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The genome portal of the Department of Energy Joint Genome Institute: 2014 updates

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ABSTRACT

The U.S. Department of Energy (DOE) Joint Genome Institute (JGI), a national user facility, serves the diverse scientific community by providing integrated high-throughput sequencing and computational analysis to enable system-based scientific approaches in support of DOE missions related to clean energy generation and environmental characterization. The JGI Genome Portal (<http://genome.jgi.doe.gov>) provides unified access to all JGI genomic databases and analytical tools. The JGI maintains extensive data management systems and specialized analytical capabilities to manage and interpret complex genomic data. A user can search, download and explore multiple data sets available for all DOE JGI sequencing projects including their status, assemblies and annotations of sequenced genomes. Here we describe major updates of the Genome Portal in the past 2 years with a specific emphasis on efficient handling of the rapidly growing amount of diverse genomic data accumulated in JGI.

INTRODUCTION

A leader in genome sequencing, the DOE JGI has significantly expanded its capabilities to achieve a deeper understanding of biological functions encoded by DNA. With the increasingly diverse data types it generates and associated computational strategies for their analysis, the DOE JGI is focused on enabling its community of users to make important new scientific discoveries that address major energy and environmental challenges (U.S. Department of Energy Joint Genome Institute Progress Report, <http://www.jgi.doe.gov/whoware/JGI-progress-report-2012.pdf>).

In 2012, JGI completed 2635 projects, a 3-fold increase over 2011, and generated >56 trillion nucleotides of

genome-sequence data from microbes and microbial communities, fungi, algae and plants. In the past year alone, JGI has added 650 genomes to the public databases. JGI sequencing efforts are mostly based on the proposals submitted to JGI by researchers and to a large extent are aligned with several large-scale JGI programs such as Community Science Program (CSP) and Genomic Encyclopedia of Bacteria and Archaea (GEBA) (1). The amount of data being produced by sequencing and analyzing genomes brings genomics into the realm of big data category. The increased scale in data has demanded a corresponding advance in the scale and robustness of the computing infrastructure underlying the Genome Portal. Since the previous publication on the JGI Genome Portal in January 2012 (2), we specifically focused on improvement of computational resources for efficient storage, access, download and analysis of these data.

DATABASES ACCESSIBLE THROUGH INTEGRATED GENOME PORTAL

The Portal home page, available at <http://genome.jgi.doe.gov>, allows a user to select the genomic data set and the tools to work with (Figure 1). It provides the information about the latest genome releases and access to several specialized JGI database resources: integrated microbial genomes (IMG) (3) and metagenomes (IMG/M) (4), Phytozome for green plant genomes (5) and MycoCosm for fungal genomes (2). It also provides access to extensive help pages as well as a recently developed interactive tutorial for novice users.

There are two major categories of data available in JGI sequencing projects and annotated genomes and metagenomes. More than 15000 DOE JGI projects of different types are publicly available and searchable in our database. These projects include different genomic products, such as standard and improved draft, finished genomes, gene expression profiling, resequencing, metagenome projects, single cell projects, transcriptomes, metatranscriptomes, exomes, specialized analysis types

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Figure 1. The Genome Portal page. Pull-down menus for the Search categories and the Amoebozoa branch of Eukaryota are shown.

and others. The Genome Portal provides access to over 17 000 annotated genomes and metagenomes available in the DOE JGI database, along with specialized analytical tools to navigate these data sets and compare genomes.

DATA ORGANIZATION AND ACCESS

Individual Genome Portal project sites ('portals') are created automatically on passage of sample quality control stage for a given sequencing project. The JGI has ~24 000 portals for isolate, metagenome, single-cell, transcriptome and resequencing projects. Portals aggregate relevant analysis tools for each project and provide download access to project data and project information such as proposal name, organism and taxonomy info as well as the names of principal investigator and other contacts relevant to an associated data set (Figure 2).

To navigate the large volume and diversity of genome projects at the JGI, the Genome Portal offers several new and improved tools to locate a genome of interest: a list of all JGI projects, a 'Search' function, an interactive 'Tree of Life' and domain-specific comparative resources. Data access and the spectrum of data depend on the stage of

each project and the role of users in these projects (e.g. administrative). Free registration allows users not only to access all data but also to initiate new projects with JGI. The 'Project List' link on the Genome Portal page (<http://genome.jgi.doe.gov>) (Figure 1) brings users to a list of all DOE JGI projects with a detailed description of each project including its scope and current status, taxon, the JGI program, the project lead and the computational resources available for this project.

The JGI Genome Portal now includes a new Portal Search function that enables searching for genomes and projects by keyword (e.g. plants, algae, single cell, water), name and other categories of data (shown in a pull-down menu, Figure 1). The user can also locate projects related to specific classifications such as a proposal or a project. Typing the beginning of the word in the text window brings up a pull-down menu with relevant search term choices.

Search results now include Project information and status, GenBank accession, taxonomic information, PI contact and much more (Figure 3). Every JGI Proposal, which can include multiple genomes, transcriptomes or other data sets, now has all related portals grouped

JGI  Home  Project List  Login finished

Microbial community impact on carbon sequestration in managed wetland "carbon farming": Wetland Surface Sediment Aug2011 Site B2 Bulk Metagenome

INFO DOWNLOAD IMG/M

Project: Wetland Surface Sediment Aug2011 Site B2 Bulk Metagenome (*Project ID:* [1015567](#))

Proposal: Microbial community impact on carbon sequestration in managed wetland "carbon farming" (*Proposal ID:* [368](#))

Program: CSP

PI: [Susannah Tringe](#)

Metagenome

Name: Microbial community impact on carbon sequestration in managed wetland "carbon farming": Wetland Surface Sediment Aug2011 Site B2 Bulk Metagenome

JGI Project ID: [1015567](#)

NCBI Project ID: [188796](#)

GOLD ID: [Gs0003483](#)

Taxonomy

NCBI Tax ID: [410658](#)

Environment

Ecosystem: Environmental

Ecosystem Category: Aquatic

Ecosystem Type: Marine

Ecosystem Subtype: Wetlands

Specific Ecosystem: Sediment

Habitat: Host

Sampling Site: California, United States

Contacts

JGI: metagenome@lists.jgi-psf.org

Collaborators: Susannah Tringe <sgtringe@lbl.gov>

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Groups

This portal belongs to the following groups

##	Name
1	Environmental Aquatic Marine
2	Microbial community impact on carbon sequestration in managed wetland "carbon farming"

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Genome Portal version:UNDEFINED.21141 content:211111 clustering:3468 synten:3468 frylock.jgi-psf.org 08-Oct-2013 13:56:18.952 PDT

Figure 2. Individual portal page for the Wetland Surface Sediment Metagenome project. Relevant information is classified into several sections including 'Groups' that specifies an appropriate proposal or large-scale JGI programs.

together, and downloads of entire segments of data are possible at the proposal level.

The Tree of Life organizes the sequenced genomes by the domains of life and metagenomes by ecological 'niche'. Clicking on a branch name produces a menu displaying available genomes in the corresponding kingdom, phylum,

class or order. Selecting an entire group of genomes or a particular genome connects a user to a corresponding organism page or pages in specialized resources indicated by associated icons (Figure 1). Microbial, archaeal genomes and metagenomes are directed to the corresponding IMG and IMG/M pages, fungal genomes to

The screenshot shows the JGI search interface. At the top, there are navigation links for Home, Project List, and Login. A search bar contains the text 'Microbial community impact on carbon sequestration in man' with a 'Search' button. Below the search bar, there are sorting options: 'Sort by: Name' with a dropdown menu, and radio buttons for 'ascending' (selected) and 'descending', along with a checked box for 'Include groups'. The results section shows 'Results per page: 100' and '11 results found' with an 'Export To Excel' button. The main table has columns: Name, Taxonomy, JGI Info, Proposal Name, Resources, Principal Investigator, and Other. Three rows are visible, each representing a different data set related to carbon sequestration in managed wetlands.

Name	Taxonomy	JGI Info	Proposal Name	Resources	Principal Investigator	Other
Group: Microbial community impact on carbon sequestration in managed wetland "carbon farming"			Microbial community impact on carbon sequestration in managed wetland "carbon farming"	Info Download	• Susannah Tringe	
Microbial community impact on carbon sequestration in managed wetland "carbon farming": Wetland Surface Sediment Aug2011 Site A1 Bulk Metagenome	Taxonomy: 410658 Ecosystem: Environmental Ecosystem category: Aquatic Ecosystem type: Marine Ecosystem subtype: Wetlands Specific ecosystem: Sediment GenBank Submission: This project has not been processed by data submission system. Aliases: • Soil metagenome	JGI Project Id: 1015561	Microbial community impact on carbon sequestration in managed wetland "carbon farming"	Info Download	• Susannah Tringe	Sample site: California, United States Habitat: Mud
Microbial community impact on carbon sequestration in managed wetland "carbon farming": Wetland Surface Sediment Aug2011 Site B2 Bulk Metagenome	Taxonomy: 410658 NCBI Project: 188796 Ecosystem: Environmental Ecosystem category: Aquatic Ecosystem type: Marine Ecosystem subtype: Wetlands Specific ecosystem: Sediment GenBank Submission: This project has not been processed by data submission system. Aliases: • Soil metagenome	JGI Project Id: 1015567	Microbial community impact on carbon sequestration in managed wetland "carbon farming"	Info Download JGI Project Status	• Susannah Tringe	Sample site: California, United States Habitat: Host img taxon oid: 2524614855

Figure 3. Search results table. 'Info' link in the Resources column leads to an individual portal of each found data set.

Mycocosm and plant genomes to Phytozome. Genomes not included in either of these specialized resources are linked to their individual portal pages containing information about the corresponding project and available tools.

INTRASTRUCTURE

The Genome Portal Web site is built on Apache HTTPD, Tomcat and MySQL. A majority of the Genome Portal components have been developed using Java and a variety of available open-sources tools and technologies. There are four load-balanced web servers, talking to two back-end database servers. A web-driven automated build system that uses Jenkins (<http://jenkins-ci.org/>) takes each machine silently out of the cluster, builds a new version of the portal and puts the machine back into the cluster. This procedure ensures that updates can be applied without disruption to users. This setup further makes the portal resilient against hardware failures.

The Genome Portal acquires data from several of JGI's annotation pipelines via an API and it makes the data available to authorized users without delays. There is an advanced monitoring system in place that allows preventing problems that may impact Web site and database performance.

Over the last 2 years, we have forged a strong alliance in high-performance computing with the National Energy Research Scientific Computing Center (NERSC). NERSC now hosts the servers on which the Genome Portal is

running and provides access to ESnet (Energy Sciences Network), which allows for top of the class transfer rates.

DATA DOWNLOAD

The Genome Portal currently supports download of multiple file types: all raw and quality control data, assemblies and various analysis files. All files can be accessed in a variety of ways, each designed with a particular class of users in mind.

In the web-driven approach to data access, the user finds a portal of interest and clicks on the download tab of that portal. Downloads are available in a tree structure that divides the files into logical groups so that the user can download raw data files, assemblies and so on with a single operation (Figure 4).

For users who need to download a large number of files or large files (with the largest being several hundred gigabytes), data are available via the public JGI endpoint on GlobusOnline (<https://www.globusonline.org/>). This requires that the user log on to globusonline.org and activate the 'jgi#portal' endpoint using their JGI credentials. GlobusOnline then provides a user-friendly interface for facilitating big data transfers. Behind the scenes the transfers are performed using GridFTP (6), which is a parallel transfer protocol and program. GridFTP has built-in checks that ensure the integrity of the transfers and guarantees that the files reach their destination intact.

The screenshot shows a web interface for downloading data from the JGI Genome Portal. At the top, there are navigation links (Home, Project List, myPortal, Logout) and a user profile (John Doe). The main title is "Microbial community impact on carbon sequestration in managed wetland 'carbon farming': Wetland Surface Sediment Aug2011 Site B2 Bulk Metagenome". Below the title are tabs for "INFO", "DOWNLOAD", and "IMG/M". A toolbar contains buttons for "Download Selected Files", "Download Page as XML", "ExpandAll", "CollapseAll", and "Rescan". The main content is a file tree with the following structure:

- Raw Data
 - Microbial community impact on carbon sequestration... Project: 1015567, Library: NCYO 6558.7.47340.GTGAAA.fastq.gz 40 GB; Fri Jan 11 20:00:44 PST 2013
- QC Filtered Raw Data
 - Microbial community impact on carbon sequestration... Project: 1015567, Library: NCYO 6558.7.47340.GTGAAA.adna.fastq.gz 40 GB; Mon Jan 14 22:59:53 PST 2013
- QC and Genome Assembly
 - Additional Files
 - 1015567_1718
 - Microbial community impact on carbon sequestration... Project: 1015567, 1015567.combined_unique.fa.contigs.agp 22 MB; Tue Apr 09 09:35:10 PST 2013
 - Microbial community impact on carbon sequestration... Project: 1015567, 1015567.combined_unique.fa.contigs.cov 14 MB; Tue Apr 09 09:35:07 PST 2013
 - Microbial community impact on carbon sequestration... Project: 1015567, 1015567.combined_unique.fa.contigs.fasta 218 MB; Tue Apr 09 09:35:23 PST 2013
 - Microbial community impact on carbon sequestration... Project: 1015567, 1015567.combined_unique.fa.readme.pdf 158 KB; Tue Apr 09 09:35:10 PST 2013
 - Microbial community impact on carbon sequestration... Project: 1015567, 1015567.combined_unique.fa.trim.unmapped.pe.MERGED.fastq.gz 11 GB; Tue Apr 09 10:58:00 PST 2013
 - Microbial community impact on carbon sequestration... Project: 1015567, 1015567.combined_unique.fa.trim.unmapped.pe.UNMERGED.fastq.gz 16 GB; Tue Apr 09 10:36:43 PST 2013
 - Sequence Alignment
 - 1015567_1718
 - Microbial community impact on carbon sequestration... Project: 1015567, 1015567.ReadsMapping.sort.bam 36 GB; Tue Apr 09 10:08:07 PST 2013
- IMG Data
 - Additional Files
 - Microbial community impact on carbon sequestration... Project: 1015567, 14112.assembled.faa 77 MB; Sat Apr 20 02:11:17 PST 2013
 - Microbial community impact on carbon sequestration... Project: 1015567, 14112.assembled.faa.COG 19 MB; Sat Apr 20 02:11:16 PST 2013
 - Microbial community impact on carbon sequestration... Project: 1015567, 14112.assembled.faa.EC 9 MB; Sat Apr 20 02:11:16 PST 2013

Figure 4. Download function access page for the Wetland Surface Sediment Metagenome project. A user can select any relevant data set/s of raw data, genome assembly and analysis results.

Finally, a web service is available for users who seek to download JGI data programmatically. This service is described in the documentation on the Genome Portal Web site.

Whether a user navigates the web user interface, uses GlobusOnline or uses the web service, the data that can be accessed are the same in each case. As the amount of data the JGI makes available is counted in petabytes, many of the files are stored on the NERSC HPSS mass storage archive. All three approaches hide this fact from the user, interacting with the tape system to cache files as required.

In addition to downloading data, The Department of Energy Systems Biology Knowledgebase (KBase) (<http://kbase.science.energy.gov/>) users can upload their data directly from the portal page to KBase. They do so by selecting files in the tree on the download page, clicking 'Push to KBase' and entering their KBase credentials.

DATA SUBMISSION TO NCBI

The increasing volume of genome data has led the NCBI to develop a new automatic submission system (7) to streamline the process of submitting complex high-throughput sequencing or functional genomic data sets. The DOE JGI has collaborated with the NCBI to develop the first major implementation for a sequencing center of a framework to use this submission system. Using this system, the JGI Genome Portal automatically generates and monitors BioSample and BioProject submissions to NCBI using an XML-based submission protocol. Internally, we use the same infrastructure to

prepare GenBank submissions. The latter are submitted to the NCBI FTP server using the ASN.1 and related GenBank-specific formats.

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