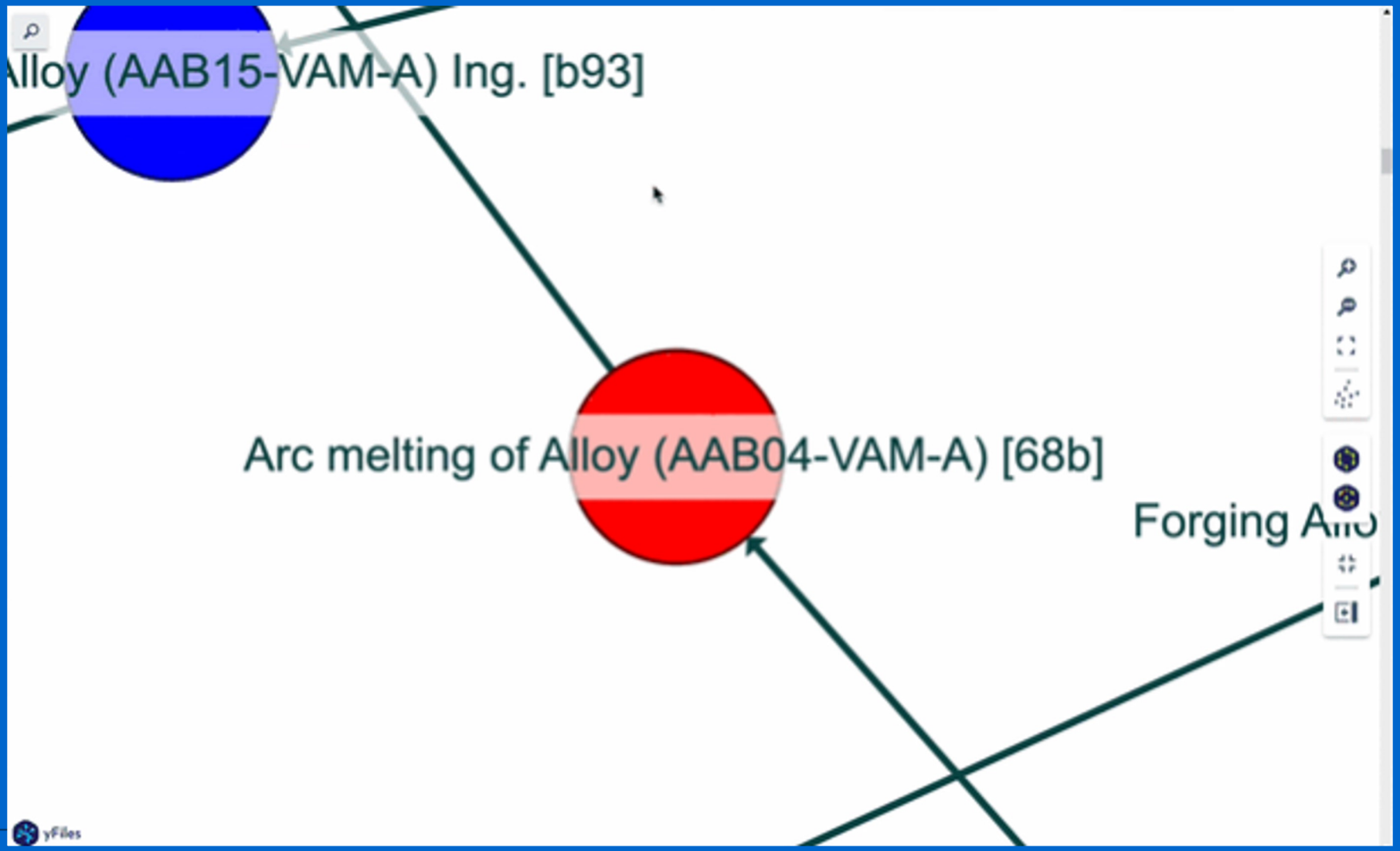
Birdshot:



Legend	
Object Type	Node Color
Process	
Material	
Ingredient	
Measurement	

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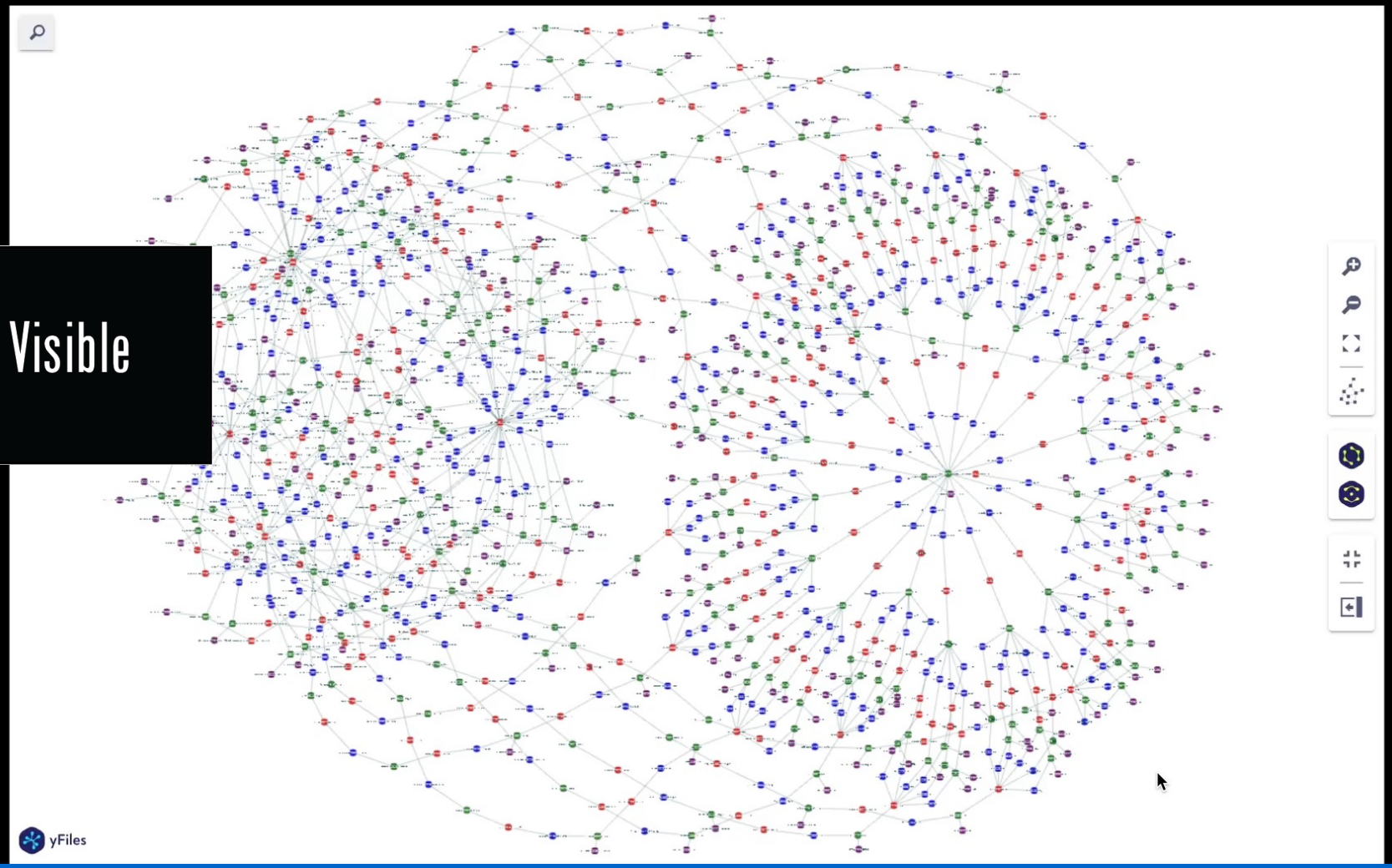
Visualize Your Materials Histories



Make the Invisible Visible

Legend	
Object Type	Node Color
Process	
Material	
Ingredient	
Measurement	

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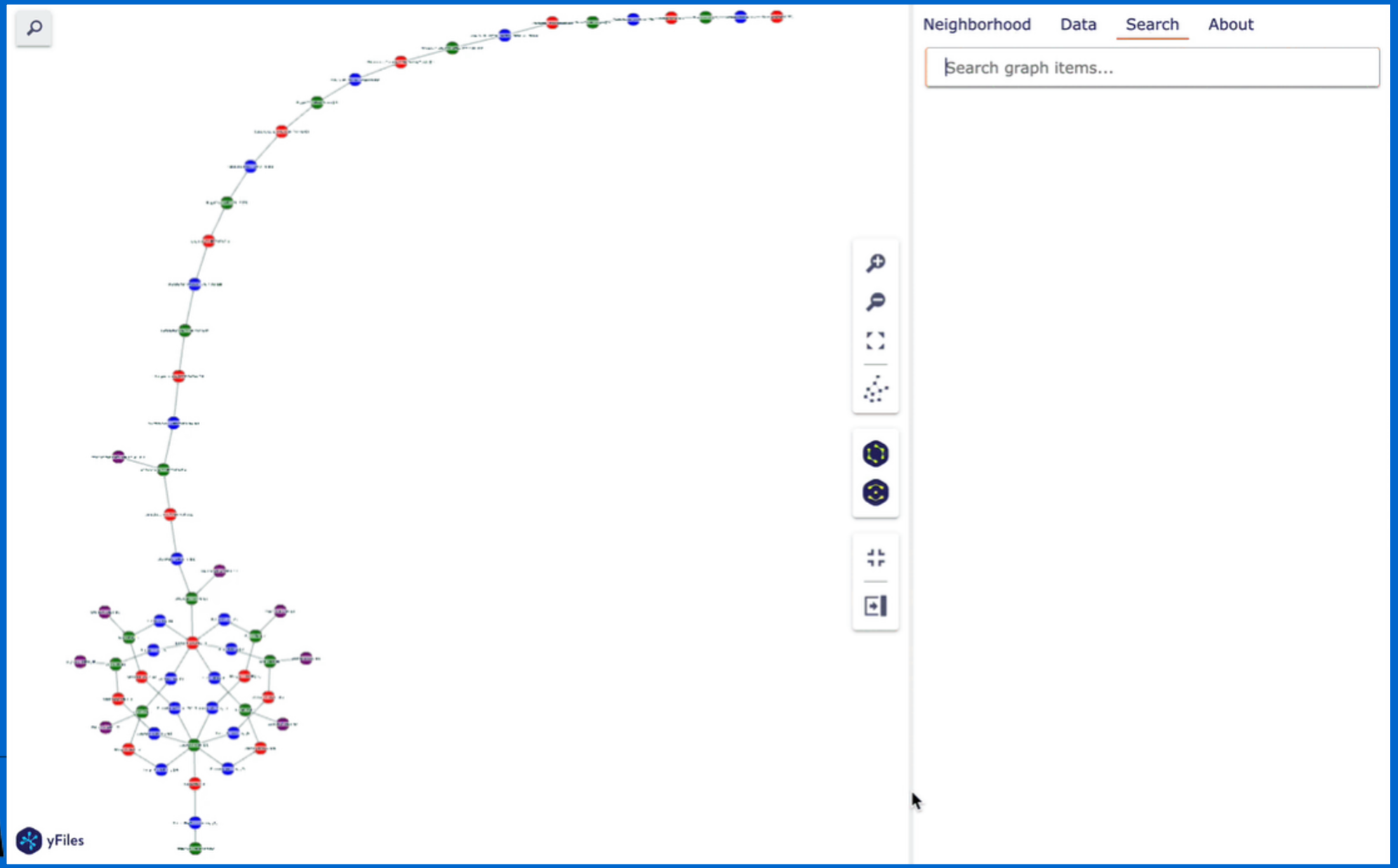
Intuitive Data Provenance



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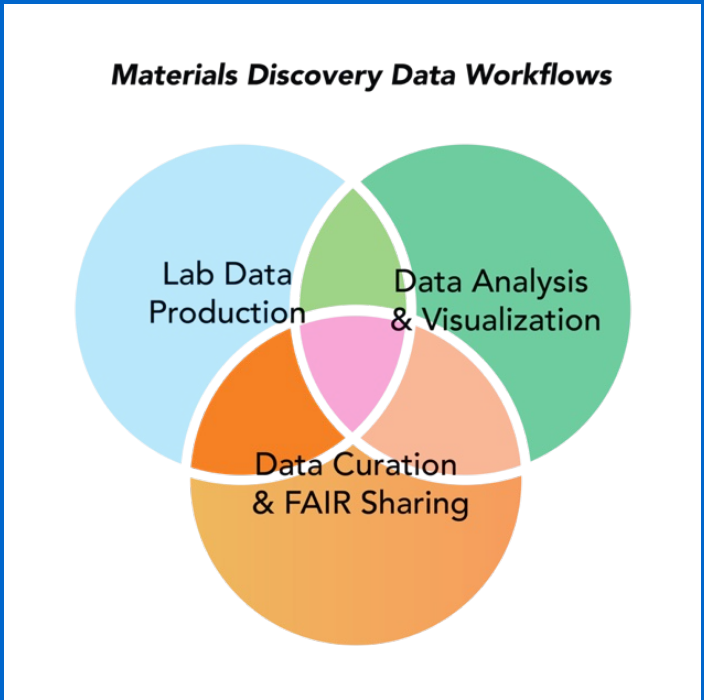
- Boromir Syndrome – Don't vilify the heroes



Scientists are the worst judges of the reuse of their own data

"People will not self organize around a system they do not understand"
– Alberto Bartolini