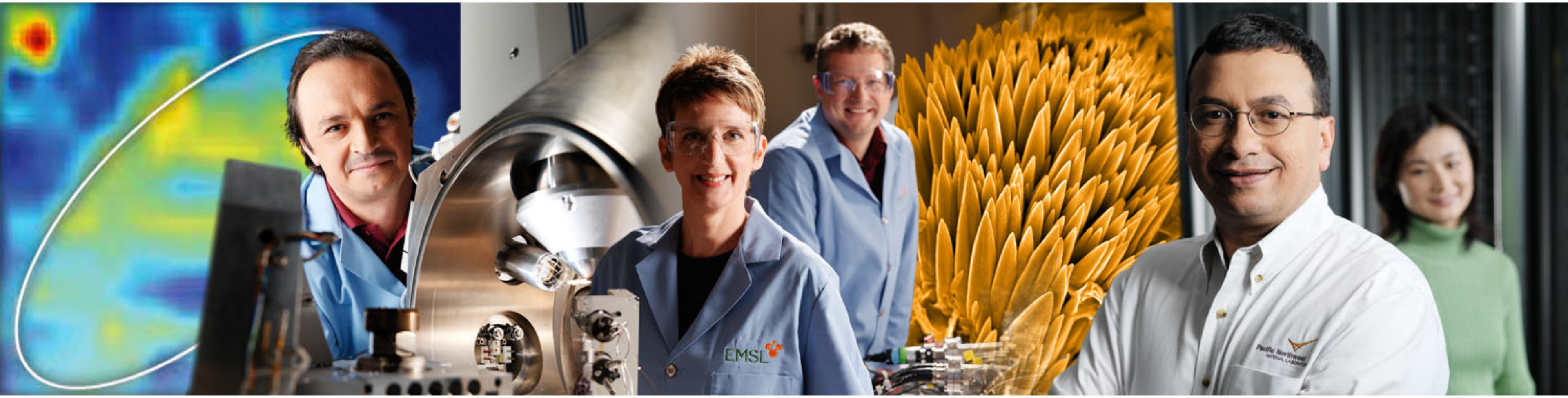
EMSL

MyEMSL & EMSLHub: Creating A flexible framework for scientific data sharing, discovery, and collaboration

PNNL-SA-96303

David Cowley



www.emsl.pnl.gov

Pacific Northwest NATIONAL LABORATORY

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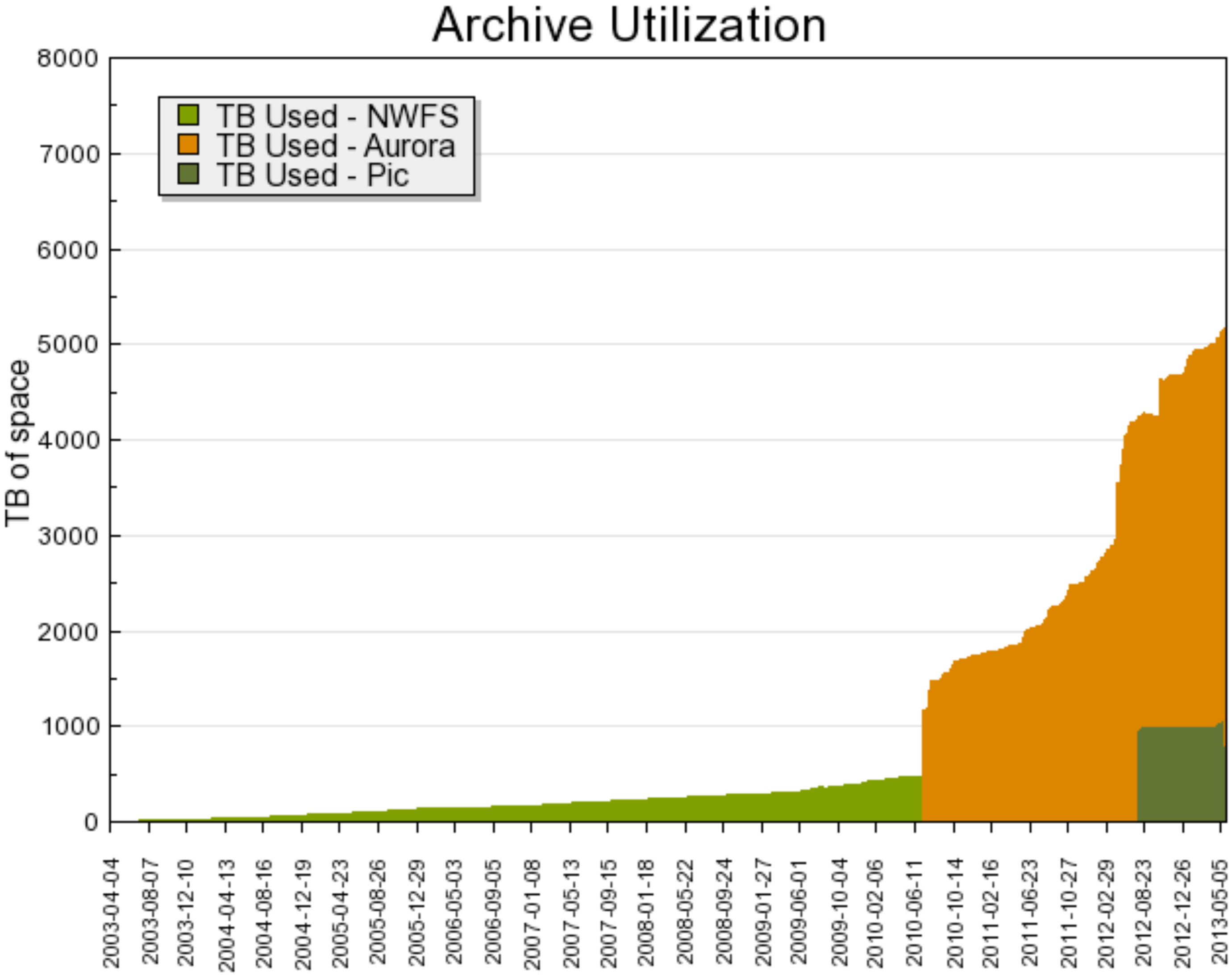
Data Growth at EMSL 2002-2013

EMSL



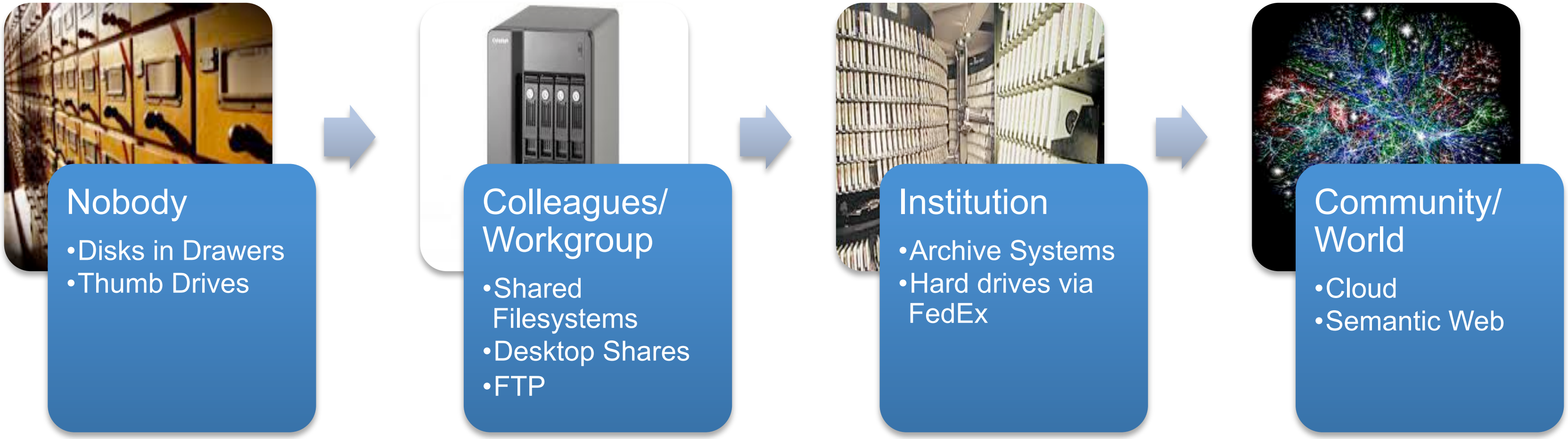
EMSL Estimated Aggregate Data Production/Transfer Rates

- At present:
  - 6 TB/day produced in EMSL
  - 5 TB/day transferred within EMSL
  - 200 GB/month transferred out of EMSL
- 2-5 years from now:
  - 20 TB/day produced
  - 40 TB/day transferred within
  - 600 TB/month transferred
  - 5 TB/month transferred into EMSL
- 5+ years from now:
  - 100 TB/day produced
  - 200 TB/day transferred within
  - 3 PB/month transferred out
  - 50 TB/month transferred in

New Directives: Expand Public Access to the Results of Federally Funded Research

- *"The Obama Administration is committed to the proposition that citizens deserve easy access to the results of scientific research their tax dollars have paid for. That's why, in a policy memorandum released today, OSTP Director John Holdren has directed Federal agencies with more than $100M in R&D expenditures to develop plans to make the published results of federally funded research freely available to the public within one year of publication and requiring researchers to better account for and manage the digital data resulting from federally funded scientific research."*
- -- Posted by Michael Stebbins on whitehouse.gov February 22, 2013 at 12:04 PM EDT

Continuum of Data Sharing



Nobody

- Disks in Drawers
- Thumb Drives

Colleagues/ Workgroup

- Shared Filesystems
- Desktop Shares
- FTP

Institution

- Archive Systems
- Hard drives via FedEx

Community/ World

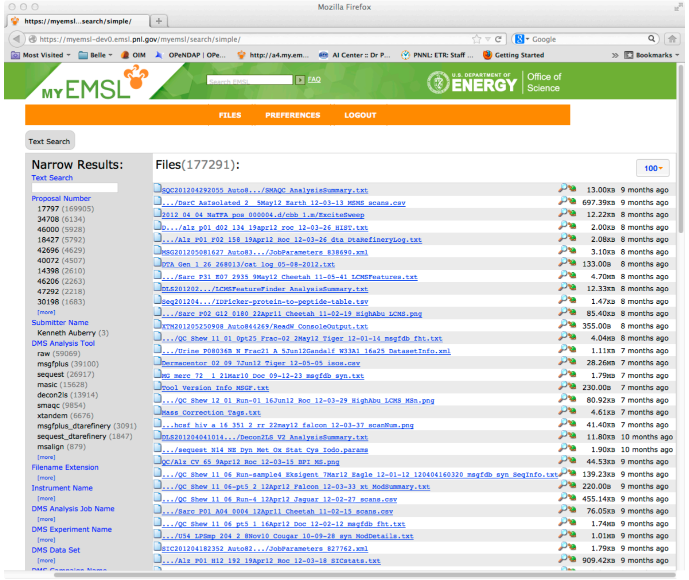
- Cloud
- Semantic Web

Limitations of our old approach

- **Aurora** is EMSL’s current archive system
- It has lots of parts:
  - Multi-petabyte robotic tape library (in CSF)
  - 1 Petabyte Disk Storage (in EMSL)
  - Many servers
  - Many services
- It’s mostly been used as a big ol’ pile of files
  - Organization (if any) was strictly DIY
  - Hard to find anything or even know it’s there!
- Access from outside EMSL is extremely limited

MyEMSL: Data Management for a diverse user facility

- Provide a system to capture, store and share data & metadata from EMSL's instruments and computers
- Create a flexible data framework that supports multiple scientific fields & approaches
- Allow scientific collaboration around data via EMSLHub (aka HubZero):
  - Workflow-based computation
  - Data integration and analysis
- Leverage high quality open source software
  - Form open source development groups
  - Easily shared with community
  - Highly efficient support and maintenance model
- Long term, create a framework to federate data sources across institutions



Narrow Results:

Text Search

Proposal Number
17797 (169905)
34708 (6134)
46000 (5928)
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[more]

Submitter Name
Kenneth Auberry (3)

DMS Analysis Tool
raw (59069)
msgfplus (39100)
sequest (26917)
masic (15628)
decon2ls (13914)
smaqc (9854)
xtandem (6676)
msgfplus_dtarefinery (3091)
sequest_dtarefinery (1847)
msalign (879)
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Filename Extension
[more]

Instrument Name
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DMS Analysis Job Name
[more]

DMS Experiment Name
[more]

DMS Data Set
[more]

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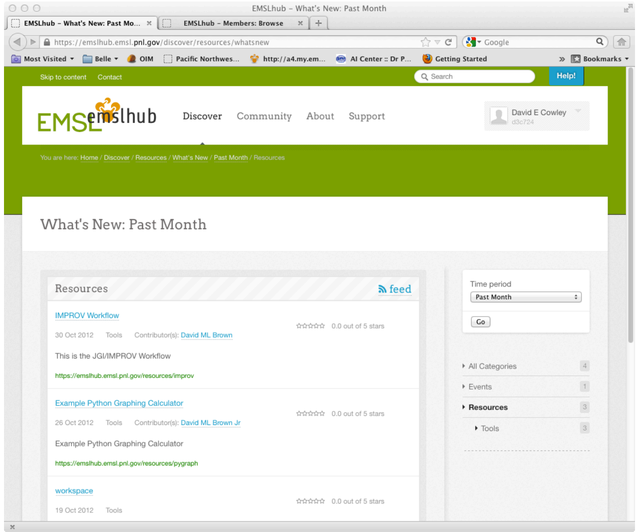

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What's New: Past Month

Resources — feed

IMPROV Workflow — ☆☆☆☆☆ 0.0 out of 5 stars
30 Oct 2012 Tools Contributor(s): David ML Brown
This is the JGI/IMPROV Workflow
https://emslhub.emsl.pnl.gov/resources/improv

Example Python Graphing Calculator — ☆☆☆☆☆ 0.0 out of 5 stars
26 Oct 2012 Tools Contributor(s): David ML Brown Jr
Example Python Graphing Calculator
https://emslhub.emsl.pnl.gov/resources/pygraph

workspace — ☆☆☆☆☆ 0.0 out of 5 stars
19 Oct 2012 Tools

Time period: Past Month
Go

All Categories	4
Events	1
Resources	3
Tools	3

Supporting Scientific Collaboration with MyEMSL

- Provide search and easy access to data & metadata for authorized users
- Facilitate and enforce data release policies
- Find enthusiastic scientists who know they have data needs and partner with them
- Provide data interaction framework to facilitate “Bring Your Own”:
    - Data catalogs & definitions
    - Workflow based computation
    - Data integration and analysis
    - Web and mobile apps

Why MyEMSL?

- **MyEMSL** aims to solve a number of problems with the old archive approach:
  - Make data easy to find by good use of metadata
  - Make files easy to get via the web
  - Set up good access control
  - Make it easy to share data with collaborators
- Leverage existing HPSS archive for bulk data storage
- Augment legacy archive with other parts:
  - Metadata Database
  - Automated uploader for instruments
  - Web portal @ https://my.emsl.pnl.gov
  - Links to EMSL's User/Resource allocation systems & EMSLHub

The importance of Metadata

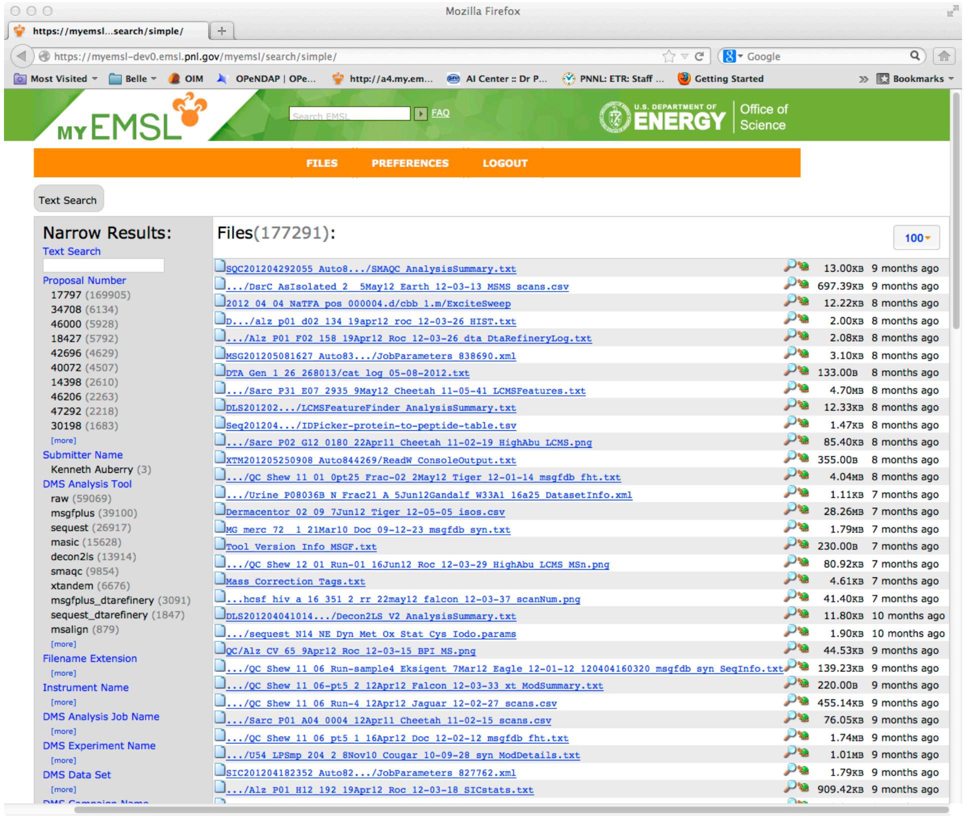
- We have a big pile of files going back 15 years, but nobody knows what all is in there!
- The key to discovering and understanding data is to have good **metadata!**
- Metadata tells you what is known about the data
- Can be trivial:
  - File name
  - File owner
  - Time and date stamps
- Can be much more interesting:
  - Instrument settings & environmental parameters
  - Sample information
  - Registration data for multimodal analyses

What we need to do about metadata

- The more we can get of it, the more powerful MyEMSL becomes
- We have defined a little essential metadata that all data must have
- MyEMSL must be **flexible and non-restrictive** about metadata and **enable metadata to evolve** over time
- We don't know whatever other metadata people may need – maybe they don't know yet
- Science partners will need to tell us what metadata will be useful to them and MyEMSL will need to support it
- How can we get it?
  - Our processes (i.e. autouploader) can capture or generate a little of it
  - Humans may need to enter it
  - Code can be written to extract/generate it, but this will require funding and people time!

What exists today

- Web and service interfaces for moving data and metadata into and out of MyEMSL
- Authentication mechanisms
- Search and "shopping cart" interfaces
- EMSLHub collaboration site with pilot workflows
- Proteomics pipeline adapted to MyEMSL interfaces
- Increasing numbers of scientific instruments uploading data



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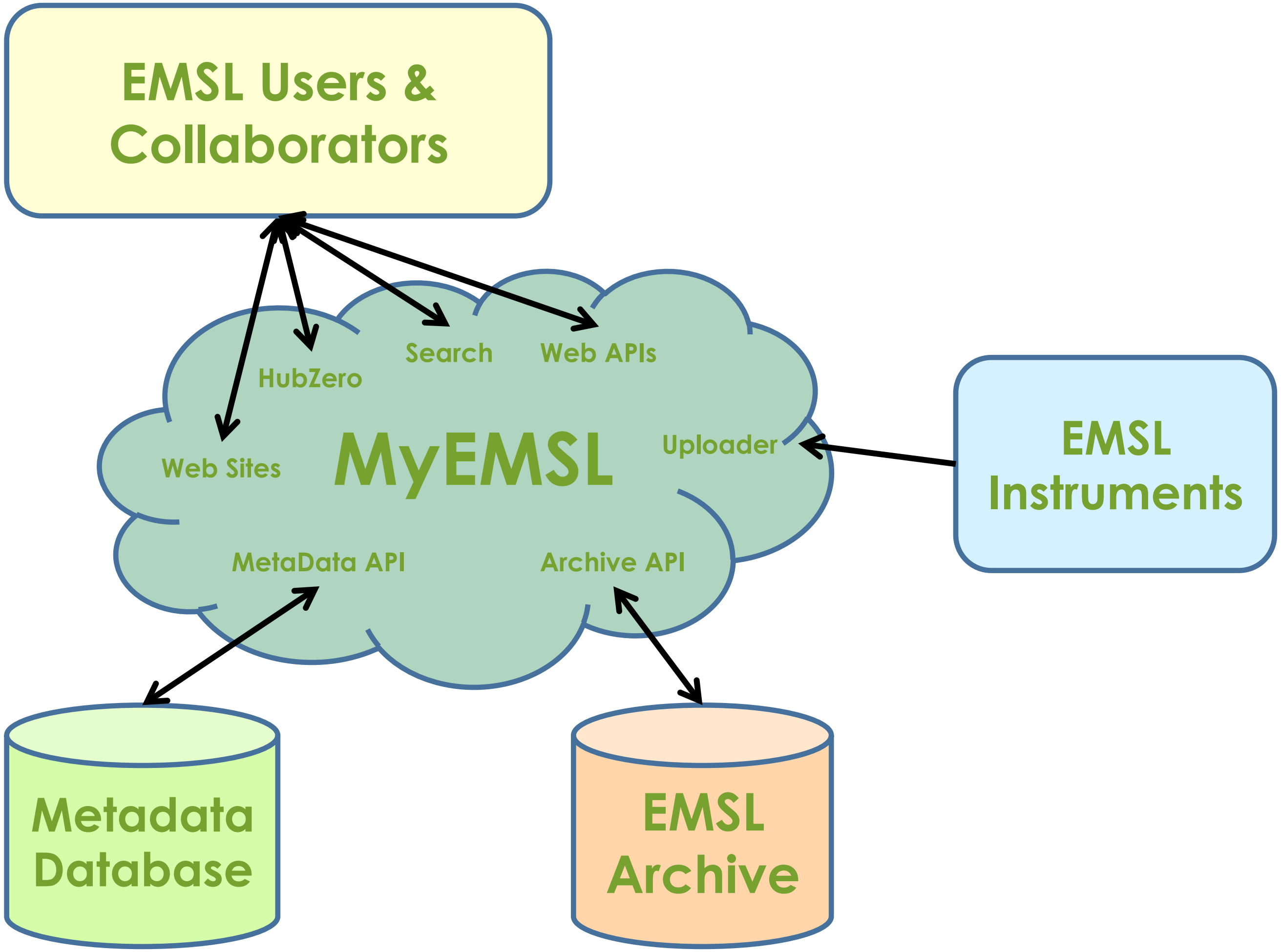
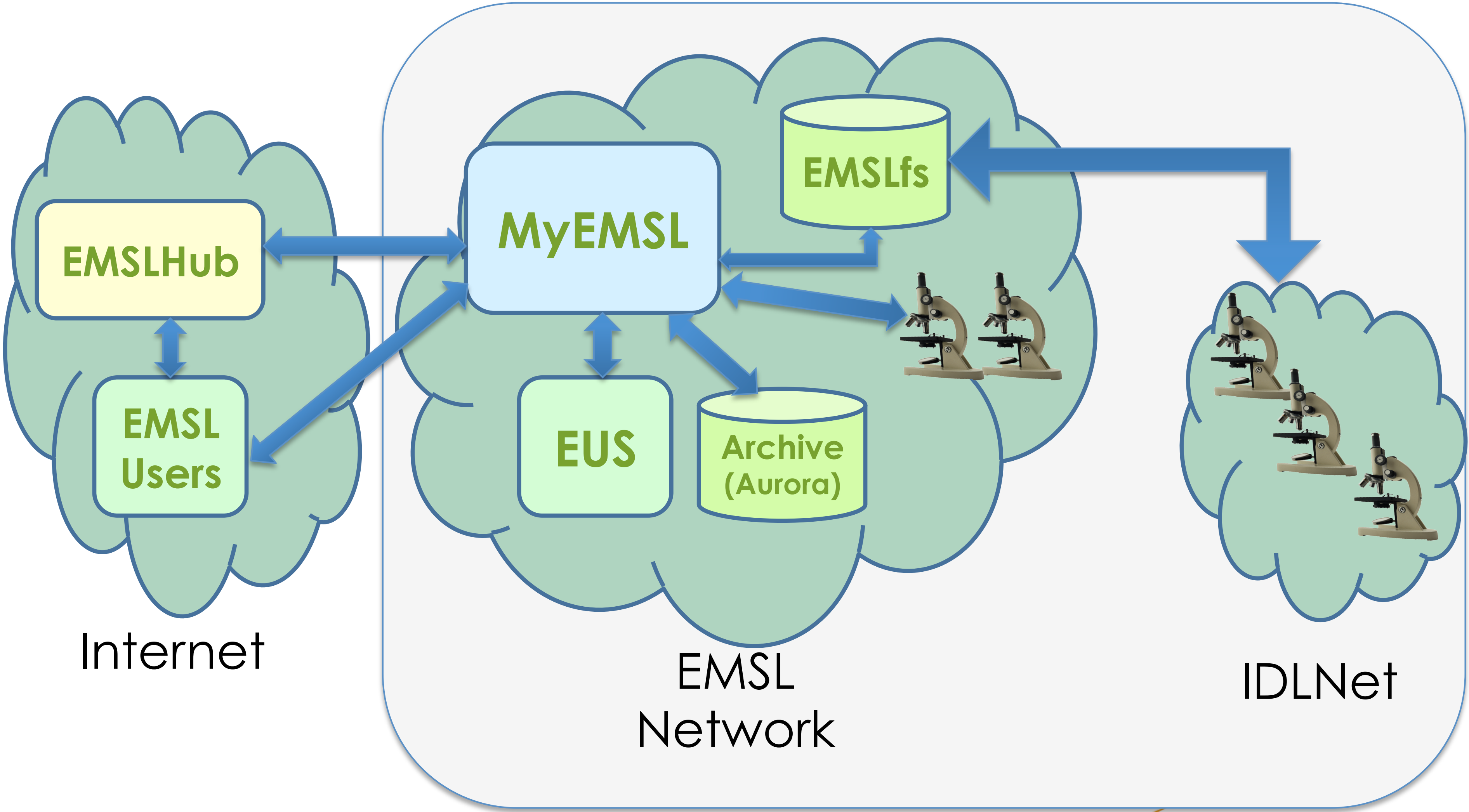
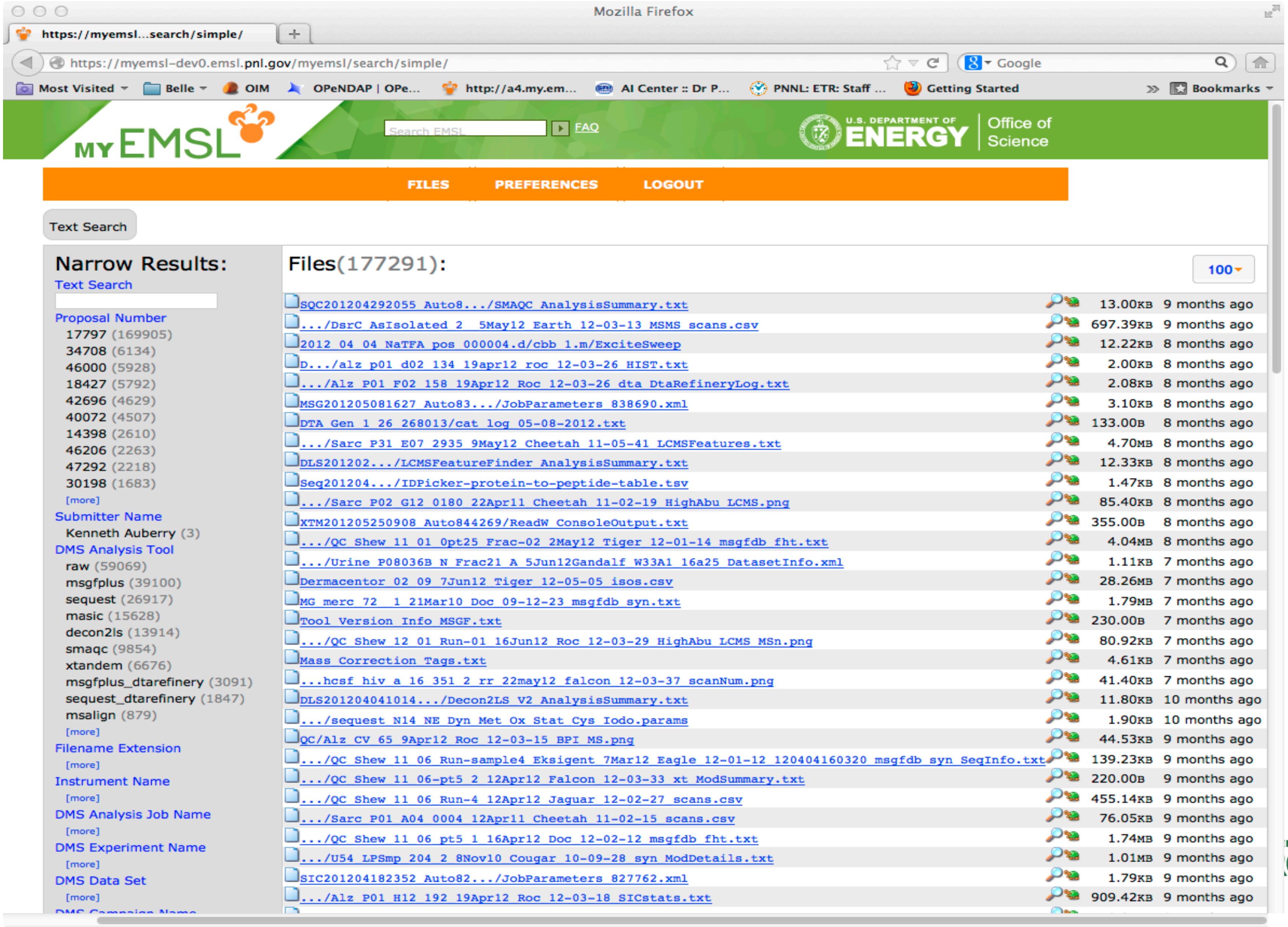
MyEMSL Conceptual Diagram



Data, Instruments in EMSL context



http://my.emsl.pnl.gov



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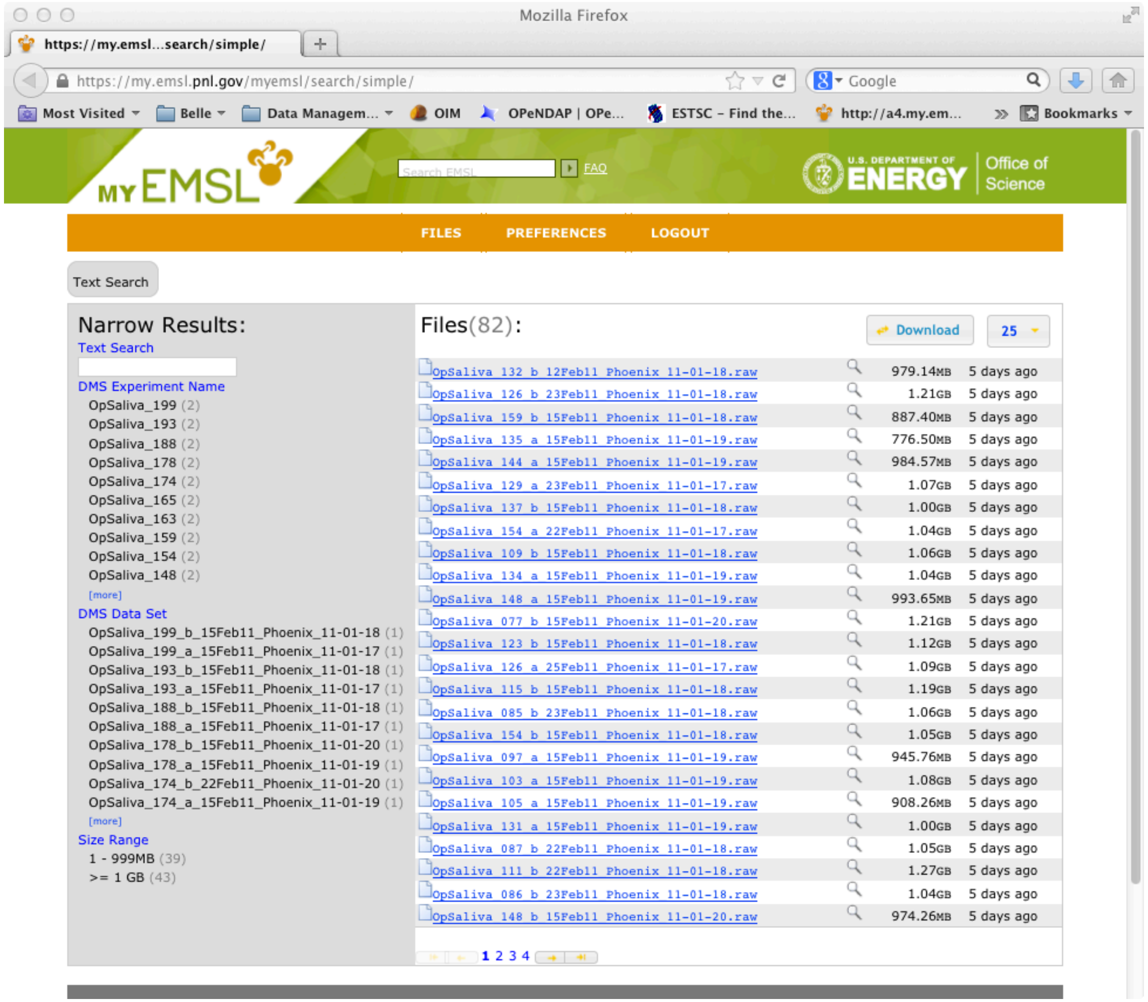
Example: Public data in MyEMSL web pages



Narrow Results:

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- OpSaliva_193 (2)
- OpSaliva_188 (2)
- OpSaliva_178 (2)
- OpSaliva_174 (2)
- OpSaliva_165 (2)
- OpSaliva_163 (2)
- OpSaliva_159 (2)
- OpSaliva_154 (2)
- OpSaliva_148 (2)
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- OpSaliva_178_a_15Feb11_Phoenix_11-01-19 (1)
- OpSaliva_174_b_22Feb11_Phoenix_11-01-20 (1)
- OpSaliva_174_a_15Feb11_Phoenix_11-01-19 (1)
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Size Range

- 1 - 999MB (39)
- >= 1 GB (43)

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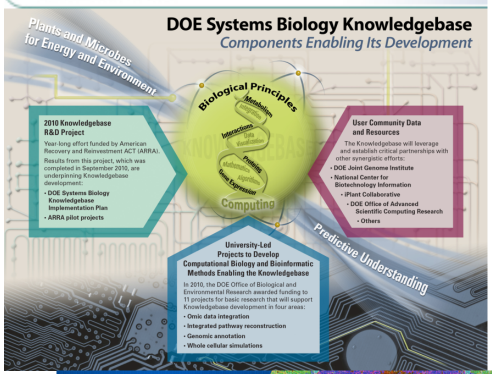
1 2 3 4

Establishing MyEMSL Collaborations

- We are establishing key collaborations with other institutions to:
  - Define tools and interfaces for data exchange
  - Leverage existing tools and frameworks
  - Establish open source consortia
- Partner organizations and activities:
  - DOE Joint Genome Institute (JGI)
  - DOE Systems Biology Knowledgebase (KBASE)
  - National Center for Microscopy and Imaging Research (NCMIR):
  - Semantic Physical Sciences (SPS) workshops

JGI
DOE JOINT GENOME INSTITUTE
US DEPARTMENT OF ENERGY
OFFICE OF SCIENCE



DOE Systems Biology Knowledgebase
Components Enabling Its Development

2010 Knowledgebase R&D Project

Year-long effort funded by American Recovery and Reinvestment ACT (ARRA).

Results from this project, which was completed in September 2010, are underpinning Knowledgebase development:

- DOE Systems Biology Knowledgebase Implementation Plan
- ARRA pilot projects

User Community Data and Resources

The Knowledgebase will leverage and establish critical partnerships with other synergistic efforts:

- DOE Joint Genome Institute
- National Center for Biotechnology Information
- iPlant Collaborative
- DOE Office of Advanced Scientific Computing Research
- Others

University-Led Projects to Develop Computational Biology and Bioinformatic Methods Enabling the Knowledgebase

In 2010, the DOE Office of Biological and Environmental Research awarded funding to 11 projects for basic research that will support Knowledgebase development in four areas:

- Omic data integration
- Integrated pathway reconstruction
- Genomic annotation
- Whole cellular simulations

NCMIR

University of BRISTOL

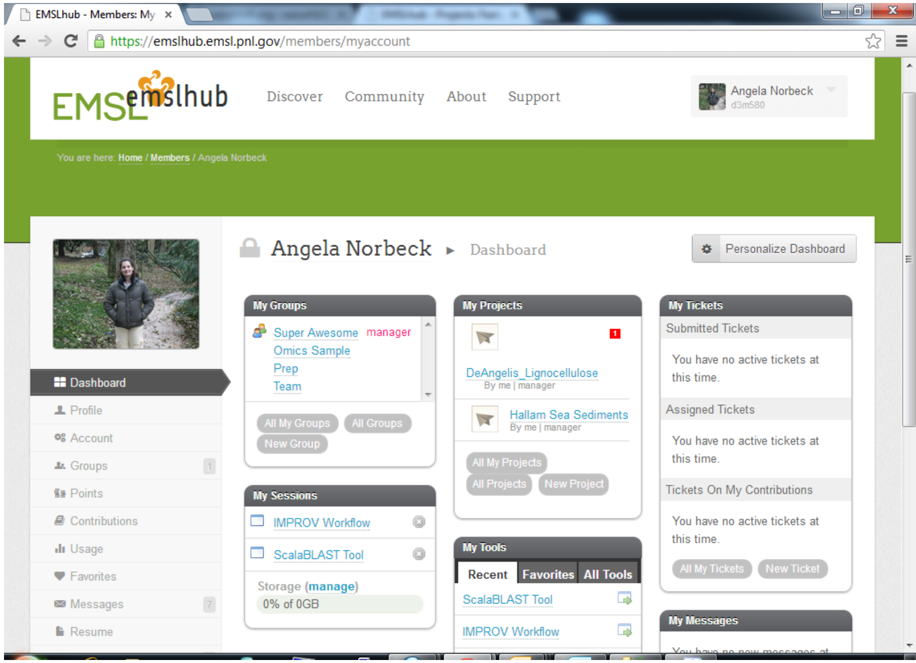
UNIVERSITY OF CAMBRIDGE

CSIRO

PENNSTATE
1855

EMSLHub

- **EMSLHub** is a collaborative web site at https://emslhub.emsl.pnl.gov
- Purpose: provide a system to allow scientific collaboration around *data* with a rich toolset
- Early collaborative efforts:
  - JGI – EMSL Data Integration
  - Proteomics project coordination & data dissemination
  - Integration of NWChem & NMR
  - Scientific Workflows



EMSLhub - Members: My

https://emslhub.emsl.pnl.gov/members/myaccount

You are here: Home / Members / Angela Norbeck

Angela Norbeck ▸ Dashboard

My Groups: Super Awesome manager, Omics Sample, Prep, Team

My Projects: DeAngelis_Lignocellulose (By me | manager); Hallam Sea Sediments (By me | manager)

My Tickets

Submitted Tickets: You have no active tickets at this time.

Assigned Tickets: You have no active tickets at this time.

Tickets On My Contributions: You have no active tickets at this time.

My Sessions: IMPROV Workflow; ScalaBLAST Tool

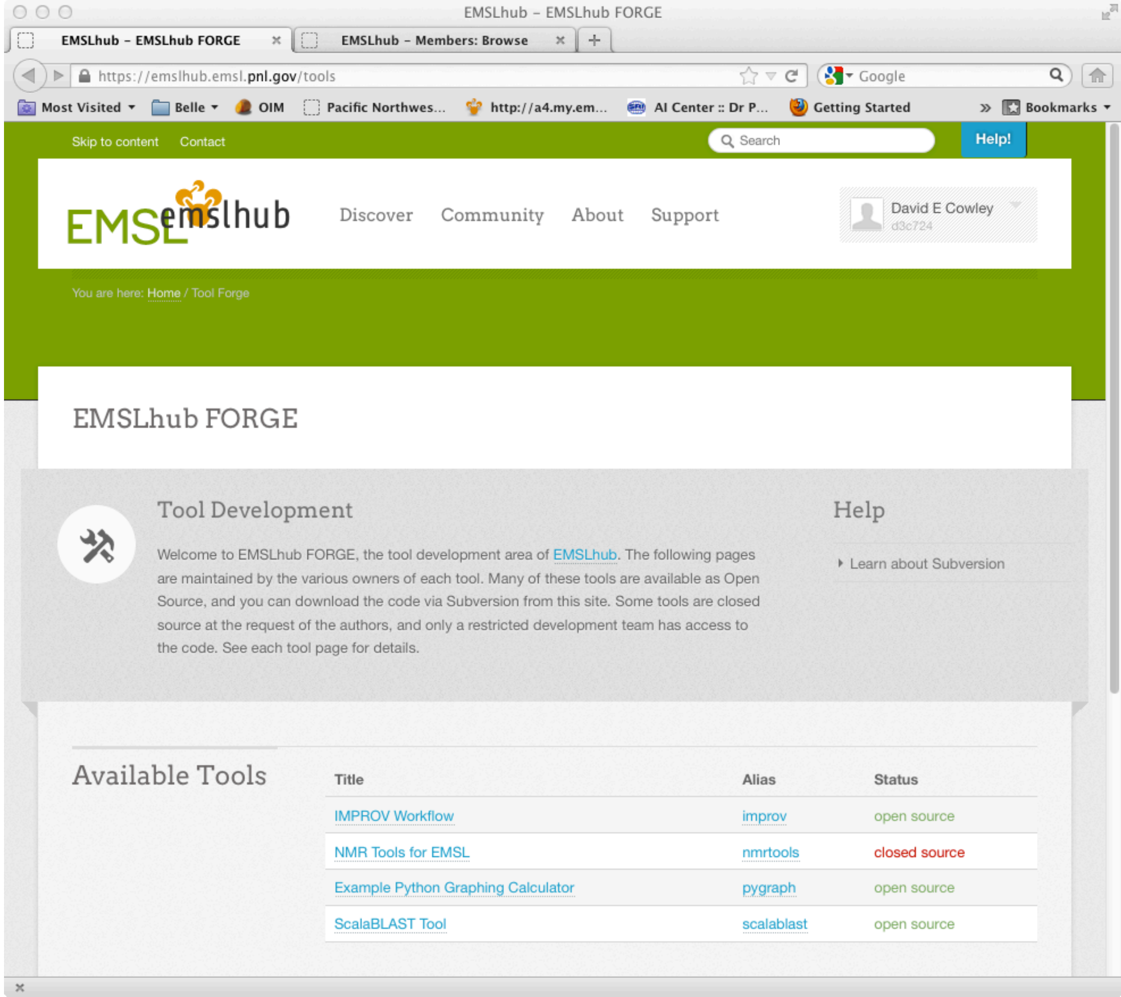
Storage (manage) 0% of 0GB

My Tools (Recent): ScalaBLAST Tool; IMPROV Workflow

My Messages

Tools Development in EMSLHub

- HubZero framework allows programs to be developed, shared, used within as “tools” in EMSLHub
- Anyone with access can submit tools
- Approved tools can be shared with groups
- First examples are:
  - NMR analysis pipeline
  - ScalaBLAST job submission
  - IMPROV in EMSLHub



EMSLhub FORGE

Tool Development

Welcome to EMSLhub FORGE, the tool development area of EMSLhub. The following pages are maintained by the various owners of each tool. Many of these tools are available as Open Source, and you can download the code via Subversion from this site. Some tools are closed source at the request of the authors, and only a restricted development team has access to the code. See each tool page for details.

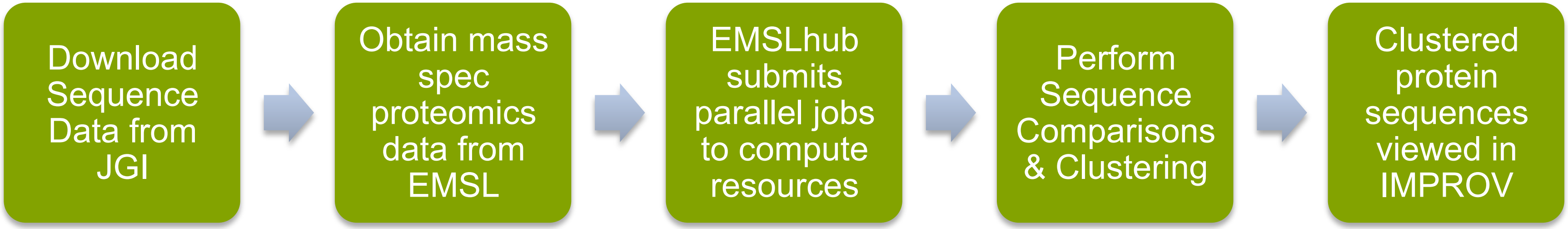
Help

- Learn about Subversion

Available Tools

Title	Alias	Status
IMPROV Workflow	improv	open source
NMR Tools for EMSL	nmrtools	closed source
Example Python Graphing Calculator	pygraph	open source
ScalaBLAST Tool	scalablast	open source

Example: Metaproteomics pipeline implementation in EMSLHub



Download Sequence Data from JGI

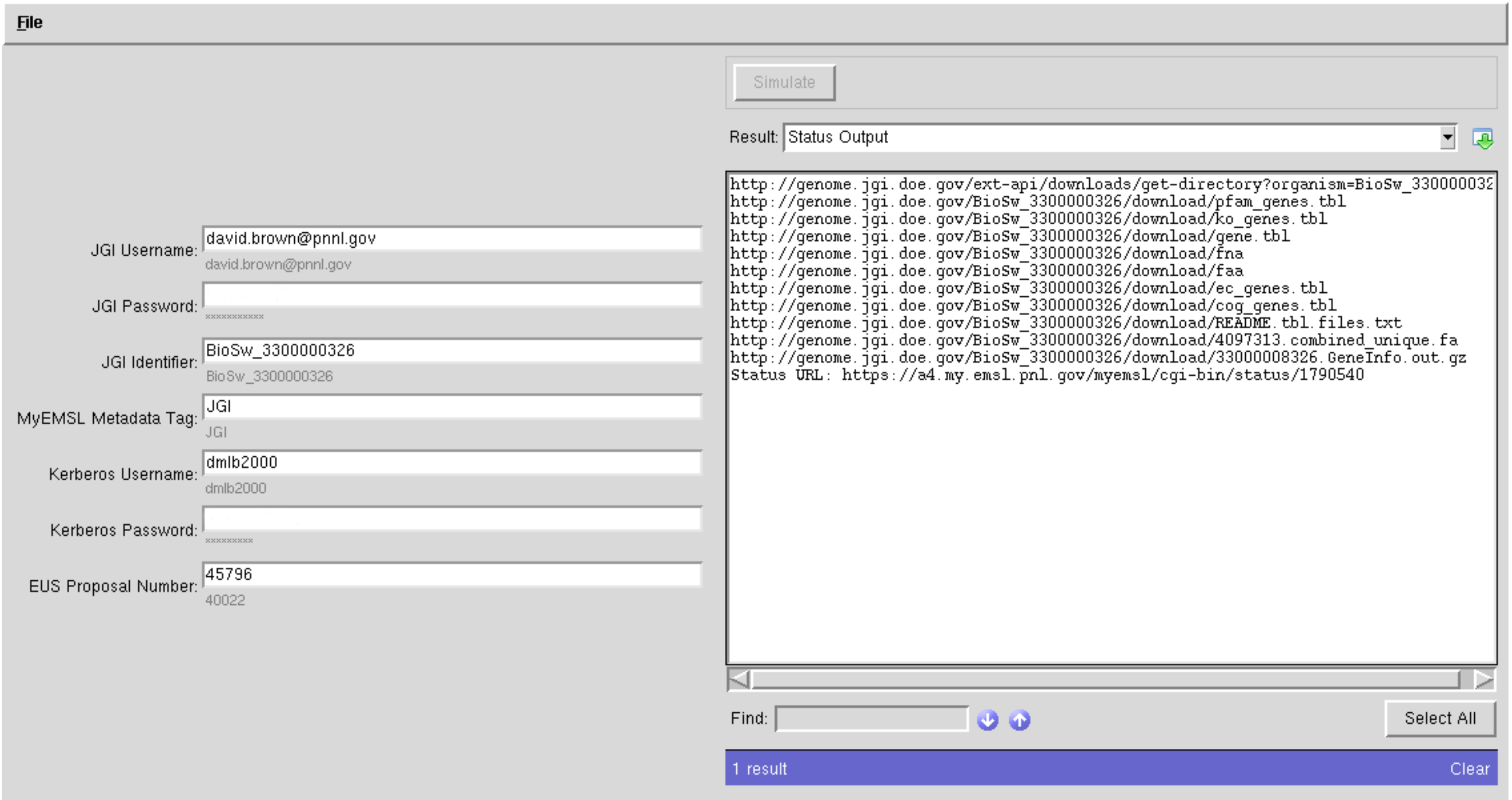
Obtain mass spec proteomics data from EMSL

EMSLhub submits parallel jobs to compute resources

Perform Sequence Comparisons & Clustering

Clustered protein sequences viewed in IMPROV

Example: Metaproteomics pipeline implementation in EMSLHub



JGI Username: david.brown@pnnl.gov
david.brown@pnnl.gov

JGI Password:
xxxxxxxxxxxx

JGI Identifier: BioSw_3300000326
BioSw_3300000326

MyEMSL Metadata Tag: JGI
JGI

Kerberos Username: dmlb2000
dmlb2000

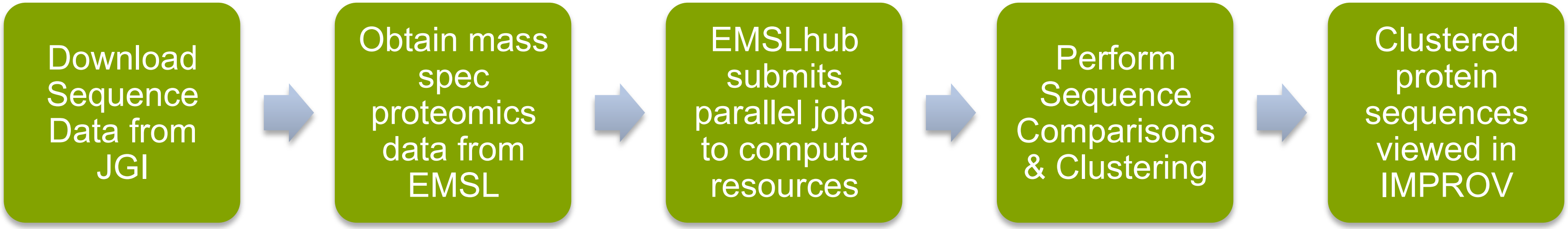
Kerberos Password:
xxxxxxxxxx

EUS Proposal Number: 45796
40022

Result: Status Output

```
http://genome.jgi.doe.gov/ext-api/downloads/get-directory?organism=BioSw_330000032
http://genome.jgi.doe.gov/BioSw_3300000326/download/pfam_genes.tbl
http://genome.jgi.doe.gov/BioSw_3300000326/download/ko_genes.tbl
http://genome.jgi.doe.gov/BioSw_3300000326/download/gene.tbl
http://genome.jgi.doe.gov/BioSw_3300000326/download/fna
http://genome.jgi.doe.gov/BioSw_3300000326/download/faa
http://genome.jgi.doe.gov/BioSw_3300000326/download/ec_genes.tbl
http://genome.jgi.doe.gov/BioSw_3300000326/download/cog_genes.tbl
http://genome.jgi.doe.gov/BioSw_3300000326/download/README.tbl.files.txt
http://genome.jgi.doe.gov/BioSw_3300000326/download/4097313.combined_unique.fa
http://genome.jgi.doe.gov/BioSw_3300000326/download/3300008326.GeneInfo.out.gz
Status URL: https://a4.my.emsl.pnl.gov/myemsl/cgi-bin/status/1790540
```

Example: Metaproteomics pipeline implementation in EMSLHub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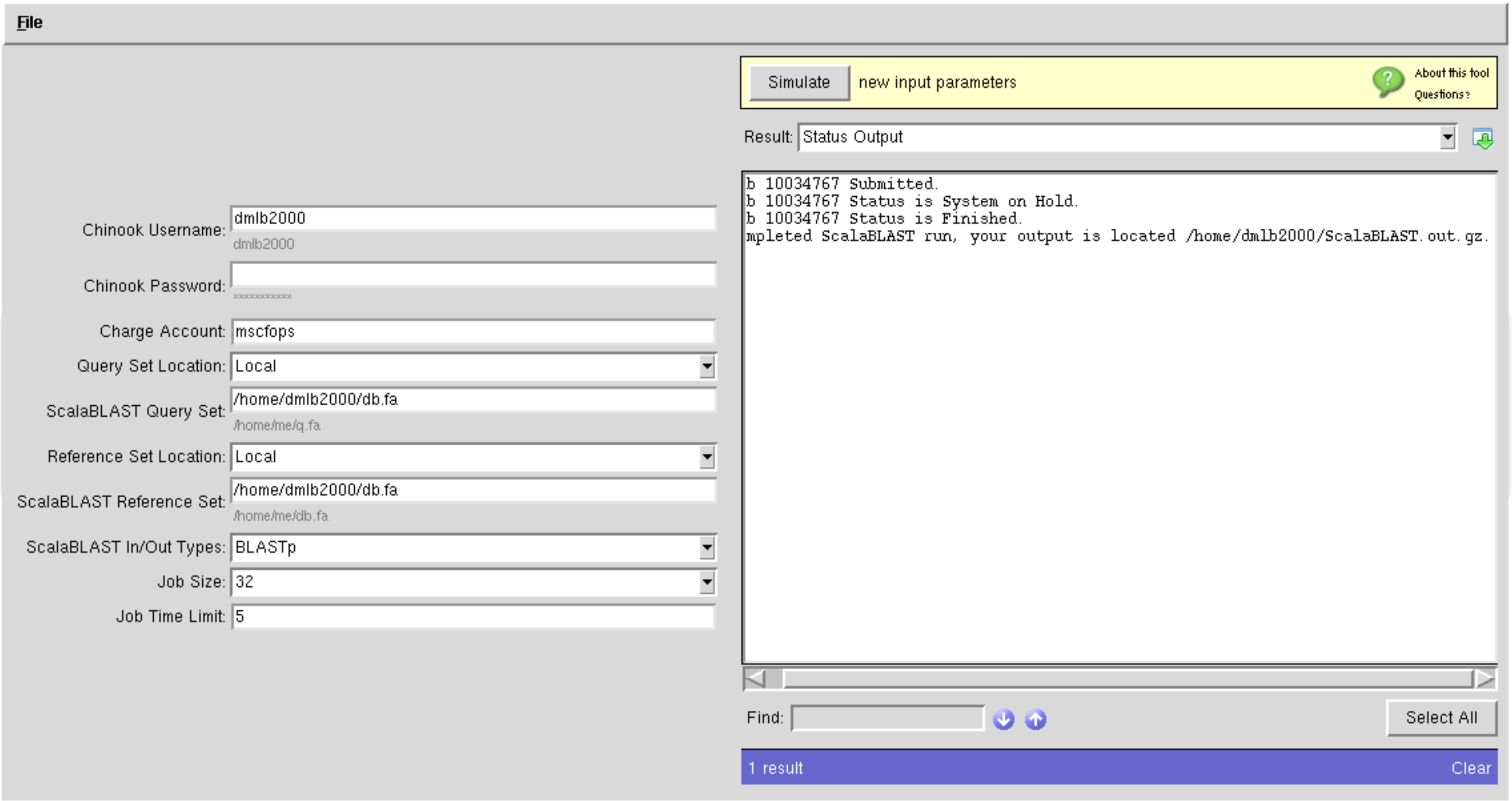
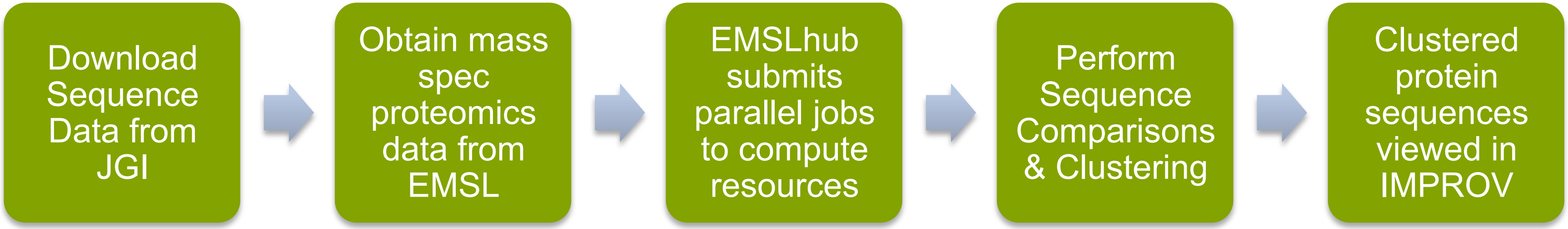


Result: Status Output

```
b 10034767 Submitted.
b 10034767 Status is System on Hold.
b 10034767 Status is Finished.
mpleted ScalaBLAST run, your output is located /home/dmlb2000/ScalaBLAST.out.gz.
```

Chinook Username:	dmlb2000 dmlb2000
Chinook Password:	××××××××××
Charge Account:	mscfops
Query Set Location:	Local
ScalaBLAST Query Set:	/home/dmlb2000/db.fa /home/me/q.fa
Reference Set Location:	Local
ScalaBLAST Reference Set:	/home/dmlb2000/db.fa /home/me/db.fa
ScalaBLAST In/Out Types:	BLASTp
Job Size:	32
Job Time Limit:	5

Example: Metaproteomics pipeline implementation in EMSLHub



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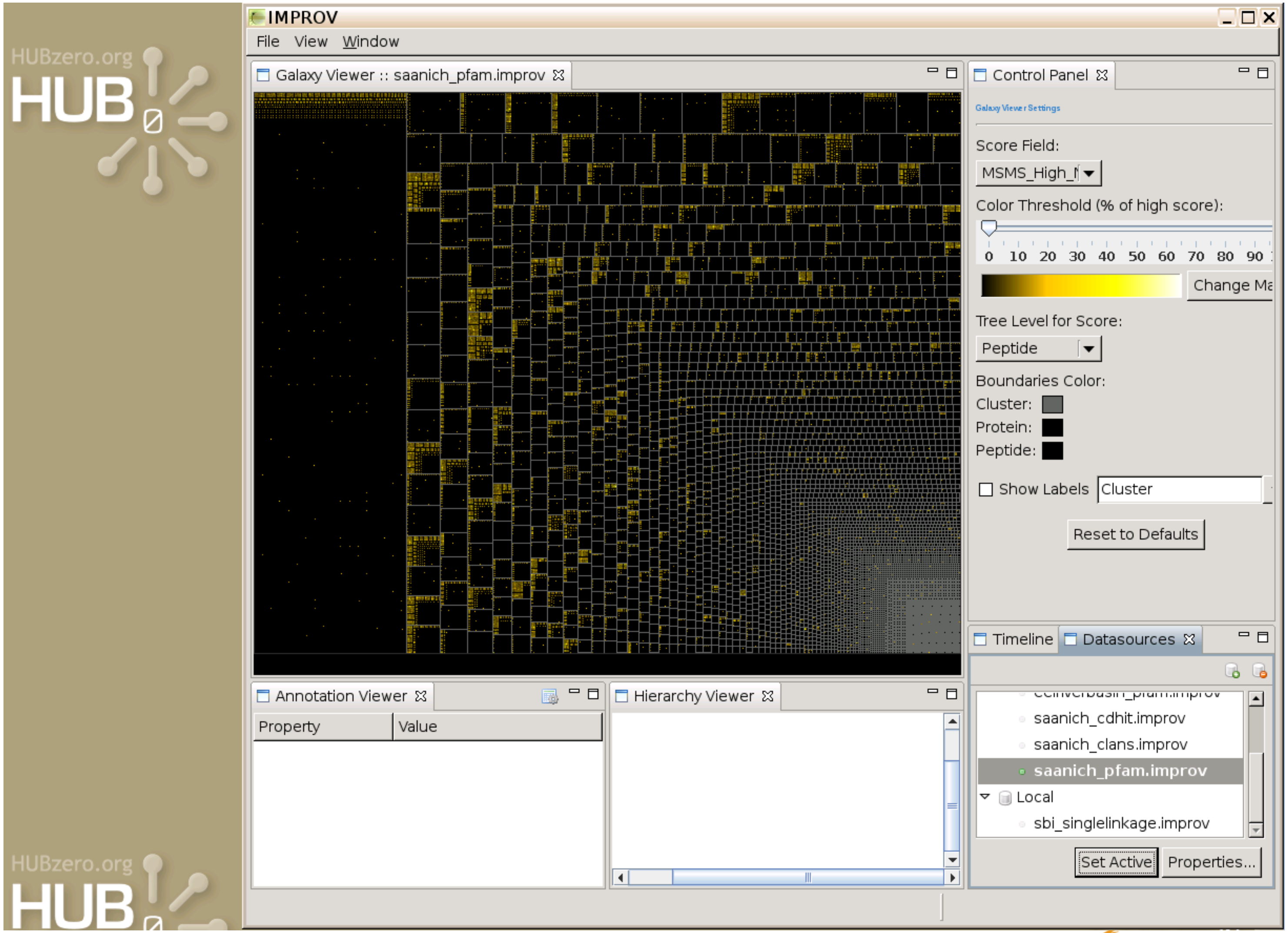


Score Field: MSMS_High_I

Color Threshold (% of high score): 0 10 20 30 40 50 60 70 80 90

Tree Level for Score: Peptide

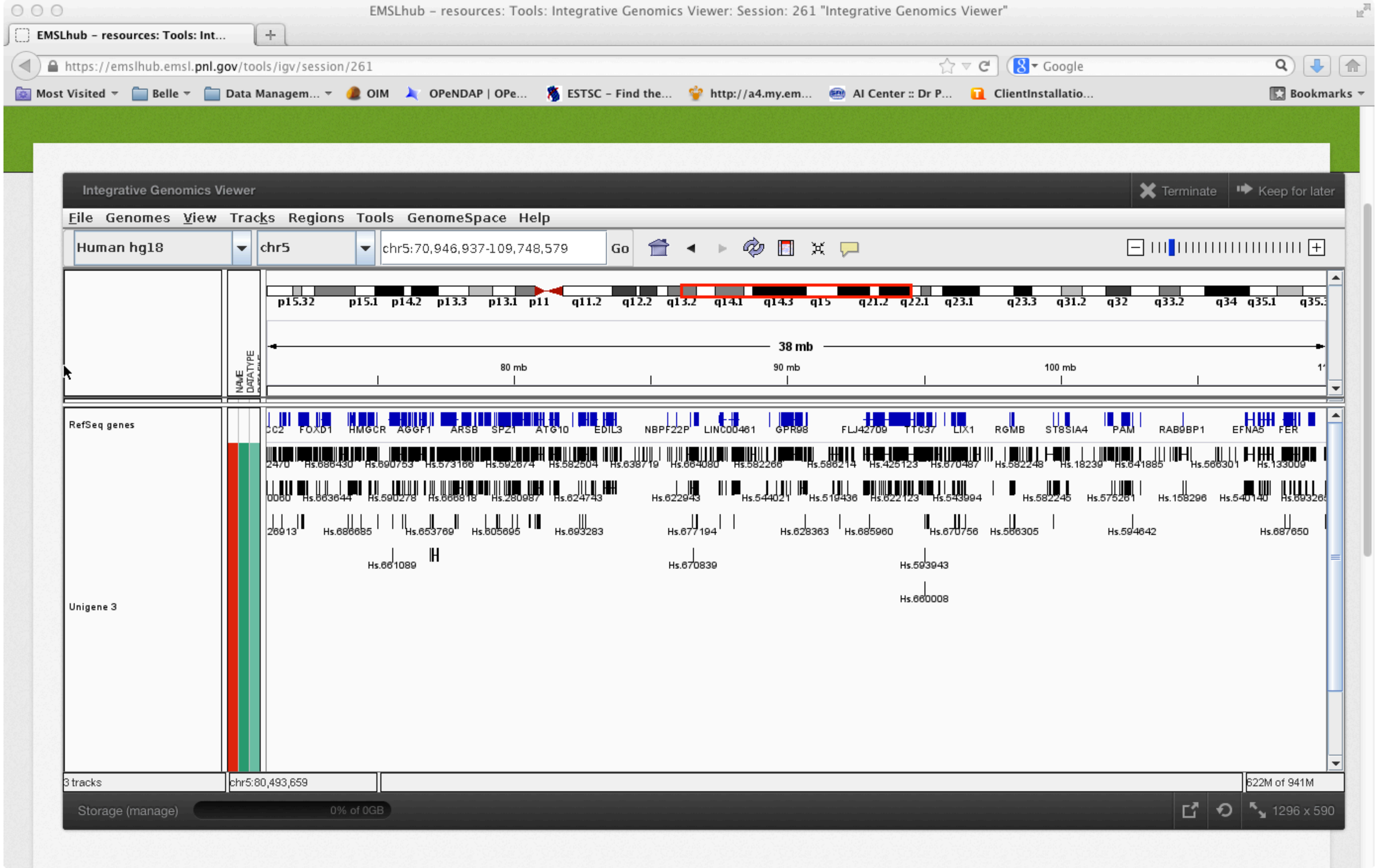
Boundaries Color:
Cluster:
Protein:
Peptide:

□ Show Labels Cluster

Property	Value

- cellverbasin_pfam.improv
- saanich_cdhit.improv
- saanich_clans.improv
- saanich_pfam.improv
- Local
  - sbi_singlelinkage.improv

Example: Genomics in EMSLHub



EMSLhub – resources: Tools: Integrative Genomics Viewer: Session: 261 "Integrative Genomics Viewer"

https://emslhub.emsl.pnl.gov/tools/igv/session/261

Human hg18

chr5

chr5:70,946,937-109,748,579

3 tracks

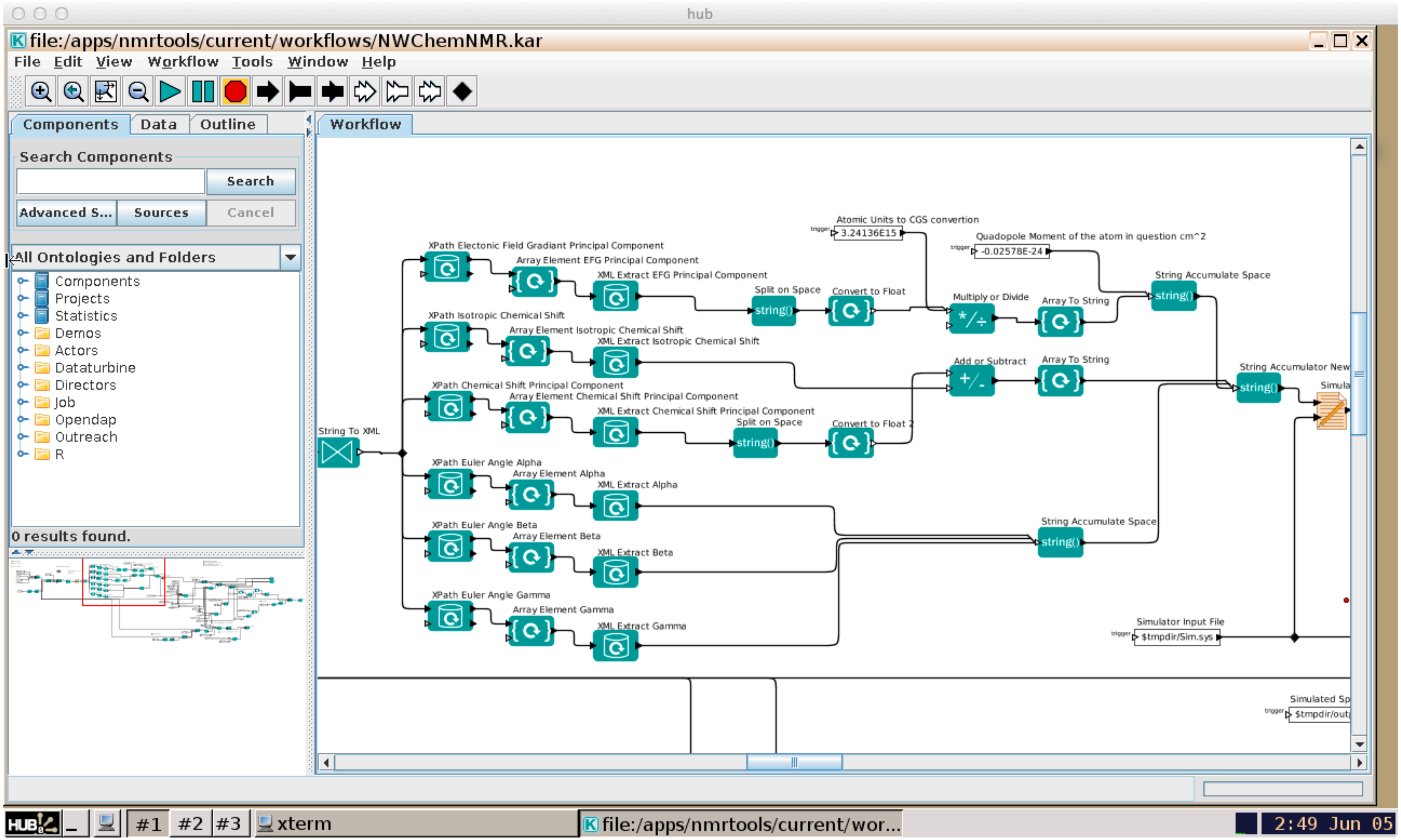
chr5:80,493,659

622M of 941M

Storage (manage) 0% of 0GB

1296 x 590

Example: Kepler workflow-based computing in EMSLHub



Pacific Northwest NATIONAL LABORATORY

Proudly Operated by **Battelle** *Since 1965*

U.S. DEPARTMENT OF ENERGY

Supporting the need for new approaches to data & collaboration

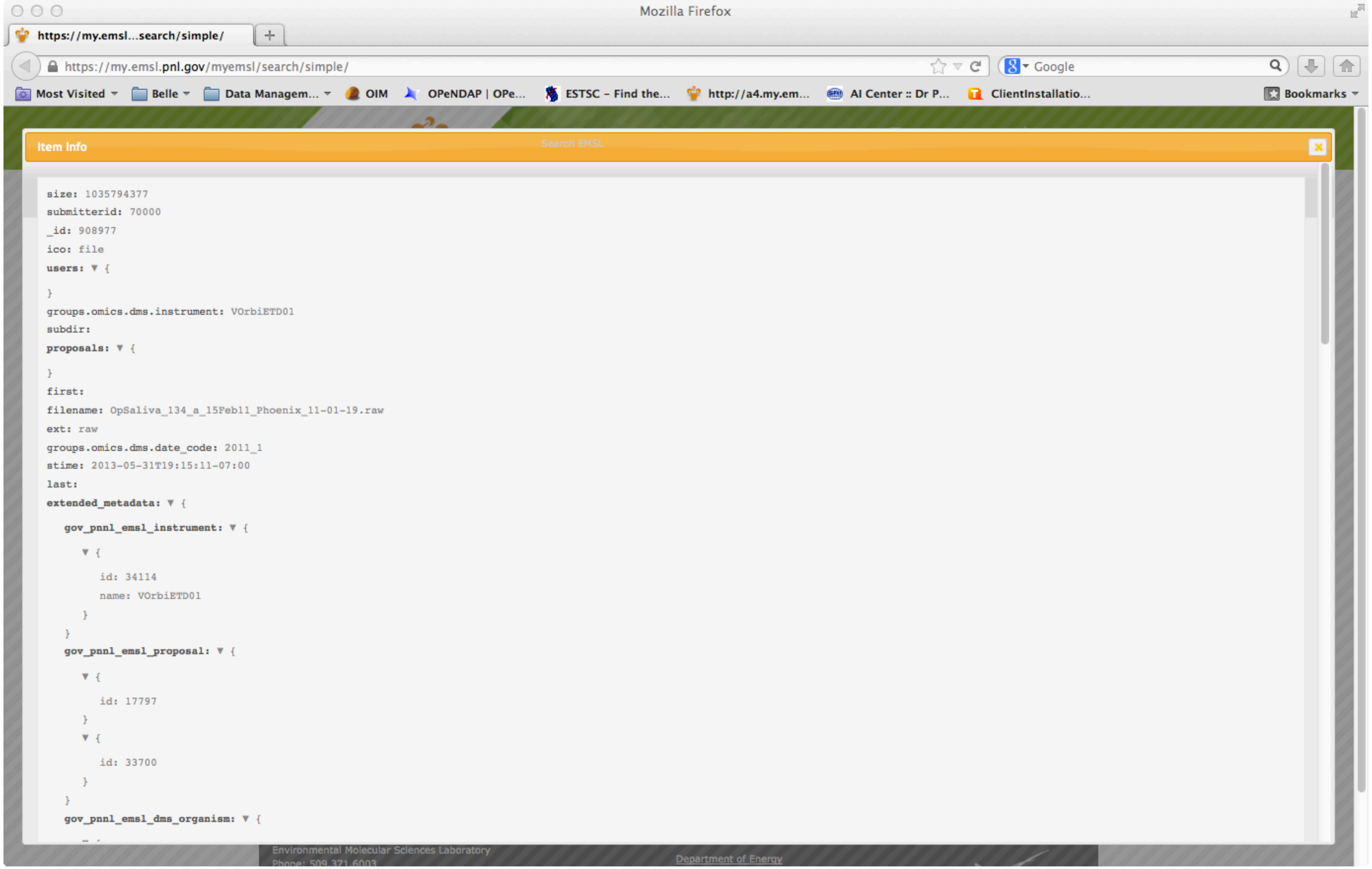
- Data is being generated both experimentally and computationally at an very rapid pace
- Islands of data are growing at institutions all over the world
- The leading edge of scientific discovery in the 21st century will be attained by collaboration and combining data in new ways
- MyEMSL & EMSLHub will help us
  - Cultivate the exchange of ideas
  - Leverage shared, searchable data
  - Foster collaborations, sharing & discovery

Team Members

- Project Management
  - William Shelton
  - David Cowley
- Core Project Team
  - Kevin Glass
  - David Brown
  - Brock Erwin
  - Kevin Fox
  - Nate Trimble
- EMSLHub
  - David Brown
  - Brock Erwin
  - Silvia Hoisie
- Metagenomics partners
  - Angela Norbeck
  - Ken Auberry
  - David Brown
- NMR partners
  - Karl Mueller
  - David Brown
  - Herman Cho
  - Bert DeJong
  - Brock Erwin
  - Nancy Washton
- Microscopy Partners
  - Nigel Browning
  - James Evans
  - James Bouwer

Thank You!

Metadata Sample



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         id: 33700
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