

Computation Institute

Networking materials data

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ianfoster.org



THE UNIVERSITY OF
CHICAGO



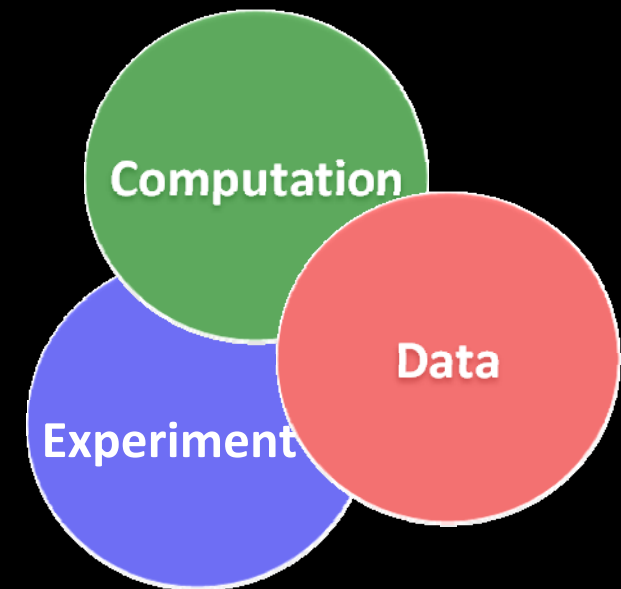
computationinstitute.org



Materials Genome Initiative — Materials Innovation Infrastructure

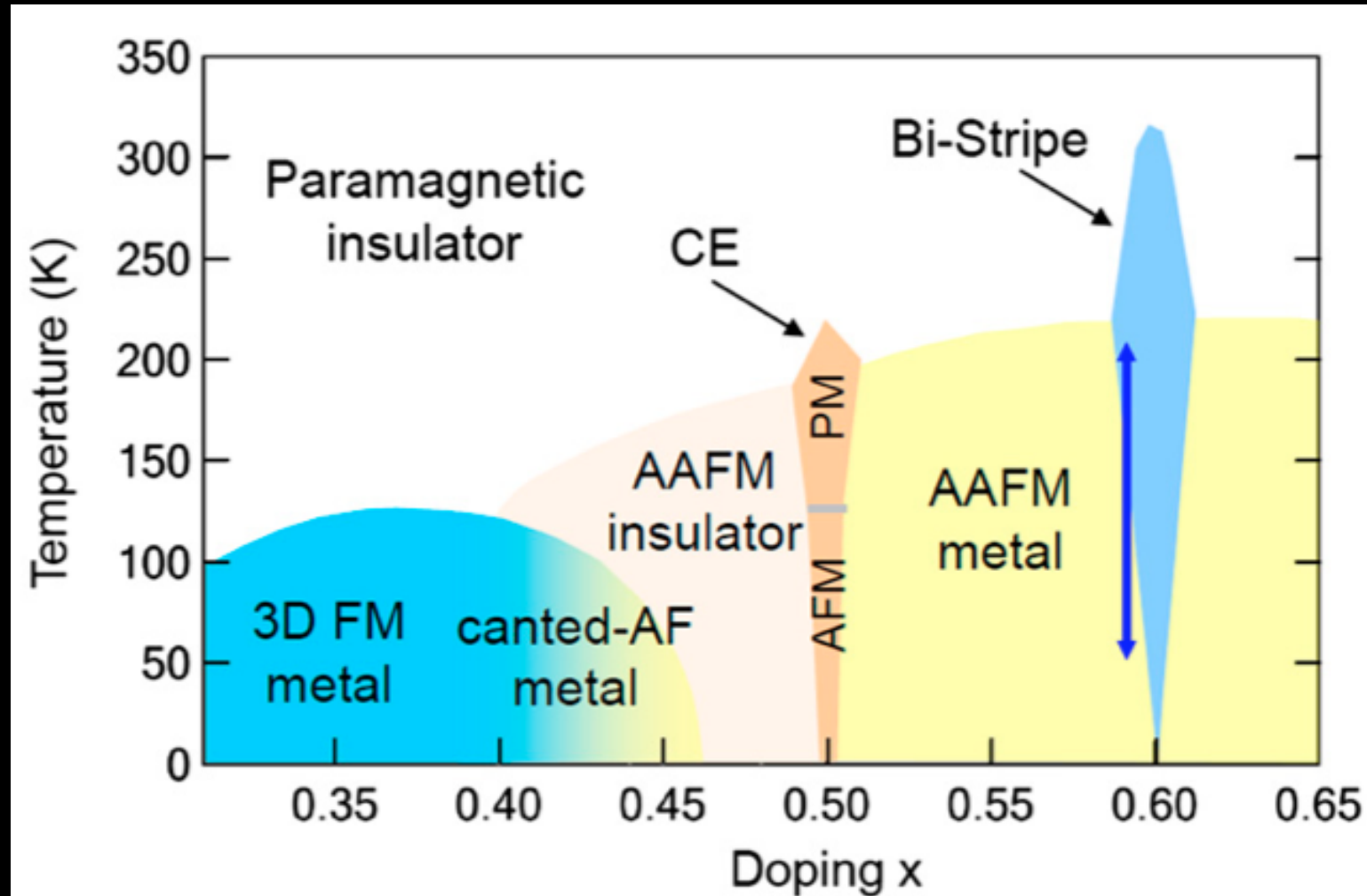
A **data sharing system** to facilitate:

- Use of a broader set of data to render more accurate models
- Multi-disciplinary communication among scientists and engineers working on different stages of materials development
- Searches for advanced materials with specific, desired properties
- Curating and sharing of reliable computational code for modeling and simulation





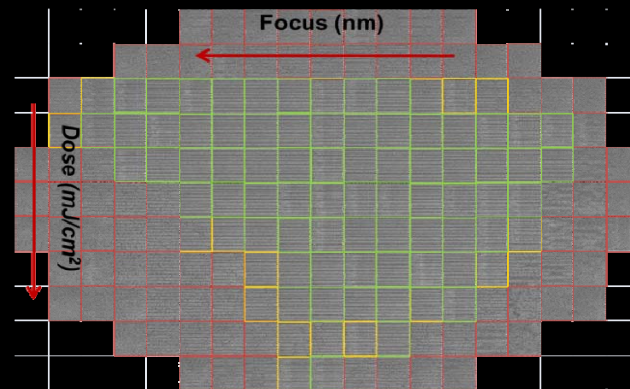
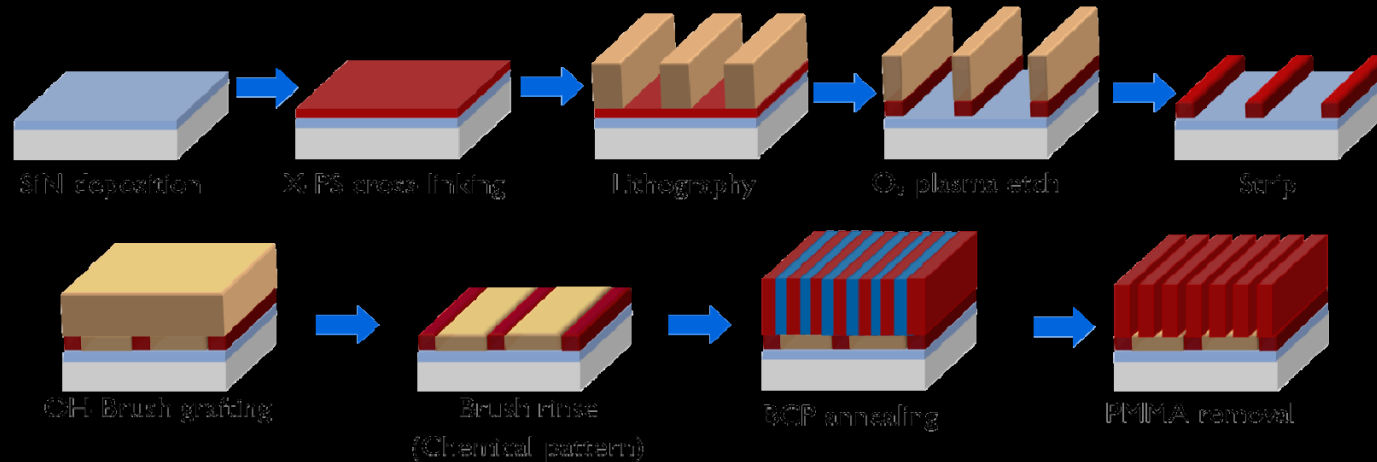
Linking simulation and experiment to study disordered structures



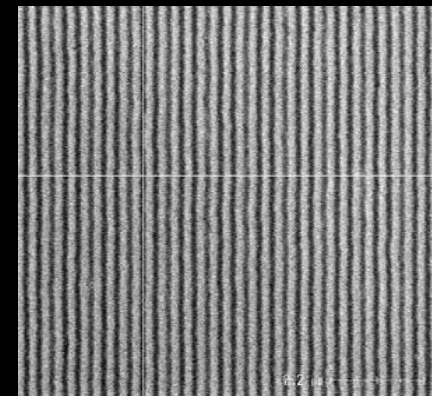


Linking simulation, experiment to study directed self-assembly of block polymers

LINE FLOW (UCL-NEALEY)



IMEC



300 nm wafers

Track processing



Materials Database Projects

- Materials Project (MIT/LBL)
- PRedictive Integrated Structural Materials Science (PRISMS) – Materials Commons
- Center for Hierarchical Materials Design (CHiMaD)
- Joint Center for Energy Storage Research (JCESR)
- NIST
- Etc.



Data: Rare treasure?





Or chaotic deluge?

It's both ...

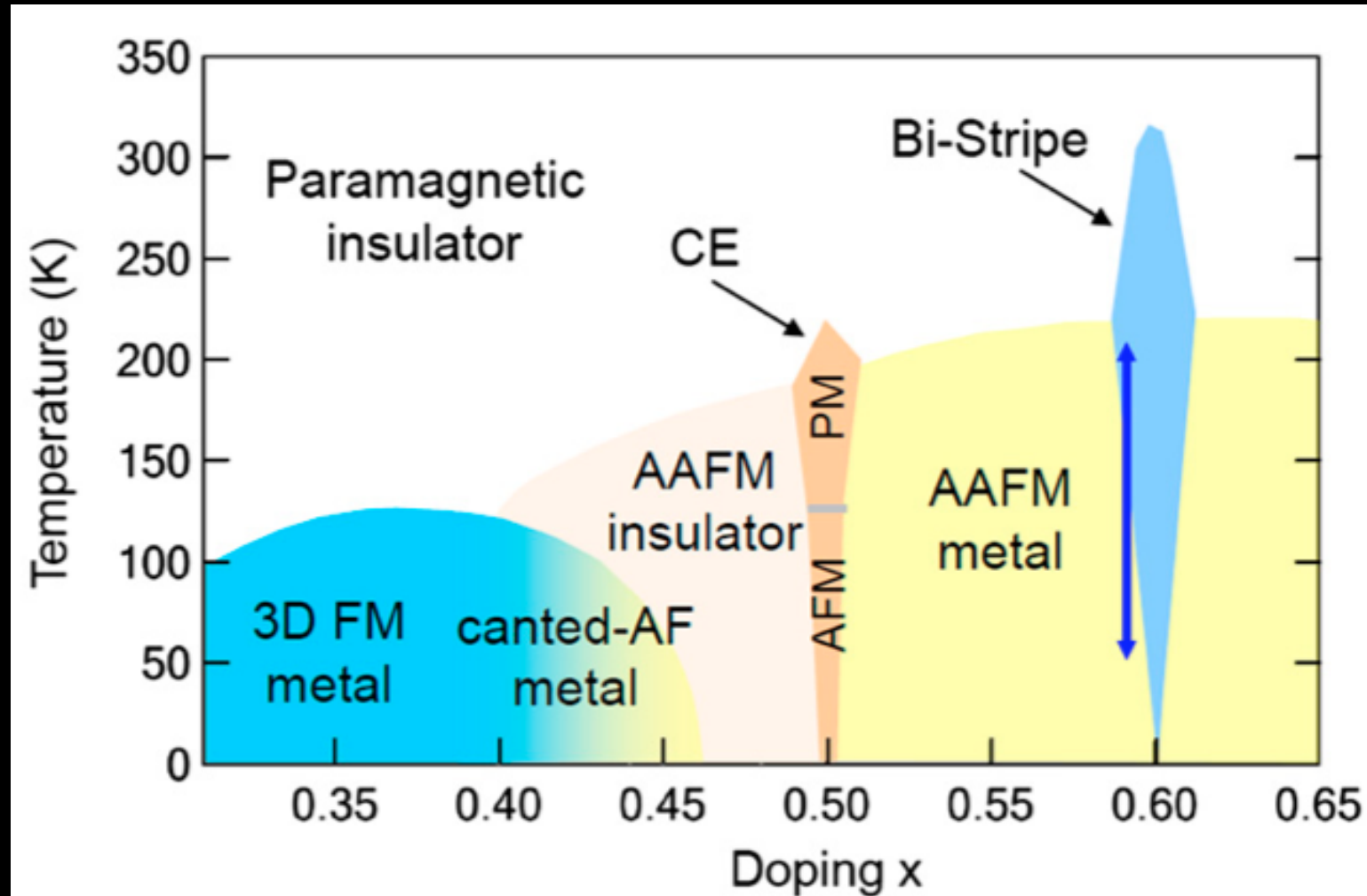
We must manage the data deluge—both to enhance user productivity and to increase data capture

→ **Network materials data**



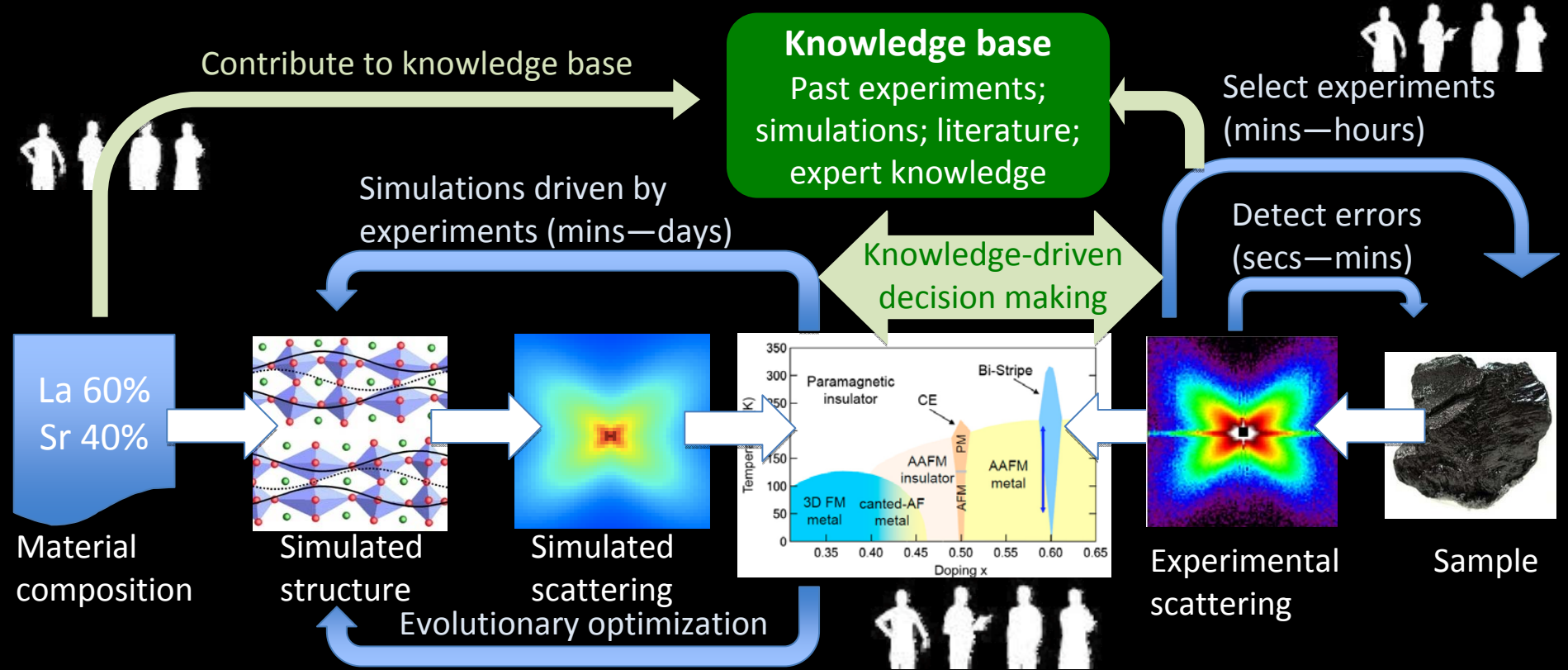


Linking simulation and experiment to study disordered structures



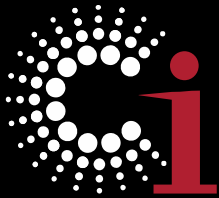


Linking simulation and experiment to study disordered structures

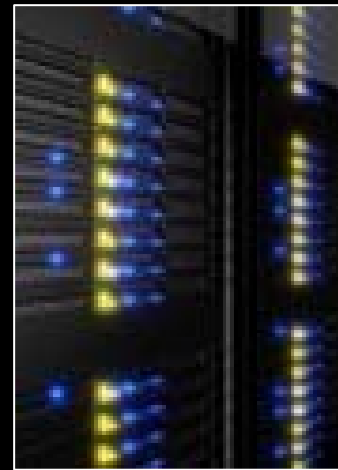
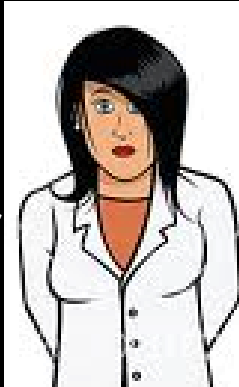
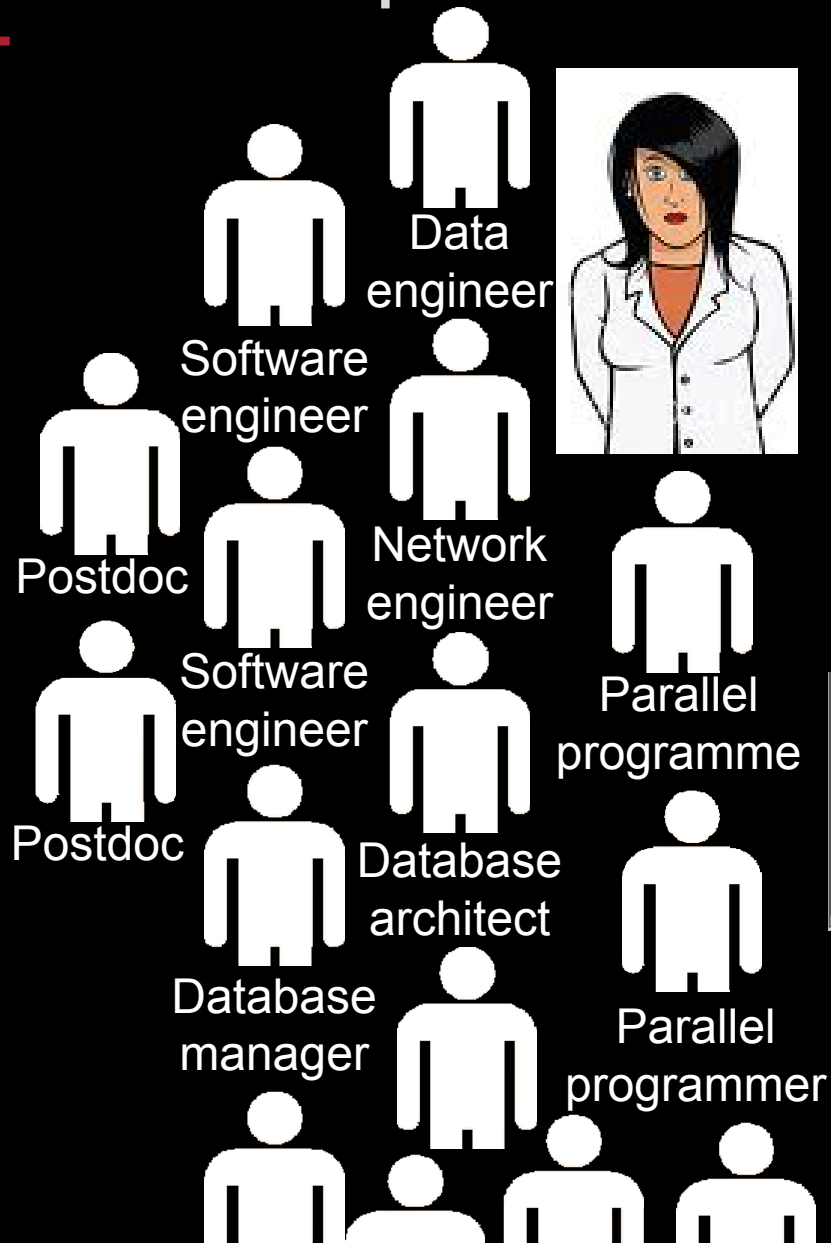


Diffuse scattering images from Ray Osborn et al., Argonne





An expensive business ...



```
40 import java.awt.image.IndexColorModel;
41 import java.awt.image.ColorModel;
42 import java.awt.image.MemoryImageSource;
43 import java.awt.event.*;
44
45 /** The representation of a chemical .xyz model */
46 class XV2ChemModel {
47     float vert[];
48     Aton atons[];
49     int lvert[];
50     int ZsortUp[];
51     int novert, maxovert;
52
53     static Hashtable atonTable = new Hashtable();
54     static Aton defaultAton;
55     static {
56         atonTable.put("C", new Aton(0, 0, 0));
57         atonTable.put("H", new Aton(210, 210, 210));
58         atonTable.put("O", new Aton(0, 0, 255));
59         atonTable.put("N", new Aton(255, 0, 0));
60     }
61 }
```



A small business, 20 years ago



```
Report java.awt.Desktop (Desktop)
Report java.awt.Desktop (Desktop)
Report java.awt.Desktop (Desktop)
Report java.awt.Desktop (Desktop)
Report java.awt.Desktop (Desktop)

// The representation of a Chemical object.
class IVChemical {
    Atom atom;
    int year;
    int yearHigh;
    int yearLow;

    static HashTable atomTable = new HashTable();
    static {
        atomTable.put("C", new Atom(6, 0, 0));
        atomTable.put("H", new Atom(1, 0, 0));
        atomTable.put("O", new Atom(8, 0, 0));
        atomTable.put("N", new Atom(7, 0, 0));
        atomTable.put("S", new Atom(16, 0, 0));
    }
}
```



A small business, today

STARBUCKS



“Business cloud”

Reduce costs
Speed innovation
Reliable, scalable, simple



salesforce

oDesk[®]
Love the way you work.



KnowledgeTree



liveops

box

xero





Can we do the same for research?

STARBUCKS



“Discovery cloud”

{ Reduce costs
Speed discovery
Reliable, scalable, simple }

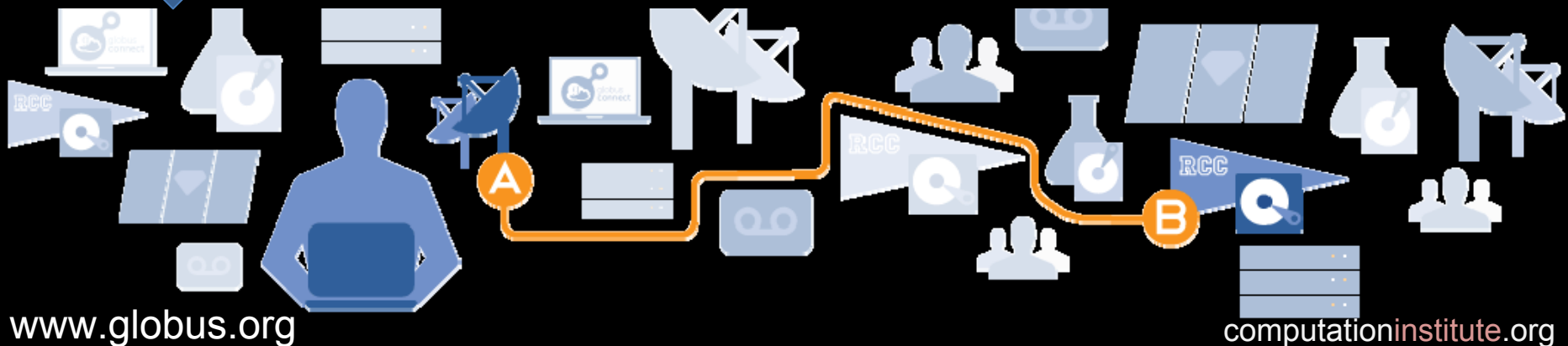
?



Discovery cloud: Globus research data management services



File transfer
& sharing



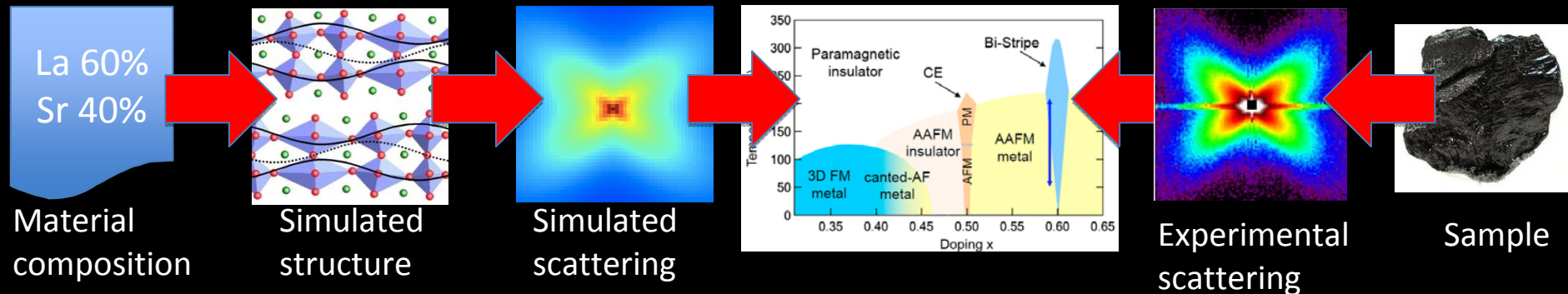


Linking simulation and experiment to study disordered structures



Globus transfer service

Cloud hosted: reliable, secure, fast
20K users, 3B files, 50 PB transferred
Available at www.globus.org





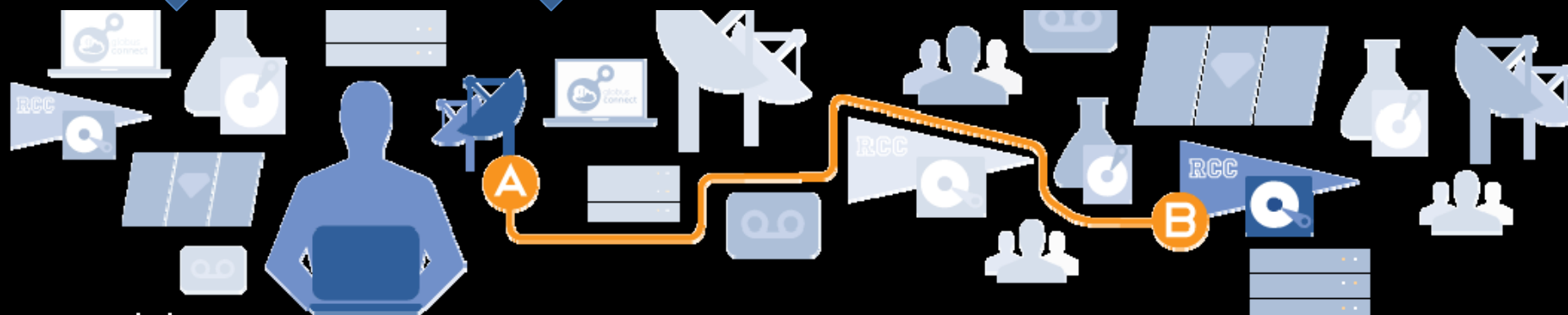
Discovery cloud: Globus research data management services



File transfer & sharing



Identity & group management



www.globus.org

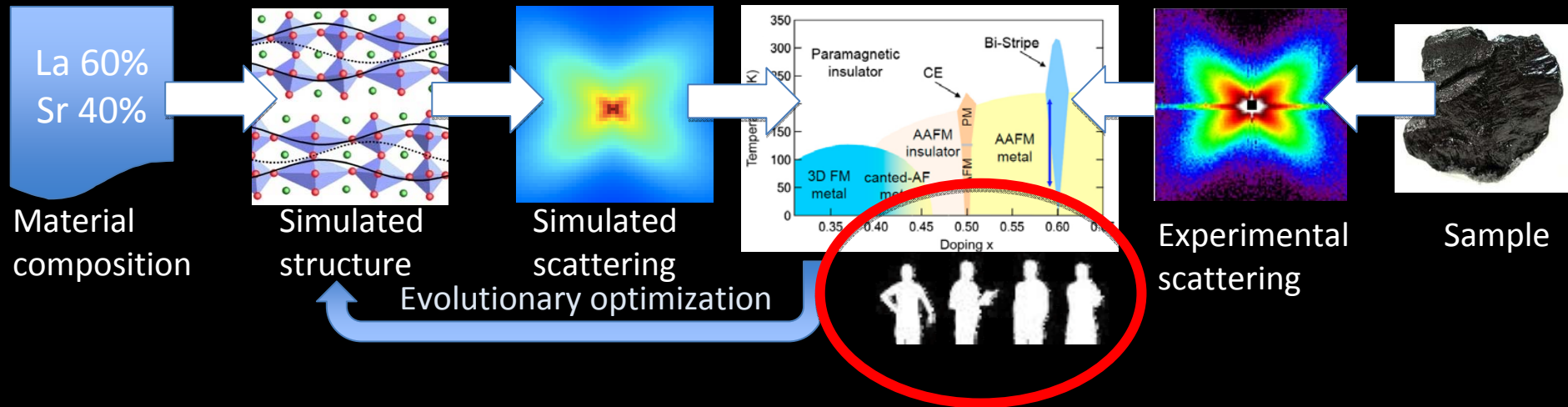
computationinstitute.org



Linking simulation and experiment to study disordered structures



Globus sharing
Identities, groups, profiles
Cloud hosted





Discovery cloud: Globus research data management services



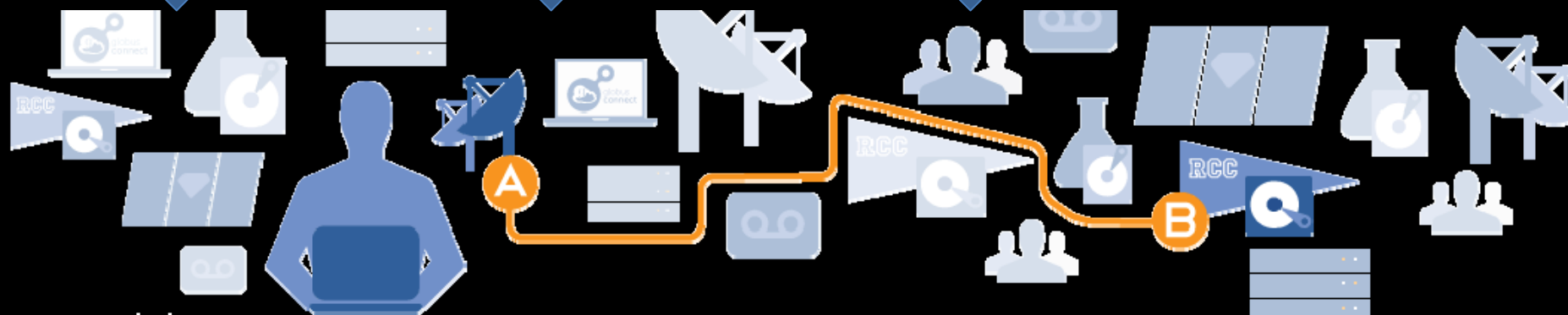
File transfer
& sharing



Identity & group
management



Data publication
& discovery

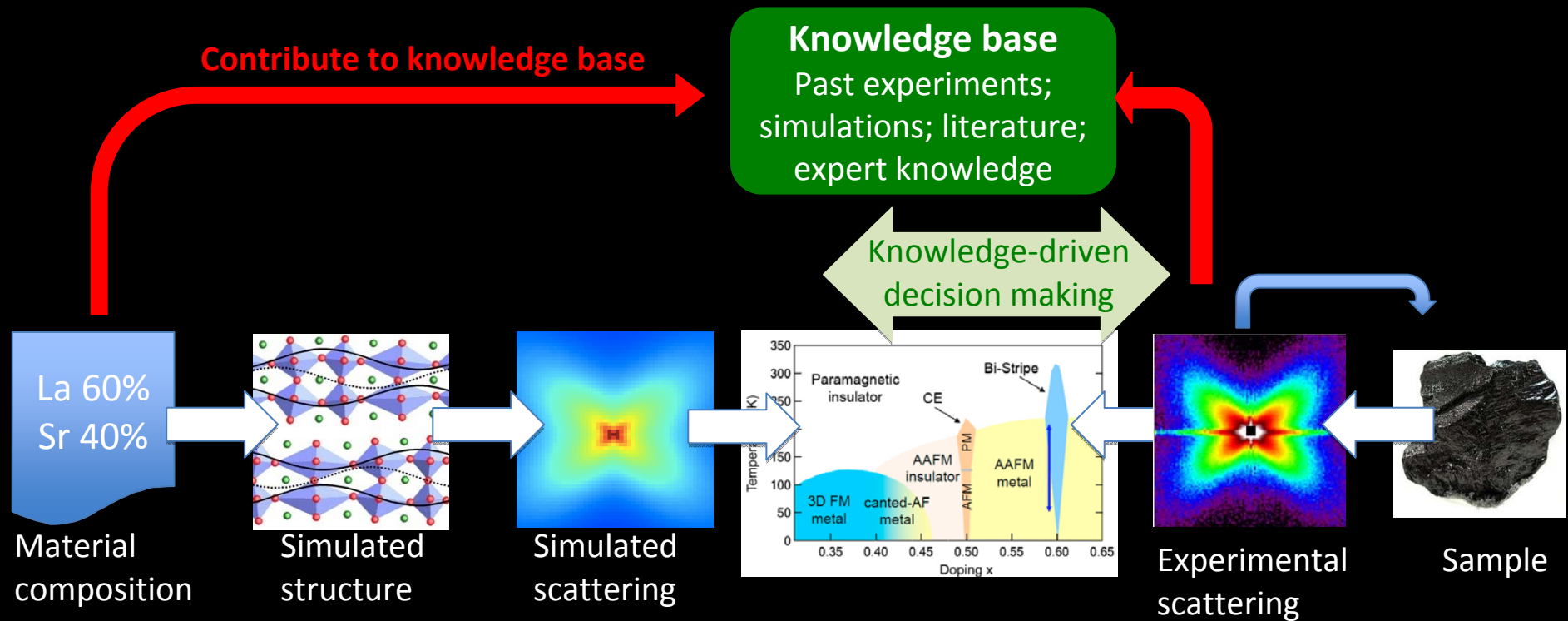


www.globus.org

computationinstitute.org



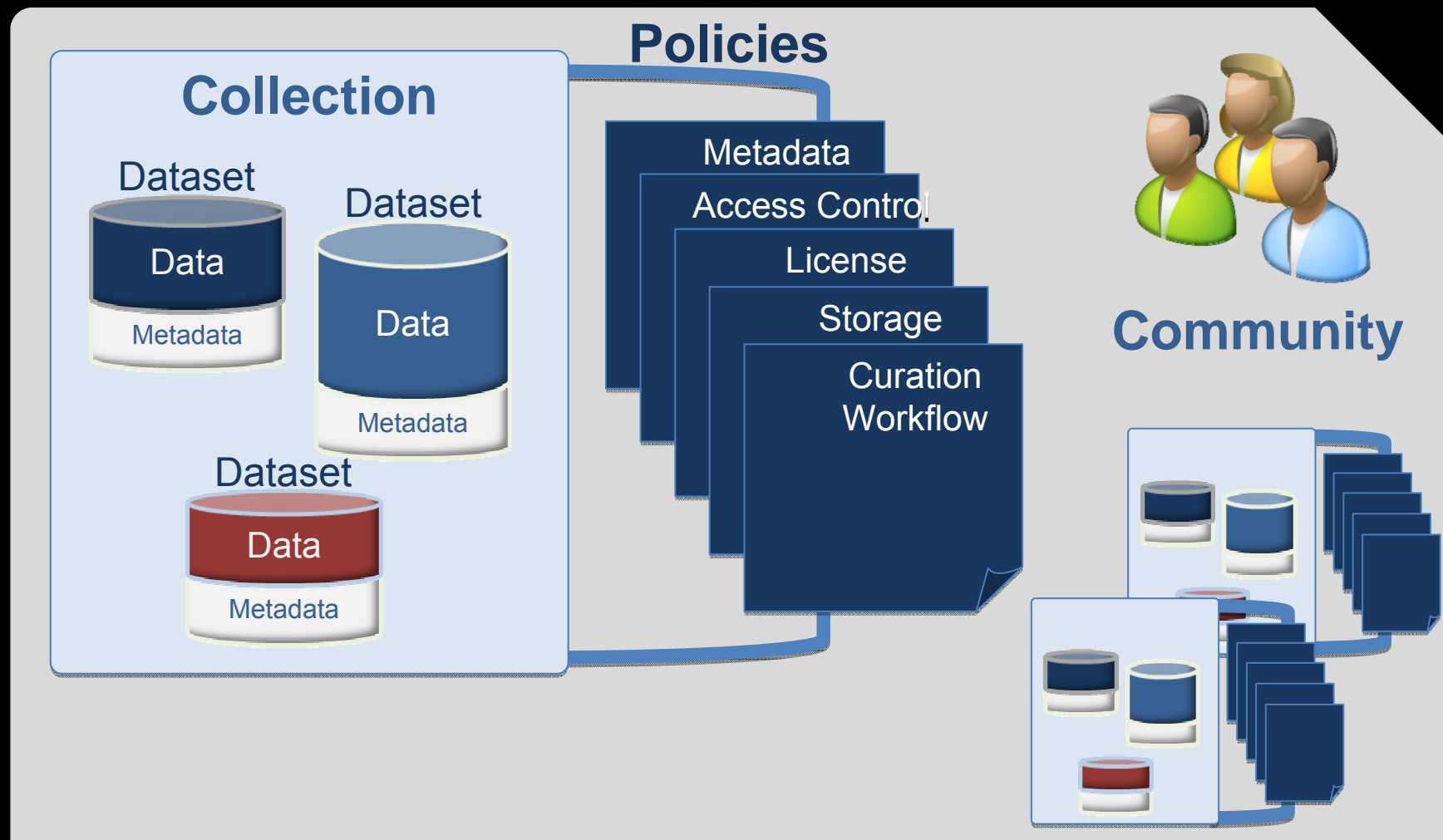
Linking simulation and experiment to study disordered structures



Globus data publication
and discovery
Cloud hosted



Data publication and discovery



We are looking for pilot users!




Publish dashboard

The screenshot shows the Globus Publish dashboard interface. At the top left is the Globus logo. To the right of the logo are navigation links: Search, Publish, Manage Data, Groups, Support, and a user profile link for 'blaiszik'. Below the navigation bar is a blue header bar with the text 'Globus'. Underneath is another blue bar indicating the user's dashboard: 'Dashboard: Ben Blaiszik'. Below this are two buttons: a green 'Start a New Submission' button and a blue 'View Accepted Submissions' button. At the bottom left of the dashboard area, it says 'powered by DSpace' with the DSpace logo.



Start a new submission


 globus blaiszik ▾

Submit: Choose Collection ?

Select the collection you wish to submit an item to from the list below, then click "Next".

Collection	
	Advanced Photon Source
	Center for Nanoscale Materials
	Chemical Sciences and Engineering
	Institute of Molecular Engineering

Go to
[Globus Publications Home](#)
[Dashboard](#)

powered by  DSpace

Submit: Describe this Item ?

Please fill in the requested information about this submission below. In most browsers, you can use the tab key use the mouse each time.

Enter the names of the authors of this item below.

Authors

Blaiszik	Ben	Remove Entry
Kramer	Sharlotte	Remove Entry
Grady	Martha	Remove Entry
Sottos	Nancy	Remove Entry
White	Scott	Remove Entry
Last name, e.g. Smith	First name(s) + "Jr", e.g. Donald Jr	Add More

Enter ORCID of the authors of this item below.

ORCID

http://orcid.org/0000-0002-5326-4789	Remove Entry	http://orcid.org/0000-0002-7346-7621	Remove Entry
http://orcid.org/0000-0001-2034-2932		http://orcid.org/0000-0124-4356-1923	Add More

Enter the main title of the item.

Title *

Please give the date of data publication. You can leave out the day and/or month if they aren't applicable.

Date of Issue *

Month: Day: Year:

Enter the standard citation for the publication associated with this item.

Citation

Enter the standard citation DOI for the publication associated with this item.

Citation DOI

Describe submission:
1) Dublin Core

Describe Describe Upload Verify License Complete

Submit: Describe this Item ?

Please fill further information about this submission below.

Enter appropriate subject keywords or phrases below.

Subject Keywords

self-healing

Remove Entry

circuit

Remove Entry

microcapsules

Remove Entry

+ Add More

Enter the names of any sponsors and/or funding codes in the box below.

Sponsors

This material is based upon work supported as part of the Center for Electrical Energy Storage - Tailored Interfaces, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number (919 DOE ANL 9F-31921 NS).

Enter a description for this item in the box below.

Description

Thermomechanical failure of conductive pathways in highly integrated circuits results in loss of function that is often impossible to repair and remains a long-standing problem hindering advanced electronic packaging. Prior approaches to restoration of conductivity rely on external intervention in the form of heating or manual delivery of relatively low conductivity materials. Here, we demonstrate autonomic healing of an electrical circuit with nearly full recovery of conductance (ca. 99%) less than one millisecond after damage. The rapid restorative

Enter the name of experiment for this item below.

Experiment

self-healing-10wtper

Enter the names of materials used in this experiment below.

Material

Gallium

Remove Entry

Gold

Remove Entry

Indium

circuitboard

+ Add More

Enter the energy density used in this experiment.

Energy Density (mAh/g)

2000

Enter the Argonne GUP that this experiment was conducted under.

GUP

345-455-2543

< Previous

Cancel/Save

Next >

Describe submission: 2) Science metadata



Assemble the dataset

The screenshot shows the Globus user interface for the 'Submit: Assemble a dataset' workflow. At the top left is the Globus logo, and at the top right is the user name 'blaiszik'. Below the header is a navigation bar with buttons for 'Describe', 'Describe', 'Upload', 'Verify', 'License', and 'Complete'. The main heading is 'Submit: Assemble a dataset' with a blue question mark icon. Below the heading is a paragraph of instructions: 'Please follow the link to assemble your dataset using Globus. A unique endpoint will be created through which you can assemble your dataset asynchronously. You may transfer files to this endpoint over time and return to this workflow when the dataset is complete. The shared endpoint will only be accessible to you. At the completion of the submission workflow you will no longer be able to write to this endpoint; however you will be able to view and download the contents.' Below this is another paragraph: 'Please also note that the system is able to preserve the content of certain types of files better than other types. [Information about file types and levels of support for each are available.](#)' In the center is a green button labeled 'Select Files'. At the bottom of the main content area is a navigation bar with four buttons: '< Previous', 'Cancel/Save', 'Skip dataset assembly >', and 'Next >'. The footer of the page contains the text 'powered by DSpace' and the DSpace logo.

Transfer Files

Get Globus Connect Personal
Turn your computer into an endpoint.

Endpoint Path

Endpoint Path

select all | none | up one folder | refresh list

20130311-Conductivity-SH-original-4.txt	92 kB
20130317-capsule-sizing-4.csv	6 kB
20130324-Healed-fracture-tomo-2.csv	93 kB
20130328-capsule-sizing-1.txt	45 kB
20130514-Conductivity-SH-healed-3.tif	72 kB
20130516-Healed-fracture-tomo-4.tif	80 kB
20130517-Galn-capsule-SEM-1.png	99 kB
20130517-Galn-capsule-SEM-4.xlsx	38 kB
20130518-Conductivity-SH-healed-4.csv	30 kB
20130519-Galn-capsule-SEM-3.tif	53 kB
20130523-Conductivity-SH-original-1.csv	91 kB
20130524-Galn-capsule-SEM-2.csv	68 kB
20130611-Conductivity-SH-healed-2.xlsx	22 kB
20130621-Healed-fracture-tomo-1.csv	89 kB
20130622-Conductivity-SH-original-3.tif	36 kB
20130714-Conductivity-SH-original-2.tif	22 kB
20130729-Conductivity-SH-healed-1.txt	69 kB
20130813-capsule-sizing-3.tif	44 kB
20130828-Healed-fracture-tomo-3.txt	85 kB
20130925-capsule-sizing-2.tif	41 kB

select all | none | up one folder | refresh list

20130311-Conductivity-SH-original-4.txt	92 kB
20130317-capsule-sizing-4.csv	6 kB
20130324-Healed-fracture-tomo-2.csv	93 kB
20130328-capsule-sizing-1.txt	45 kB
20130514-Conductivity-SH-healed-3.tif	72 kB
20130516-Healed-fracture-tomo-4.tif	80 kB
20130517-Galn-capsule-SEM-1.png	99 kB
20130517-Galn-capsule-SEM-4.xlsx	38 kB
20130518-Conductivity-SH-healed-4.csv	30 kB
20130519-Galn-capsule-SEM-3.tif	53 kB
20130611-Conductivity-SH-healed-2.xlsx	22 kB
20130621-Healed-fracture-tomo-1.csv	89 kB
20130622-Conductivity-SH-original-3.tif	36 kB

[more options](#) Label This Transfer This will be displayed in your transfer activity.

**Transfer files to
submission endpoint**

Activity

publish#publish-server to publish#submission_11
transfer completed a few seconds ago

Describe Describe Upload Verify License Complete

Submit: Dataset Assembled Successfully ?

Your dataset was successfully assembled.

The table below shows the files which are included in this item.

Primary bitstream	File		Size	Description	File Format	
<input type="radio"/>	20130311-Conductivity-SH-original-4.txt	Remove	94208 bytes	None	Text (known)	Change
<input type="radio"/>	20130317-capsule-sizing-4.csv	Remove	6144 bytes	None	Unknown (unsupported)	Change
<input type="radio"/>	20130324-Healed-fracture-tomo-2.csv	Remove	95232 bytes	None	Unknown (unsupported)	Change
<input type="radio"/>	20130328-capsule-sizing-1.txt	Remove	46080 bytes	None	Text (known)	Change
<input type="radio"/>	20130514-Conductivity-SH-healed-3.tif	Remove	73728 bytes	None	TIFF (known)	Change
<input type="radio"/>	20130516-Healed-fracture-tomo-4.tif	Remove	81920 bytes	None	TIFF (known)	Change
<input type="radio"/>	20130517-Galn-capsule-SEM-1.png	Remove	101376 bytes	None	image/png (known)	Change
<input type="radio"/>	20130517-Galn-capsule-SEM-4.xlsx	Remove	38912 bytes	None	Microsoft Excel XML (known)	Change
<input type="radio"/>	20130518-Conductivity-SH-healed-4.csv	Remove	30720 bytes	None	Unknown (unsupported)	Change
<input type="radio"/>	20130519-Galn-capsule-SEM-3.tif	Remove	54272 bytes	None	TIFF (known)	Change
<input type="radio"/>	20130611-Conductivity-SH-healed-2.xlsx	Remove	22528 bytes	None	Microsoft Excel XML (known)	Change
<input type="radio"/>	20130621-Healed-fracture-tomo-1.csv	Remove	91136 bytes	None	Unknown (unsupported)	Change
<input type="radio"/>	20130622-Conductivity-SH-original-3.tif	Remove	36864 bytes	None	TIFF (known)	Change

Add Another File

Check dataset is assembled correctly



Submission now in curation workflow

The screenshot displays the Globus user interface. At the top, the Globus logo is on the left, and navigation links for Search, Publish, Manage Data, Groups, Support, and a user profile (blaiszik) are on the right. Below the navigation bar, a blue header bar contains the text "Globus". Underneath, a sub-header indicates the user's dashboard: "Dashboard: Ben Blaiszik". Two buttons are visible: "Start a New Submission" (green) and "View Accepted Submissions" (blue). The main content area is titled "Submissions In Workflow Process" and contains a table with one entry.

Title	Submitted to
Autonomic Restoration of Electrical Conductivity	Center for Nanoscale Materials

At the bottom of the interface, it is noted that the system is "powered by DSpace" with the DSpace logo.



Search published datasets



globus

Search Publish Manage Data Groups Support

Discover Data

energy_density | num_samples | protocol_version | 2000

Refine Search All Endpoints Collections

*

Transfer Tag Analyze

Start Destination: Home (blaiszik#laptop/) | SNS (go#ep2/home/SNS)
New Destination

All None Inverse

7 results found | > 0.0 B

0 selected | > 0.0 B

TiO₂-luciferase Nanoconjugates for Enhanced Photodynamic Therapy

Blaiszik, Ben; Rajh, Tijana;

Photodynamic therapy (PDT) is an emergent technology used for the treatment of cancers, psoriasis, and other autoimmune diseases.¹ In this method, light energy is converted to chemical energy, creating highly reactive oxygen species (ROS), which under appropriate conditions are highly disruptive for cell metabolism and lead to cell death. PDT critically depends on the possibility of delivering light in the vicinity of the tumor. At present the small penetration depth of light in the body is the primary limitation of PDT, and the tumor has to be at most within 1 cm of the light source. This eliminates the possibility for treatment of tumors that are located deep in the tissues.

04/15/2014

9:51 PM

12 files

Center for Nanoscale Materials

[View Dataset](#)

TiO₂ nanoconjugates photodynamic

sample_id:1 protocol_version:7

Detection and role of trace impurities in high-performance organic solar cells

Nikiforov, Maxim; Lai, Barry; Chen, Wei; Schaller, Richard; Darling, Seth;

Trace impurities in organic solar cells, such as those from residual catalyst material in conjugated polymers, are often ignored but are known to deleteriously affect device performance. Batch-to-batch variations in the nature and quantity of such impurities leads to widespread issues with irreproducible optoelectronic function, yet to date no technique has emerged that is reliably capable of identifying the character of impurities or their concentration in organic photovoltaic active layer blends. Here we focus on state-of-the-art, high-performance bulk heterojunction blends and show that synchrotron-based X-ray fluorescence can detect and quantify trace concentrations of metal impurities in these systems.

04/15/2014

10:04 PM

13 files

Center for Nanoscale Materials

[View Dataset](#)

solar impurities x-ray fluorescence organic solar cells

num_samples:7 protocol_version:2



Search across collections



globus

Search Publish Manage Data Groups Support

Discover Data

energy_density | num_samples | protocol_version | 2000

Refine Search All Endpoints Collections

Li-ion autonomic



Transfer

Tag

Analyze

Start

Destination: Home (blaiszik#laptop/) | SNS (go#ep2/home/SNS)

New Destination

All None Inverse

8 results found | > 0.0 B

0 selected | > 0.0 B

Autonomic Shutdown of Lithium-Ion Batteries Using Thermo-responsive Microspheres

Baginska, Marta; Blaiszik, Ben; Sottos, Nancy; White, Scott;

Autonomic, thermally-induced shutdown of Lithium-ion (Li-ion) batteries is demonstrated by incorporating thermo-responsive polymer microspheres (ca. 4 μm) onto battery anodes or separators. When the internal battery environment reaches a critical temperature, the microspheres melt and coat the anode/separator with a nonconductive barrier, halting Li-ion transport and shutting down the cell permanently. Scanning electron microscopy images of electrode surfaces from cells that have undergone autonomic shutdown provides evidence of melting, wetting, and resolidification of PE into the anode and polymer film formation at the anode/separator interface.

04/15/2014

9:20 PM

16 files

Chemical Sciences and Engineering

View Dataset

Li-ion battery safety autonomic shutdown

energy_density:250 num_samples:15

Synthesis, Characterization, and Structural Modeling of High-Capacity, Dual Functioning MnO₂ Electrode/Electrocatalysts for Li-O₂ Cells

Trahey, Lynn; Chan, Maria; Blaiszik, Ben;

It has become clear that cycling lithium-oxygen cells in carbonate electrolytes is impractical, as electrolyte decomposition, triggered by oxygen reduction products, dominates the cell chemistry. This research shows that employing an α -MnO₂/ramsdellite-MnO₂ electrode/electrocatalyst results in the formation of lithium-oxide-like discharge products in propylene carbonate, which has been reported to be extremely susceptible to decomposition. X-ray photoelectron data have shown that what are likely lithium oxides (Li₂O₂ and Li₂O) appear to form and decompose on the air electrode surface, particularly at the MnO₂ surface, while Li₂CO₃ is also formed.

04/16/2014

9:56 AM

4 files

Center for Nanoscale Materials

View Dataset

Li-ion Li-air manganese

energy_density:2500



Discover a published dataset



globus

Search Publish Manage Data Groups Support

Discover Data

energy_density | num_samples | protocol_version | 2000

Refine Search All Endpoints Collections

energy_density>1500 microcapsules



Transfer

Tag

Analyze

Start

Destination: Home (blaiszik#laptop/) | SNS (go#ep2/home/SNS)

New Destination

All None Inverse

3 results found | > 0.0 B

0 selected | > 0.0 B

Autonomic Restoration of Electrical Conductivity

Blaiszik, Ben; Kramer, Charlotte; Grady, Martha; Sottos, Nancy; White, Scott;

Thermomechanical failure of conductive pathways in highly integrated circuits results in loss of function that is often impossible to repair and remains a long-standing problem hindering advanced electronic packaging. Prior approaches to restoration of conductivity rely on external intervention in the form of heating or manual delivery of relatively low conductivity materials. Here, we demonstrate autonomic healing of an electrical circuit with nearly full recovery of conductance (ca. 99%) less than one millisecond after damage. The rapid restorative mechanism relies on the triggered release and transport of microencapsulated eutectic gallium–indium (Ga–In) liquid metal into the broken conductive pathway. For a relatively small volume fraction of microcapsules that are patterned on gold (Au) lines, all of the damaged circuits heal with high efficiency. This autonomic healing system shows the potential for more sustainable electronic devices with increased fault-tolerance, improved circuit reliability, and extended service life.

04/21/2014

2:26 PM

13 files

Center for Nanoscale Materials

View Dataset

self-healing

circuit

microcapsules

energy_density:2000

Synthesis, Characterization, and Structural Modeling of High-Capacity, Dual Functioning MnO₂ Electrode/Electrocatalysts for Li-O₂ Cells

Trahey, Lynn; Chan, Maria; Blaiszik, Ben;

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04/16/2014

9:56 AM

4 files

Center for Nanoscale Materials

View Dataset

Li-ion

Li-air

manganese

energy_density:2500



Select a published dataset



globus

Search Publish Manage Data Groups Support

Discover Data

energy_density | num_samples | protocol_version | 2000

Refine Search All Endpoints Collections

energy_density>1500 microcapsules



Transfer

Tag

Analyze

Start

Destination: Home (blaiszik#laptop/) | SNS (go#ep2/home/SNS)

New Destination

All None Inverse

3 results found | > 0.0 B

0 selected | > 0.0 B

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self-healing circuit microcapsules

energy_density:2000

04/21/2014

2:26 PM

13 files

Center for Nanoscale Materials

View Dataset

Synthesis, Characterization, and Structural Modeling of High-Capacity, Dual Functioning MnO₂ Electrode/Electrocatalysts for Li-O₂ Cells

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Li-ion Li-air manganese

energy_density:2500

04/16/2014

9:56 AM

4 files

Center for Nanoscale Materials

View Dataset

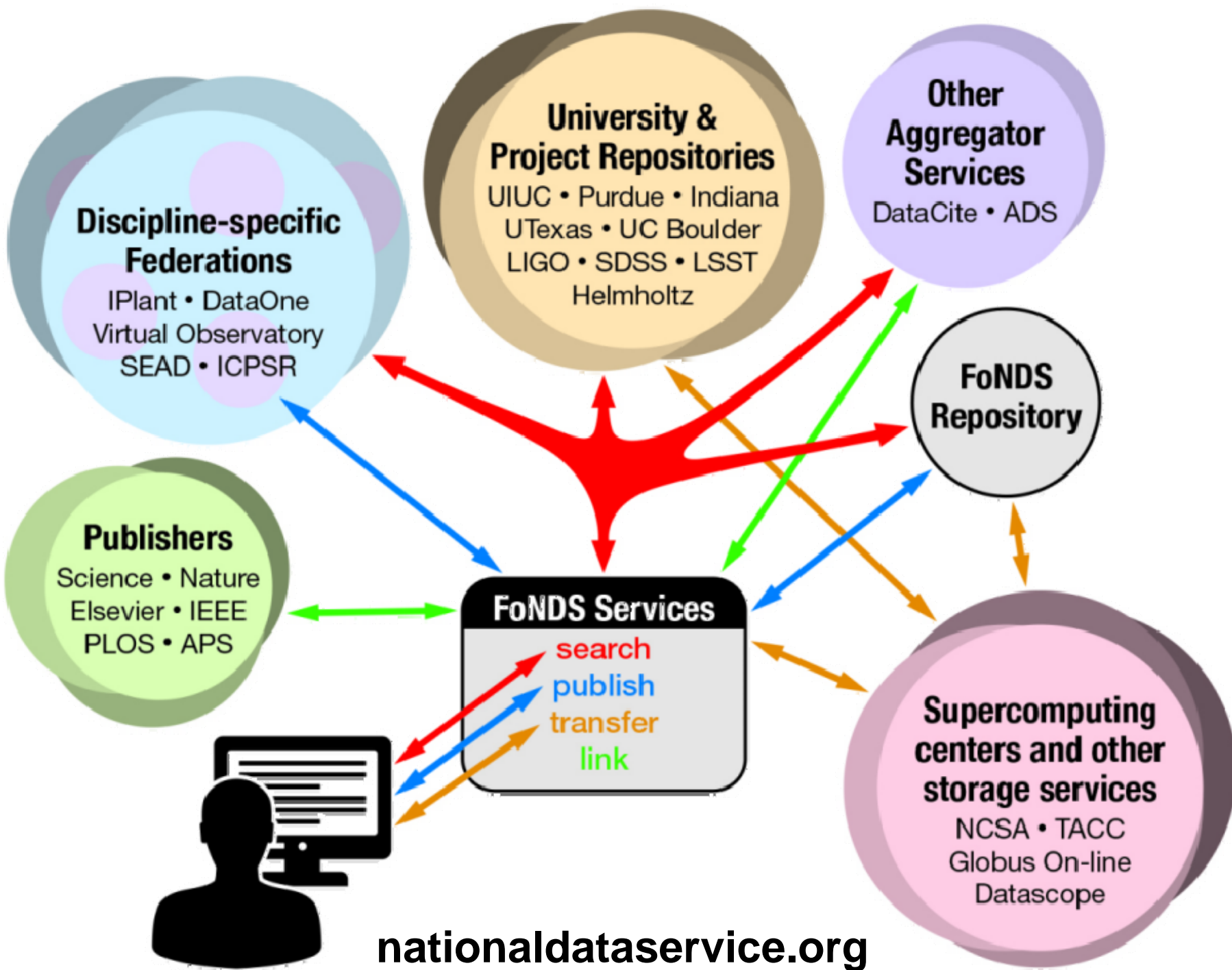


View downloaded dataset

The screenshot displays a Mac OS desktop environment. A file browser window titled "SynthesisData" is open, showing a list of files:

Name	Date Modified	Size	Kind
20120101 - Atomic-configurations.png	Today 2:45 PM	1.2 MB	Portab...image
20120108 - Cycling.png	Today 2:45 PM	1.6 MB	Portab...image
20120110 - Lithiation.jpeg	Today 2:45 PM	135 KB	JPEG image
20120201 - Overview.png	Today 2:45 PM	617 KB	Portab...image

Two image windows are also open. The window titled "20120110 - Lithiation.jpeg" shows a molecular simulation of a material structure with green and blue spheres, labeled "Li Si". The window titled "20120108 - Cycling.png" displays two scanning electron microscopy (SEM) images of a material. The left image shows a dense, granular surface, and the right image shows a porous, fibrous structure. A scale bar of 10µm is visible at the bottom of the right image.



MATERIALS DATA FACILITY LAUNCHED IN SUPPORT OF MATERIALS GENOME INITIATIVE

06.19.14 - *Permalink*

The National Data Service Consortium is launching a materials data facility for the advancement of materials science research through open data access and sharing.

On the third anniversary of President Barack Obama establishing the Materials Genome Initiative (MGI)—a multi-agency effort to transform materials science research in the United States through a national infrastructure—a consortium of research universities, national laboratories, and academic publishers announced the Materials Data Facility today.

This new facility is being established as a pilot program under the [National Data Service](#) (NDS) and will provide a repository where scientists can preserve and share materials research data, produced by both simulations and experiments.

NDS is a new emerging vision for a national data infrastructure that enables the discovery, reuse, and publication of data for scientists and researchers across all disciplines. Sharing in this vision, the Materials Data Facility will push the MGI's goals of doubling the pace of development of advanced materials research.



Discovery cloud: Globus research data management services



File transfer & sharing



Identity & group management



Data publication & discovery

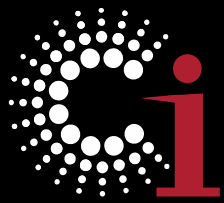


Simulation & data analysis

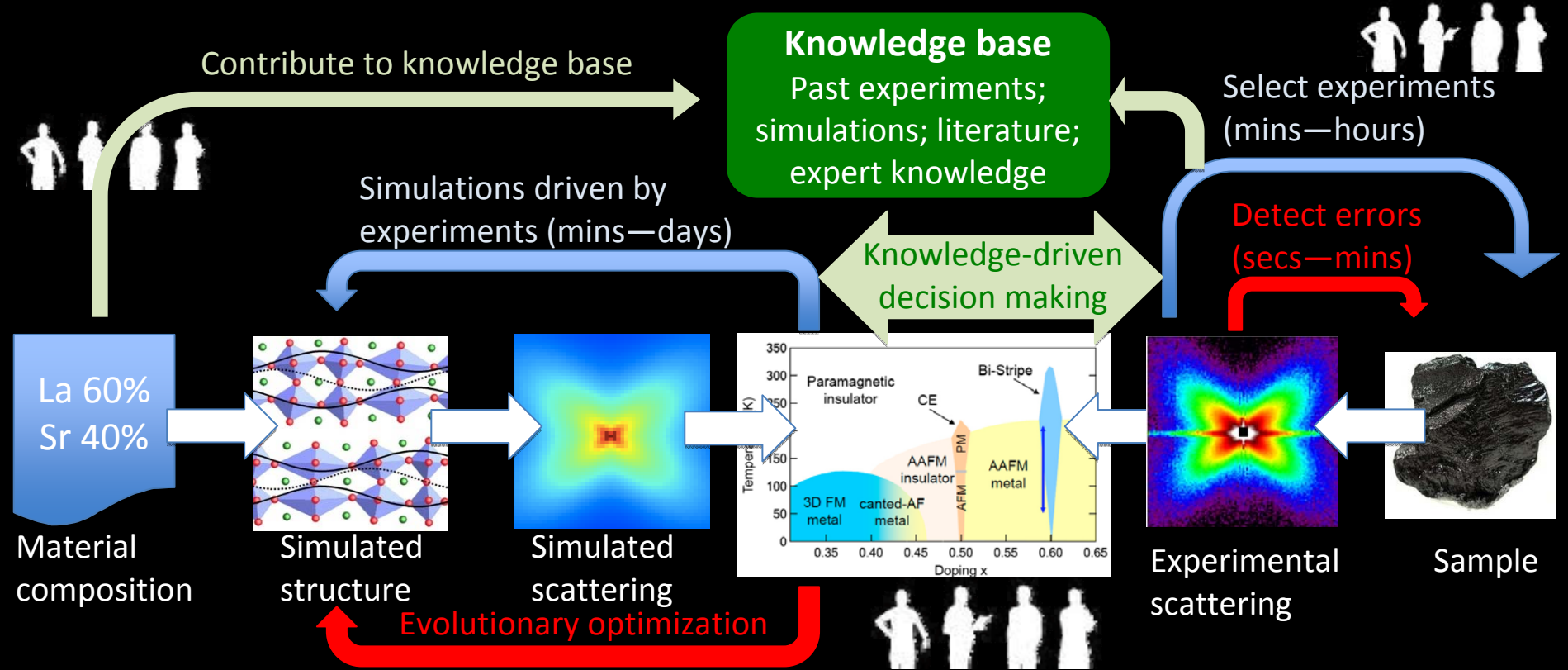


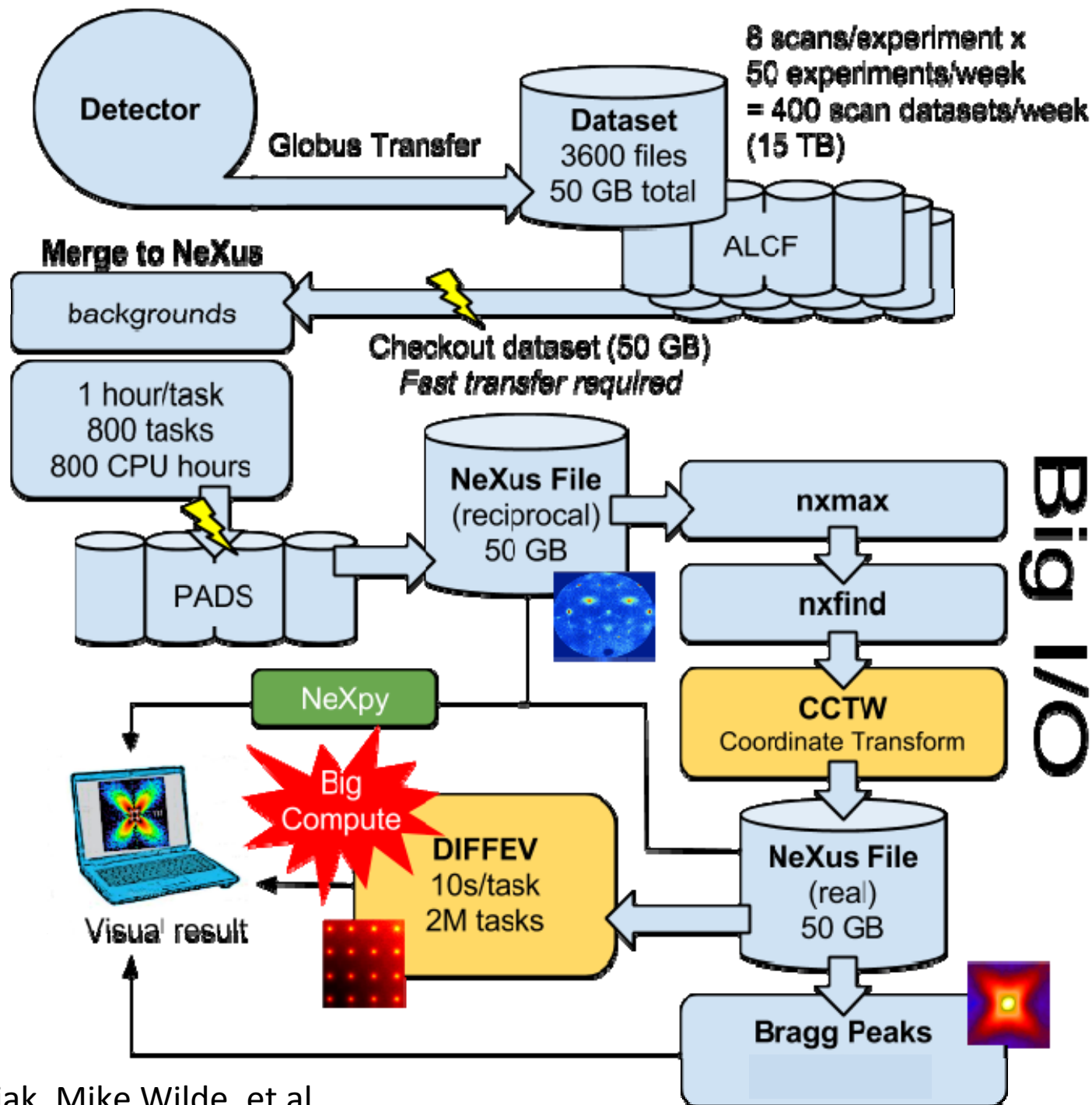
www.globus.org

computationinstitute.org



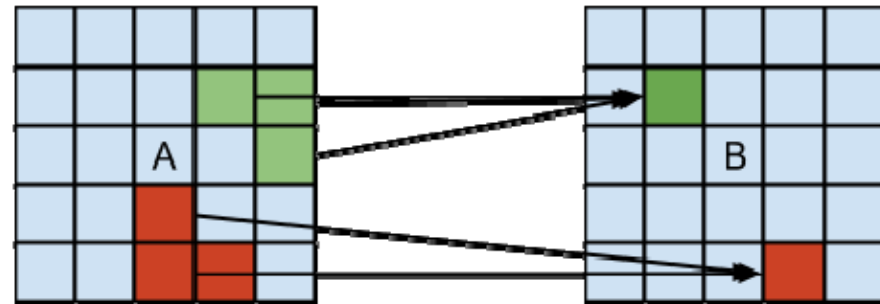
Linking simulation and experiment to study disordered structures



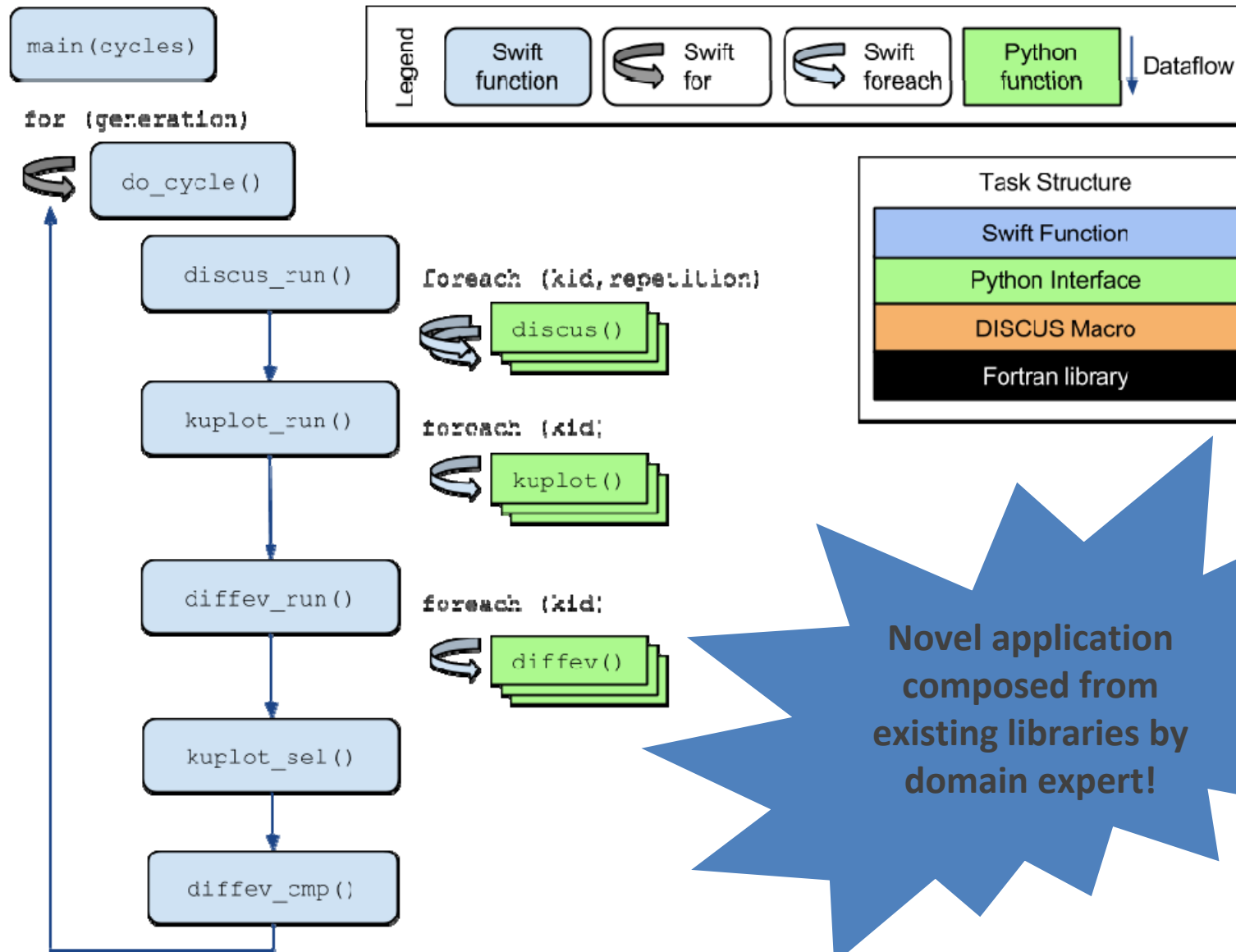


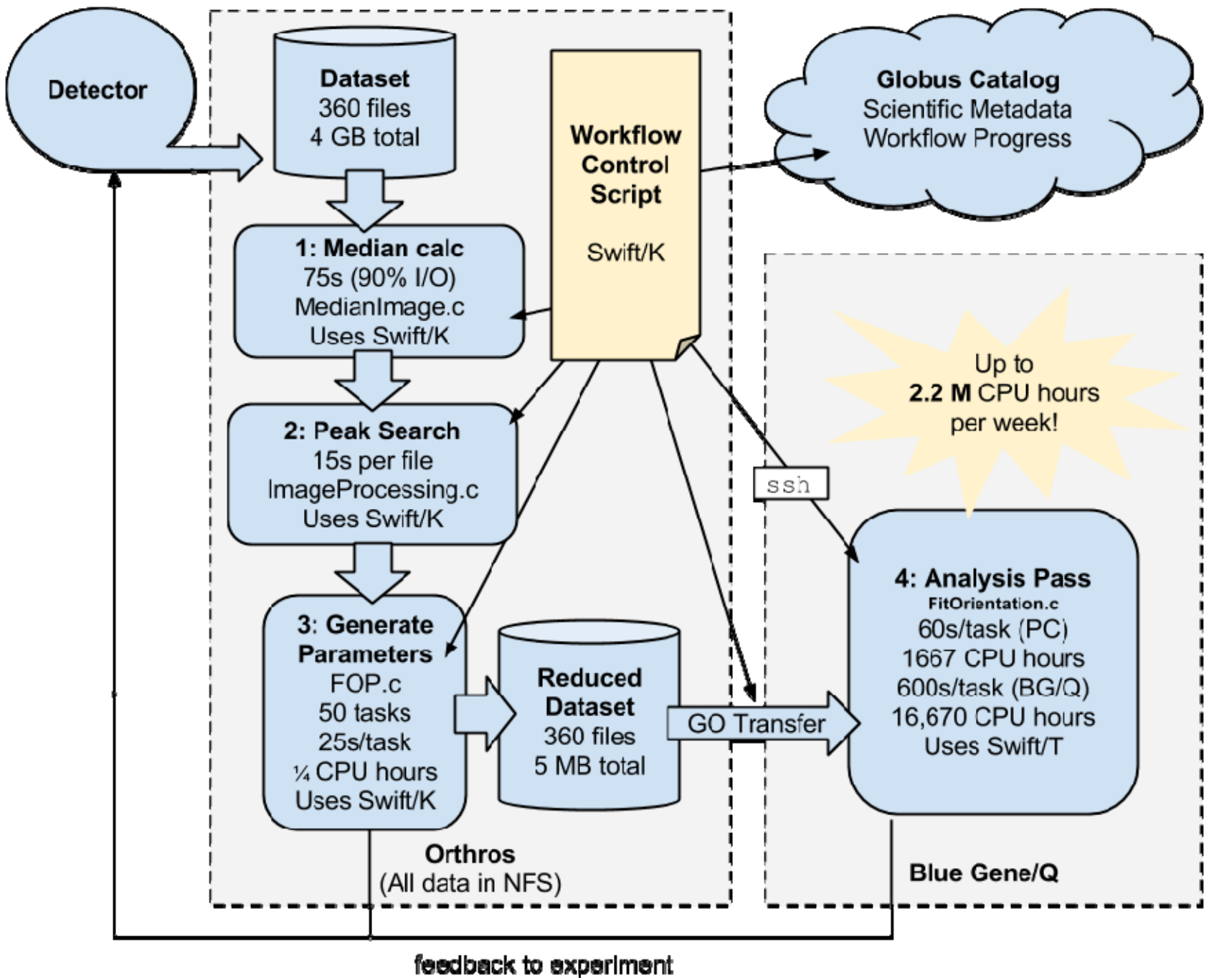
CCTW: Swift/T application (C++)

```
bag<blob> M[];  
foreach i in [1:n] {  
    blob b1= cctw_input("pznpt.nxs");  
    blob b2[];  
    int outputId[];  
    (outputId, b2) = cctw_transform(i, b1);  
    foreach b, j in b2 {  
        int slot = outputId[j];  
        M[slot] += b;  
    }  
    foreach g in M {  
        blob b = cctw_merge(g);  
        cctw_write(b);  
    }  
}
```



DIFFEV: Genetic algorithm via dataflow







Simulation and data analysis: Point and click parallelism

**Capture domain
knowledge: data
and code**

Data space

Local and remote
datasets

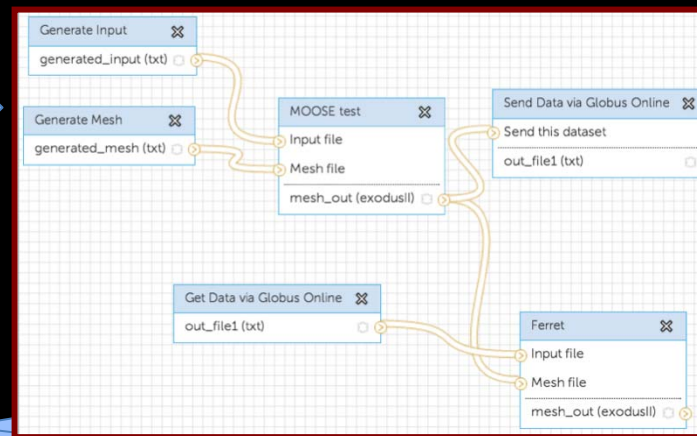
Tool shed

Simulation
models & analysis

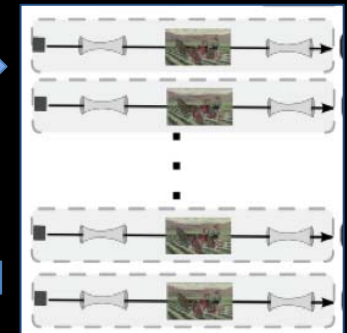
Workflows

Link data, tools in
reusable form

**Reusable workflows encode
commonly used modeling
and analysis pipelines**



**Large
simulation
campaigns**

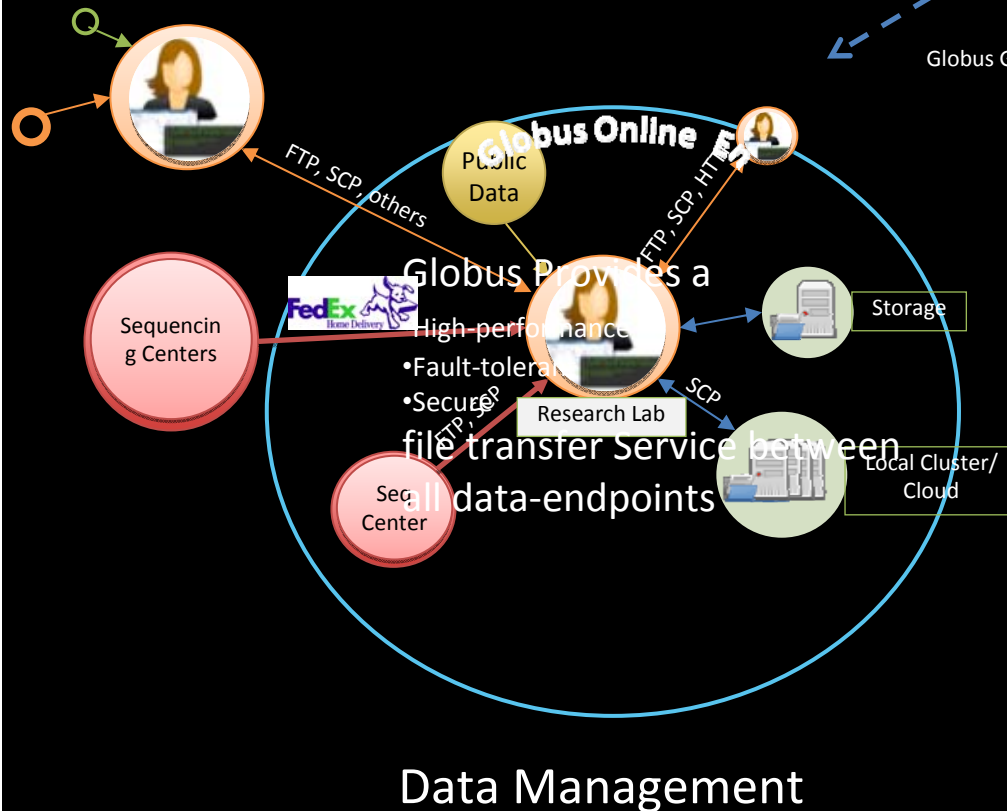


Hosted on Amazon cloud for reliable, on-demand access and scalability

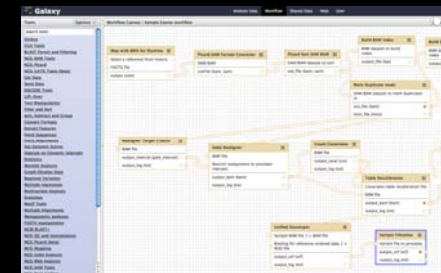
Builds on widely used Galaxy, Globus, and Swift systems
galaxyproject.org globus.org swift-lang.org

computationinstitute.org

Experiences in genomics



Galaxy Based Workflow Management System



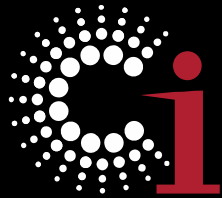
Globus Integrated within Galaxy
 Web-based UI
 Drag-Drop workflow creation
 Easily modify Workflows with new tools



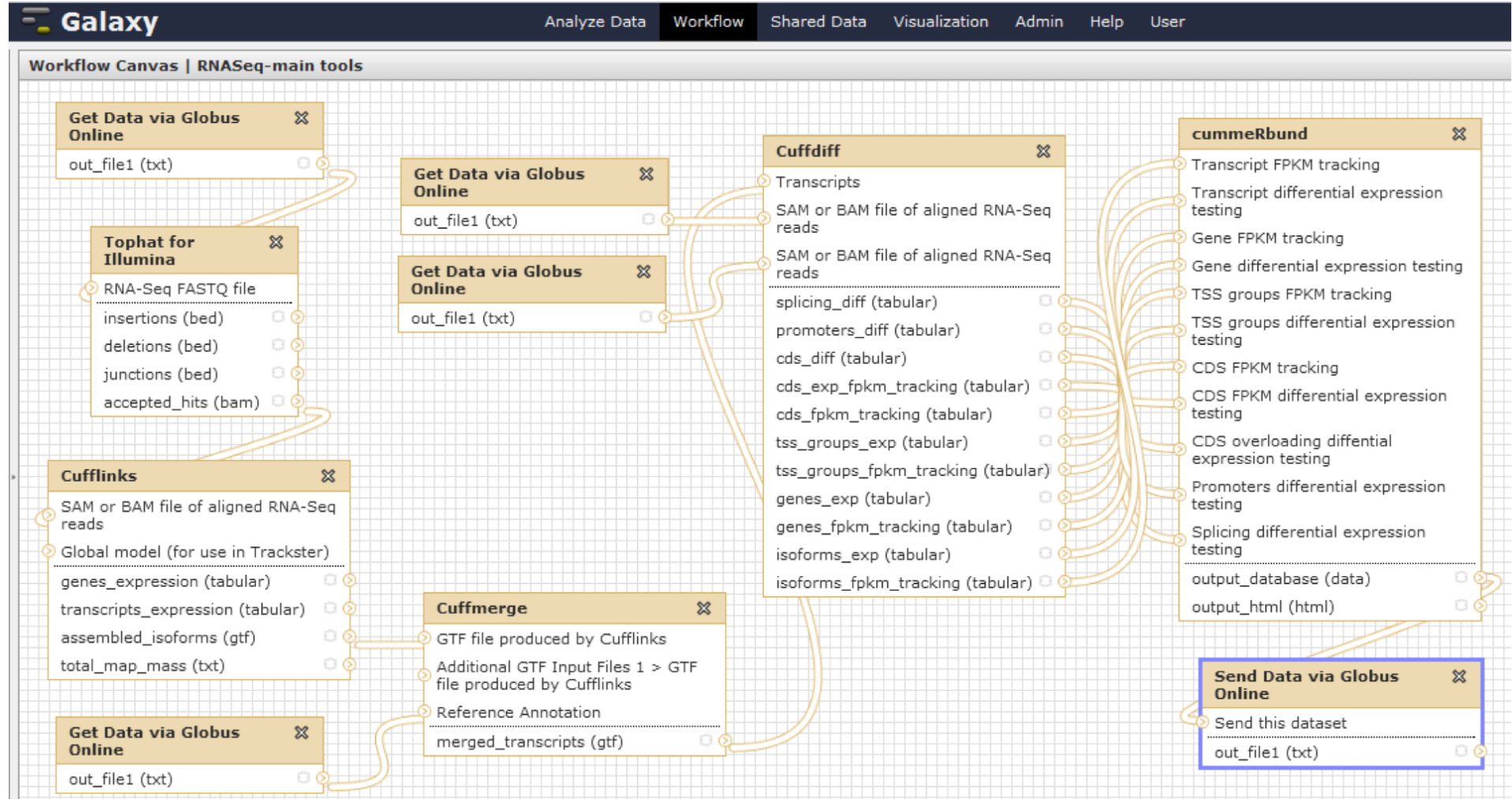
Analytical tools are automatically run on scalable compute resources when possible

Amazon Web Services

Data Analysis

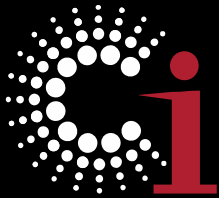


RNA-Seq pipeline

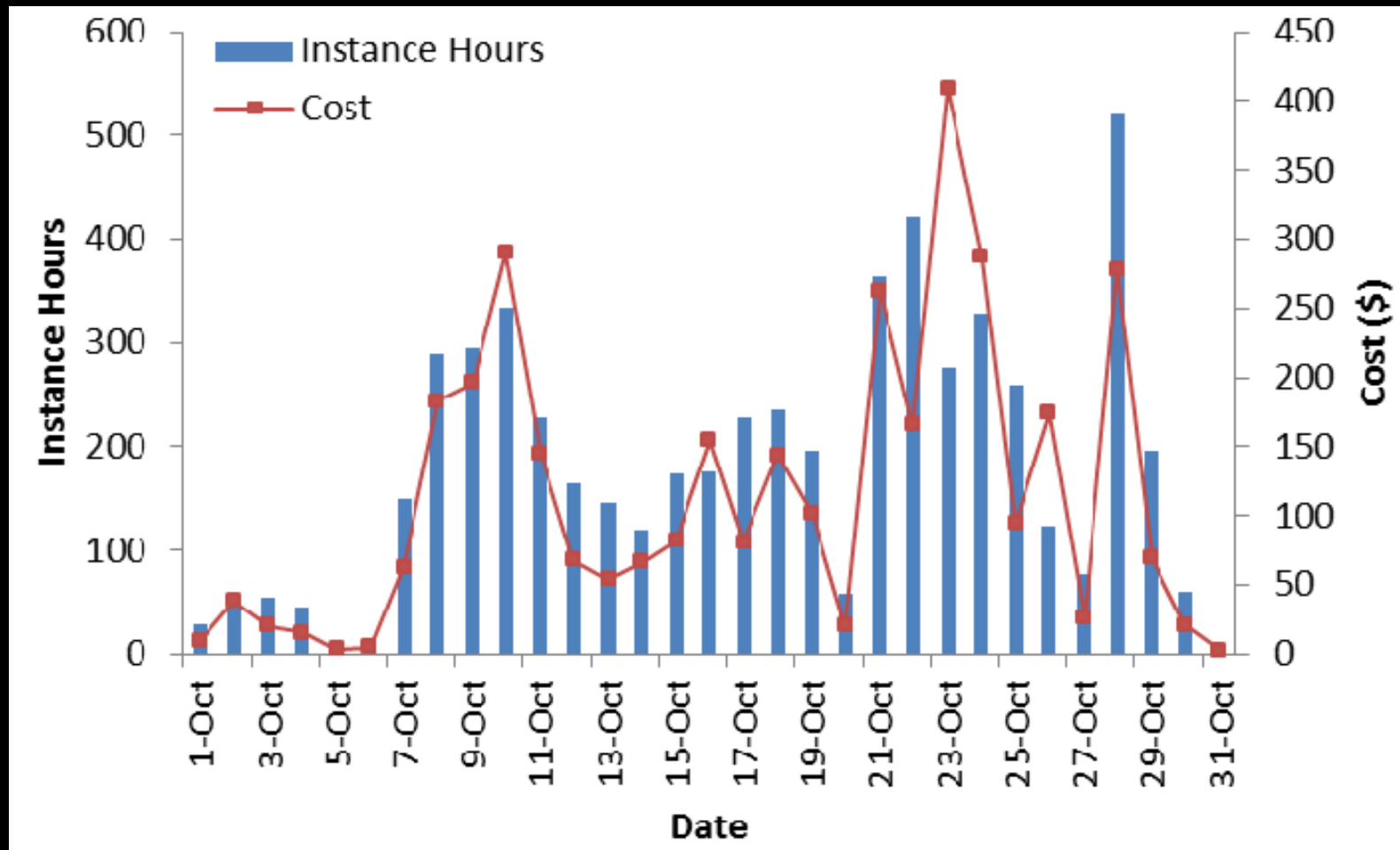


Ravi Madduri, Paul Davé, et al.

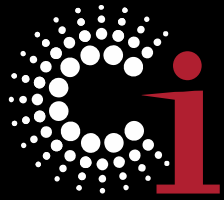
computationinstitute.org



Globus Genomics on AWS



800K Core hours in last 6 months



Discovery Cloud: Three common themes

1) Accelerate discovery via automation



2) Slash costs of trying new methods

- No local software installation
- No need to read manual
- On-demand, elastic scalability
- Low operational costs, proactive support



3) Make data preservation trivial





Take away messages


- **Data has a dual nature: rare treasure and chaotic deluge**



- **Science must embrace this duality**
 - **Treasure:** Store, curate, index, preserve
 - **Deluge:** Slash management costs, to both accelerate use & facilitate data preservation
- **Cloud services can help in both areas**



Thanks to great colleagues and collaborators

- Rachana Ananthakrishnan, Ben Blaiszik, Kyle Chard, Raj Kettimuthu, Ravi Madduri, Tanu Malik, Steve Tuecke, Justin Wozniak, and other CS colleagues
- Ray Osborn, Francesco de Carlo, Chris Jacobsen, Nicola Ferrier, and other Argonne scientists
- Juan de Pablo, Peter Voorhees, and other NIST  participants



Thank you to our sponsors!

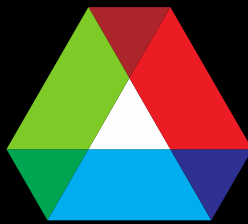


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