

JGI-NERSC Partnership: lessons in data-intensive computing at scale

NERSC Celebrates 50 years July 22, 2024



Continued Evolution into an Integrative and Collaborative User Facility

User Facility



2021...

tructure

Science

Mission

N 19

1997

The Human

Humans & animals

Genome

Project

Sequence, assemble, and annotate

GENOMES

Understand gene and genome FUNCTION

A Next-Generation An Integrative An Integrative
Genome Science Genome Science and Collaborative

2018

User Facility

INTEGRATIVE OMICS





Leverage key partnerships for multidisciplinary science

User Facility



Plants & microbes

Sequencing User

A Production

Facility



2004

Organismal interactions, DNA synthesis, metabolism

2012





Integrate sequence and functional capabilities for systems-level **BIOLOGY**

Expand interactions to characterize

BIOLOGICAL PROCESSES

User Programs and Science Programs



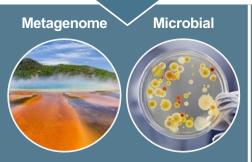
SCIENTIFIC PEER REVIEW

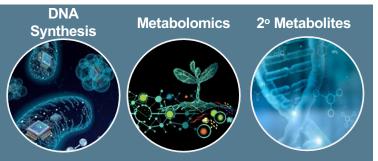
40%
Community
Science
Program (CSP)

10%
Facilities
Integrating
Collaborations for
User Science
(FICUS)









2023: JGI by the Numbers





Total Funding

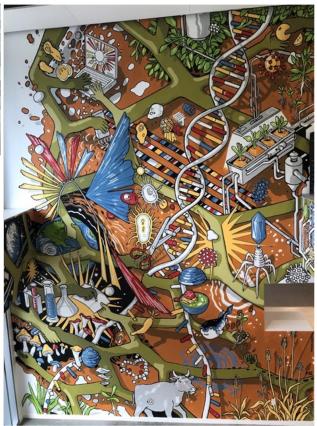


DOE BER \$89.4M

2,373 Primary Users

22,262 Secondary Users

238 Publications





- 716.9 Terabases sequence generated
- 11 Megabases DNA synthesized
- 11.56K metabolomics analyses runs
- 161 proposals submitted
- 64 proposals approved
- Total files requested: 7.9M
- JGI Archive size grew to: 15.2 million file records
- 15.95 Petabytes (PB) of data











in 3.3K

The mission of the JGI is to provide the global research community with access to the most advanced integrative genome science capabilities in support of the DOE's research

2,243

Primary Users leveraging JGI data generation capabilities in FY22

15,219

Secondary Users that engaged with JGI science gateways

14PB

JGI Data Repository size as of December 2020

Publications





Office of Biological and Environmental Research













Samples become data











Primary and Secondary Users leverage data through JGI Flagship Science Gateways







JGI X







Data Portal

















JGI User Groups



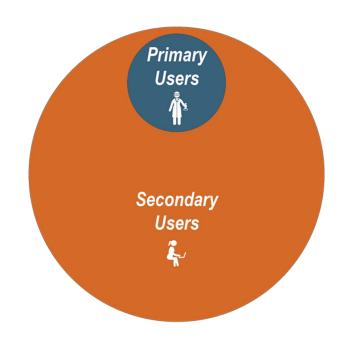
Primary and Secondary Users

Primary Users

are associated with one or more JGI **User Program proposals**

Secondary Users

build on the work of JGI personnel and primary users through direct downstream use of JGI data, systems, and tools.



Example Outcomes

- Publications
- Patents
- Software Adaptations
- New Technologies
- Marketable Products
- Methods & Standards
- Start-ups
- Grant Funding

JGI and NERSC, a brief history



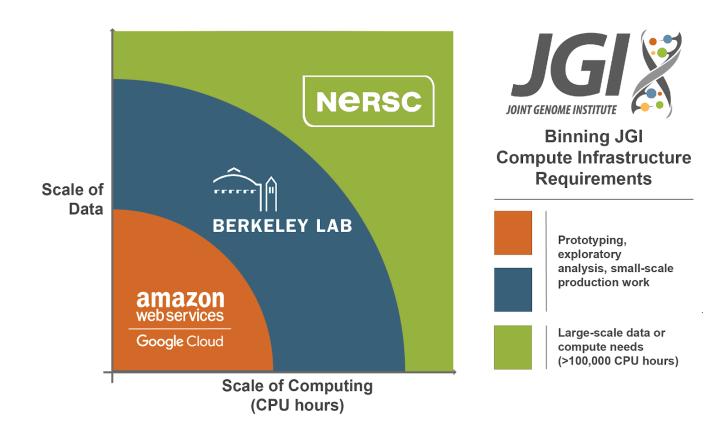
 2010 – JGI data and computing was growing too fast for the Walnut Creek facility



- New hardware was redirected to NERSC facility in Oakland
- 2011 JGI hardware unified to become the Genepool system
- 2012 Consultants hired to help support the JGI use of shared storage and computing resources
- 2013 Mendel deployed (consolidate Genepool and PDSF)
- 2019 Mendel retired (moved to LBL IT), JGI had a cabinet of Cori
- 2023 Cori retired, JGI stands up Dori at LBL IT

JGI's Computing Infrastructure Spectrum

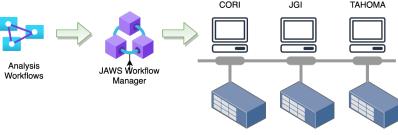




Unifying Workflow Execution Across JGI Resources



Developed a workflow manager called JGI Analysis
Workflow Service (JAWS) to run complex
computational workflows with support for distributed
computation across multiple HPC enabled sites.



- Provides a user-friendly common interface to seamlessly route jobs and data across multiple sites.
- Uses Cromwell to execute workflows in a common Workflow Description Language (WDL), standardizing the workflow language.
- Improves the reusability and robustness of bioinformatics workflows in evolving and/or diverse high-performance computing (HPC) and cloud environments.





NERSC (LBL)





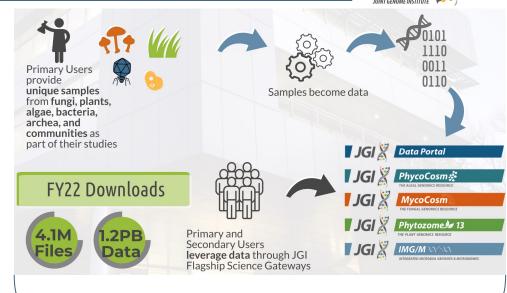




Centralized Data Access and Movement across Distributed Resources

JG S

- The JGI Archive and Metadata
 Organizer (JAMO) deployed in 2013
- Holds the metadata and locations for data produced by JGI
- Powers data distribution across JGI storage systems (file system and archives)
- Makes centralized search possible
- Supports reusability research





JAWS: Write Once, Run anywhere





JGI staff analyze JGI data on distributed resources

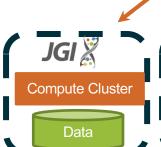


Containerized workflow, executable anywhere



Unifying Workflow Execution Layer







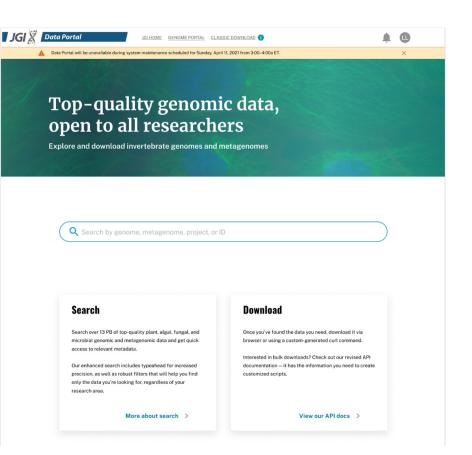






The JGI Data Portal – Access to all Public JGI Data





Our data

The U.S. Department of Energy (DOE) Joint Genome Institute (JGI) is a DOE Office of Science User Facility located at Lawrence Berkeley National Laboratory (Berkeley Lab). The JGI takes great pride in producing high-quality genomic and metagenomic data outputs for our users and the community. We ensure consistent quality by taking the following measures:

- · Starting with top-quality samples
- · Conducting ongoing quality control
- · Drawing on accumulated knowledge
- · Producing deeper metagenome sequences
- · Developing new tools
- Learn more

New releases New genomes will be released in Spring 2021! See the full list of new genomes

JGI in the news Get links to recently published studies that incorporate JGI-sequenced data.

Upcoming events

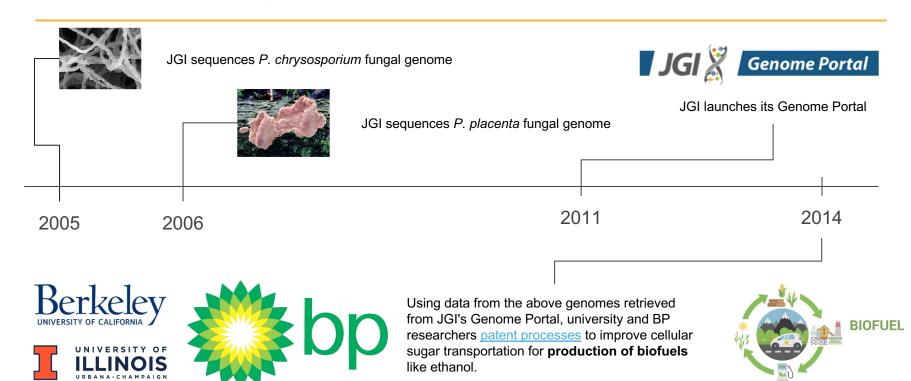
Register for upcoming JGI webinars on a variety of topics.

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GUI: https://data.jgi.doe.gov API: https://files.jqi.doe.gov/apidoc



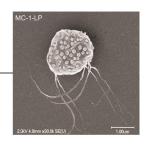
How does 'impact' begin?





2016

How does 'impact' begin?



JGI sequences the genome of *Magnetococcus* MC-1, a bacterium with special mobility traits that thrives in low-oxygen marine environments

2007

Aided by available genomic information, researchers determine that this bacteria is a very effective **medication delivery tool** for tumors in hard-to-reach areas of the brain.



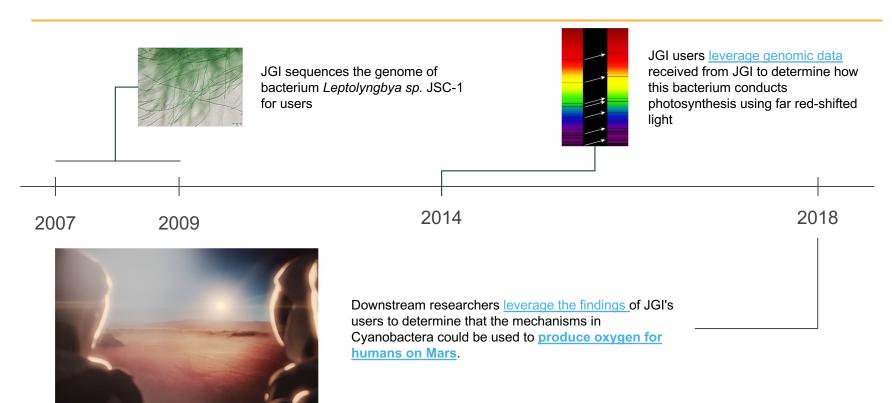


How does 'impact' begin?





How does 'impact' begin?



Highlight: The Megadata of Lake Mendota



- 3-part podcast arc released November-December 2023
- 20-year field samples from UW-Madison
- Highlighted JGI, NERSC, ExaBiome resources and capabilities harnessed to sequence and assemble 25Tb of metagenome data
- Episode interludes highlight that these are projects approved through JGI proposal calls





Host: Menaka Wilhelm





And they turned to MetaHipMer, a software developed by @LBNLcs & JGI computer scientists to tackle this task: bit.ly/MetaHipMer LM





Amazing Podcast - Genome Insider







Host: Menaka Wilhelm

Season 4 Eps 6-8 highlight the combination of supercomputing and sequencing to understand environmental microbiomes!

Supercomputing, MetaHipMer and the Mega Dataset of Lake Mendota



David Buoy sits at the deepest part of Lake Mendota, where microbial samples have been collected for over two decades.

Sequencing technology has changed dramatically over the last <u>25-plus years</u> since the JGI's inception, making it possible for researchers to get a close look at more ecosystems and organisms than ever before. In 2006, the JGI produced 33 billion base pairs of sequence; by 2023, that number was almost 717 trillion. Last year, the JGI surpassed three Petabases of data sequenced — that's three-quadrillion base pairs of DNA sequence!