

The DOE Systems Biology Knowledgebase

KBase Progress and Goals

Adam Arkin

Physical Biosciences Division

Lawrence Berkeley National Laboratory















Plants and Microbes for Energy and Environment

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

Biological Principles

Computing

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

Predictive Understanding



Complex Missions, Sophisticated Mission Analysis

- DOE mission: predict, control and design the biological components of energetic processes and environmental balance.
- Complex missions with rapidly expanding, intricately related diverse data types require ways to augment scientists' ability to:
 - Filter information
 - Focus attention
 - Ask the right questions
 - Leverage other minds
 - Make the impossible possible. [©]







Enable DOE Mission Science

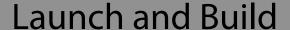
Communities Microbes **Plants** Carbon Cycl Atmosphere 750 zune (AF418169.1) Thermodesulfob NRB10 (1/223, 0/235, 0/242) sediment and soil sturry clone Er-LLAYS-96 (EU542535.1) Sediment Backer horizongensis HKU2 (AF433166.1) pacter sacchardermentans 2-79520 (AY-3124U3.2) NRB15 (07223, 07235, 2/242) Delwabbacter sp. enrichment clone WL (FJ157998.1 TCE-dechlorinating groundwater clone TANB55 (AY6 NRB16 (07223, 2/235, 4/242) Transport Across Scales in the Subsurface Respiration (Glycolysis)





Before I tell you how... DID WE MEET SPECIFICATIONS?







Distributed Development

- Four major National Labs and more than 10 collaborating universities/ research centers
- 50 people with diverse cultures and expertise and with different institutional and group alliances
- Enthusiasm to create a system to revolutionize understanding and application of biological systems.
- Deliver version 1 in 18 months and prove it can support DOE scientists!

Building an airplane in the sky







Community Specifications for KBase: 2011

- A Federated infrastructure and 10GBit/s transfer capabilities.
- 2 petabytes data storage and 2000 cores for data processing including interface and between high performance computing and cloud computational resources
- Development of core Knowledgebase integrated data and workflow analysis management tools including Application Programming Interfaces, semantic and user Interfaces.
- For microbial systems, from 100-1000 microbes: Reconstruct and Predict Metabolic and Gene Expression Regulatory Networks to Manipulate Microbial Function
- ii. For plant systems, for 10 key plants related to DOE missions: Integrate Phenotypic and Experimental Data and Metadata to Predict Biomass Properties from Genotype and Assemble Regulatory Data to Enable Analysis, Cross- Comparisons, and Modeling
- iii. For Microbial Communities: Model Metabolic Processes within Microbial Communities and Mine Metagenomic Data to Identify Unknown Genes





KBase 2013: 18 Months Deliverables Exceed Spec.

- A Federated infrastructure and 10GBit/s transfer capabilities.
 - Built for high speed data transfer over ESNET using 100 GBit/s rates.
- 2 petabytes data storage and 2000 cores for data processing including interface and between high performance computing and cloud computational resources
 - KBase Magellan has 12,000 cores for data processing via both Open Stack Cloud interfaces and Cluster Services
 - KBase has >3 Petabytes of storage capacity
- Development of core Knowledgebase integrated data and workflow analysis management tools including Application Programming Interfaces, semantic and user Interfaces.
 - Integrated KBase API specified and operational. Used by third parties to integrate function and build apps.
 - Integrated data model aware of 925 data types encompassing sequence reads, contigs, genomes, genome features, transcription data, fitness data and more.
 - 40 Interface description documents leading to 821 functions that can be compiled into use for PERL, Python, Java, and R.
 - Prototype Search, Workflow and Novel Narrative/Notebook interfaces for navigating, analyzing and building knowledge in KBase



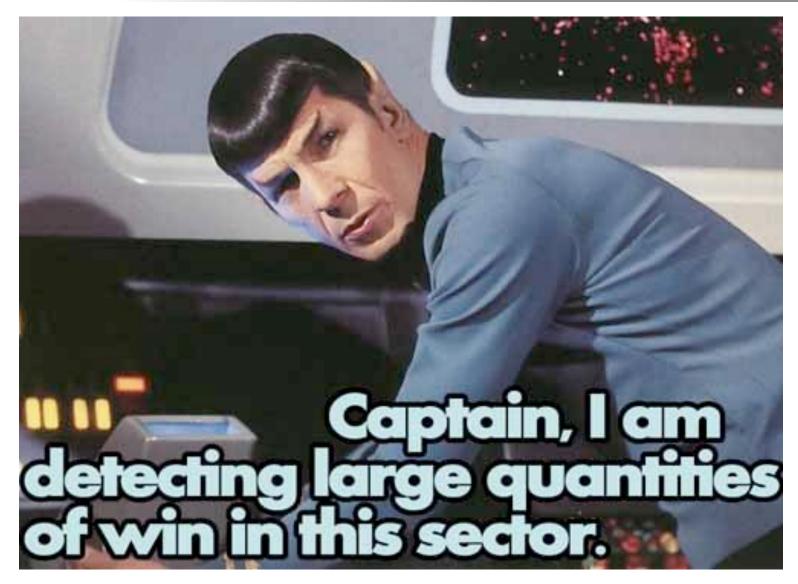


KBase 2013: 18 Months Deliverables Exceed Spec.

- i. For microbial systems, from 100-1000 microbes: Reconstruct and Predict Metabolic and Gene Expression Regulatory Networks to Manipulate Microbial Function
 - i. Metabolic and regulatory reconstructions for 5534 prokaryotic and 161 archaeal genomes
 - ii. 7830 genome annotations, 23,058,670 features predicted
 - iii. 12,620 regulons with 266,345 protein families inferred
 - iv. 4985 metabolic models including a total of 16,196 compounds and 13,428 reactions
 - v. 6202 growth curves, 1,947,690 strain fitness measurements; 3227 gene expression data sets
 - vi. Services for assembly, annotation, phylogenomics, regulatory and metabolic networks inference, FBA and PROM modeling of metabolism, reconciliation and improvement of models against data
- ii. For plant systems, for 10 key plants related to DOE missions: Integrate Phenotypic and Experimental Data and Metadata to Predict Biomass Properties from Genotype and Assemble Regulatory Data to Enable Analysis, Cross-Comparisons, and Modeling
 - i. Over 175 eukaryotic genomes including many variants of Poplar, Arabidopsis, Sorghum, Chlamydomonas, Brachypodium, Miscanthus, Switchgrass as well as many other algae and fungi.
 - ii. Phenotypes for genome variants of plants and services for calling the genetic variation among individuals.
 - iii. Services for variation calling, mapping genotype-to-phenotype via GWAS style analysis and tools for candidate gene filtering, trait modeling, and pathway enrichment,
 - iv. 731 gene expression experiments in Arabidopsis and Poplar; Plant co-expression network analysis for all.
 - v. Initial plant metabolic modeling
- iii. For Microbial Communities: Model Metabolic Processes within Microbial Communities and Mine Metagenomic Data to Identify Unknown Genes
 - i. Access to 11,000 metagenomes(>21 TBp)
 - ii. Integrated KBase access to QIIME functionality
 - iii. New tools for metagenome sequence quality assessment and experimental design
 - iv. Services for taxonomic and gene identification, abundance, and a host of other functions











The community document is not a specification, though...

WHY DO WE NEED KBASE?





Our goals drive our specification

- We believe it is necessary to solve the grand challenges in biological control of environmental and energy process.
- We believe it is necessary to deal with deep issues in scientific communication and reproducibility
- We need to lower the barriers to computationally efficient use of advanced algorithms and data from diverse producers.
- We believe we need to do this together-- leveraging many minds.



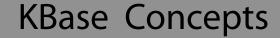


The number of bioinformatics resources is huge

An increasing number of data warehouses since biology is becoming a big data discipline (e.g., NCBI, Ensembl, etc.)
Specialized applications and databases for relatively generic analyses (e.g., MG-RAST and MicrobesOnline)
Evolving libraries of sophisticated computational biology algorithms for use in programming environments (e.g., Bioconductor)
Workflow tools that allow the chaining of these algorithms together by non-programmers (e.g., Galaxy and Taverna)
Workflow sharing tools to allow people to use each other's work products
Open-access publication of journal articles with increasing use of semantic tagging
Scientific social networks (e.g., ResearchGate, Epernicus, etc.)

So what is missing?I







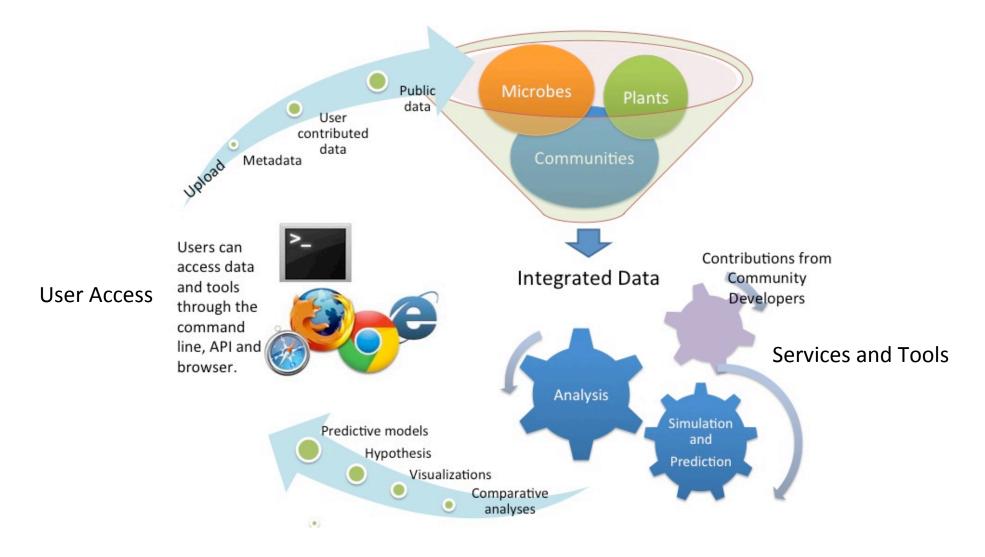
- KBase drives data through models to predictions and experimental design.
- KBase accelerates reproducible, reusable, and transparent science.
- KBase deeply enables scientists to work together to approach complex biological problems.
- KBase gives credit where it is due and privacy where it is needed.
- KBase is an open software and data environment to which others can contribute and with which others can build.







Empowering Users

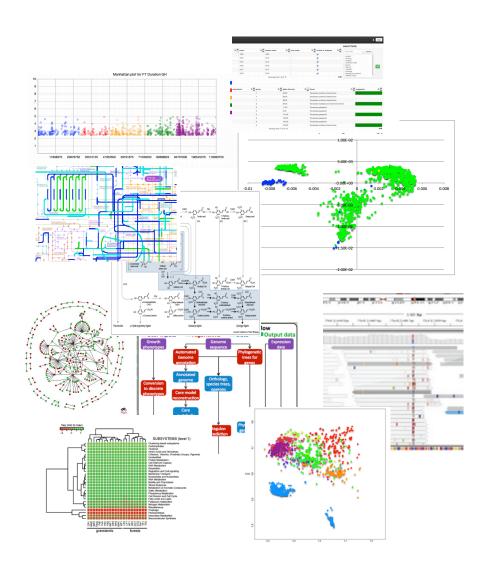






What can we do that was hard before?

- Transparently access multiple heterogeneous datasets and bioinformatics tools.
- Efficiently annotate new microbial genomes and infer metabolic and regulatory networks.
- Transform network inferences into metabolic models and map missing reactions to genes using novel data reconciliation tools.
- Design effective sequencing strategies for complex multi-sample metagenomic projects
- Test microbial ecological hypotheses through taxonomic and functional analysis of qualityassessed metagenomic data
- Predict plant gene function and molecular phenotype via navigation and analysis of tissuespecific co-expression networks.
- Discover genetic variations within plant populations and map these to complex organismal traits.
- Share data, analysis tools, workflows and scientific conclusions with the community.

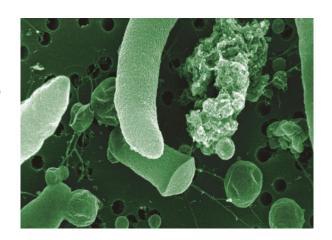


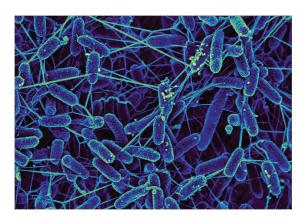




Our overall goals are to:

- Reconstruct and predict metabolic and gene expression regulatory networks to manipulate microbial function
- Vastly increase the capability of the scientific community to communicate and utilize their existing data
- Enable the planning of effective experiments and maximize our understanding of microbial system function

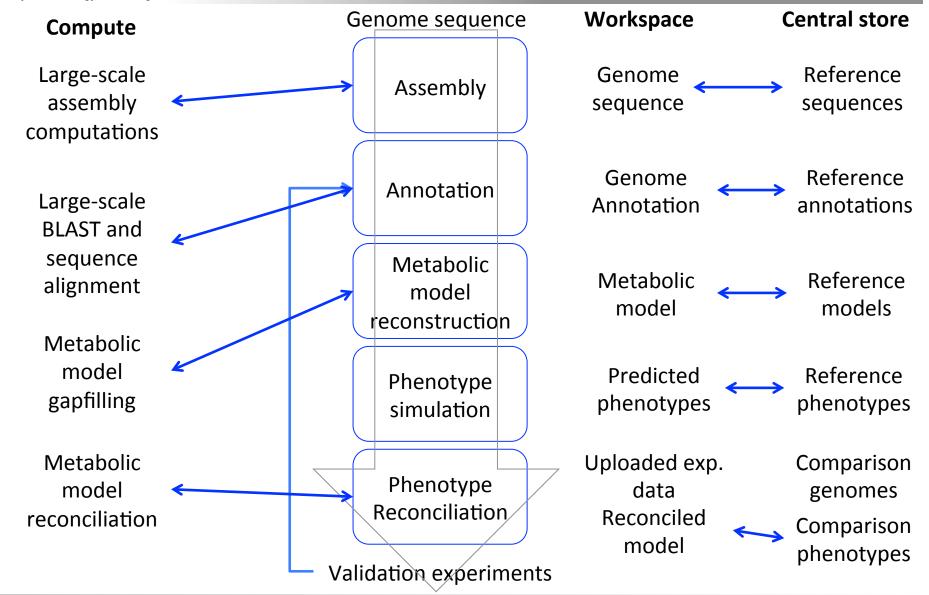








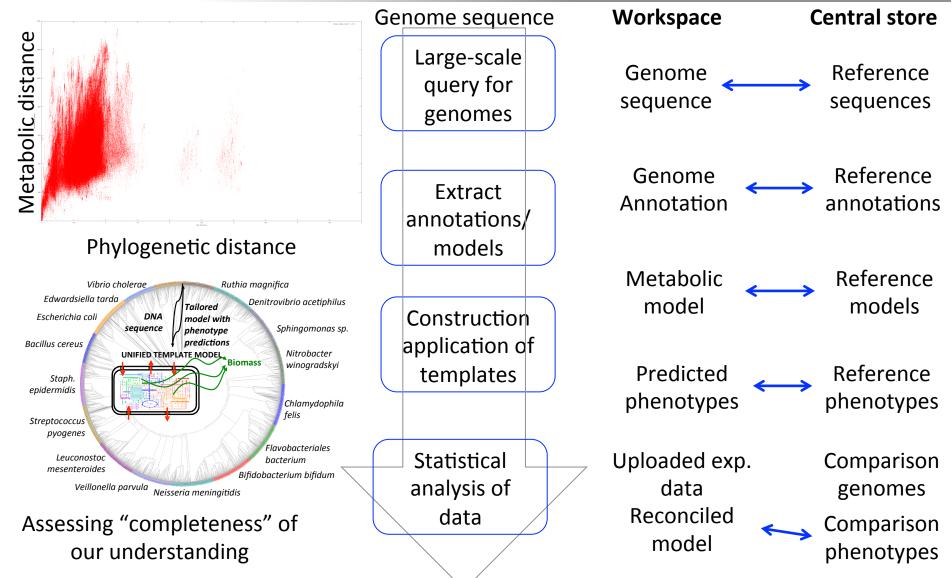
Rapidly building understanding of microbe behavior







Biological trends across the tree of life







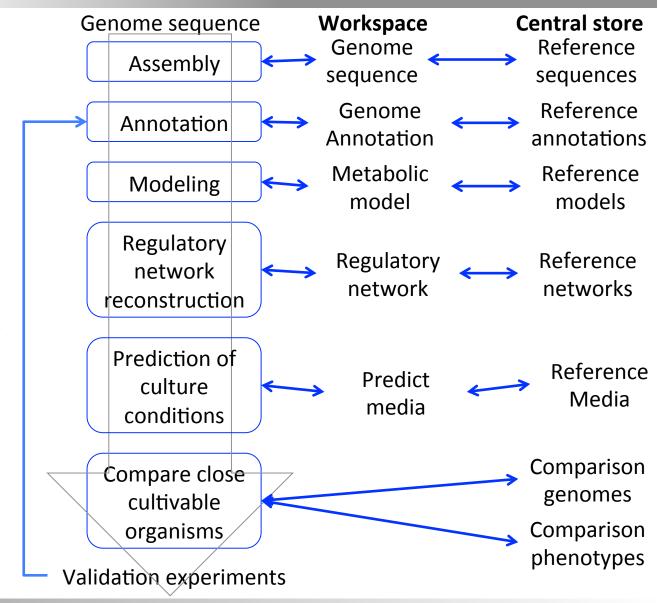
Driving discovery in experimental biology

Predict nutrients required for biomass biosynthesis

Predict potential nutrients that may inhibit growth

Compare models and predicted growth behavior of nearby cultivable microbes with genome of interest

Explore microbe-microbe codependency or microbe-host dependency hypotheses



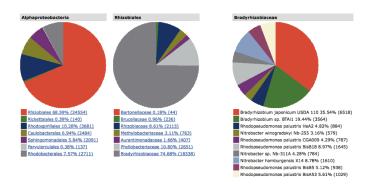




KBase Communities Supports Massive Metagenomics

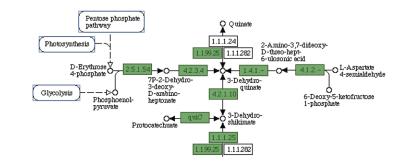
- Automated processing and analysis of metagenomic data (16s/18s, shotgun metagenome, meta transcriptome)
- Incorporation of MG-RAST and QIIME functionality
- Novel sequence QC pipelines (DRISEE)
- Evidence-based design of metagenomic experiments

Who are they?



What are they doing?

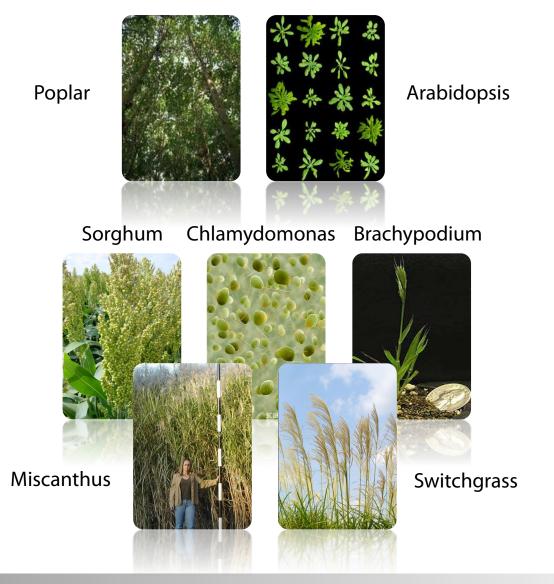
PHENYLALANINE, TYROSINE AND TRYPTOPHAN BIOSYNTHESIS







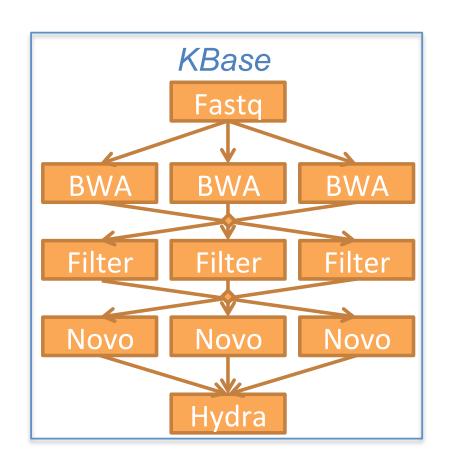
KBase-Plants: Targeted genomes

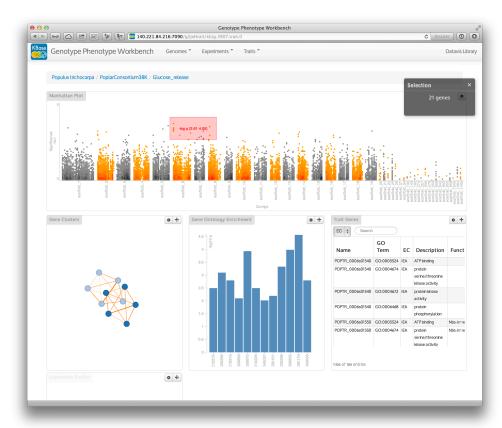






From reads through variants to phenotypes











Align and call SNPs from 35M 80bp (14Gbp) reads with maize genome (zmb73v2) Identified 372k high confidence SNPs

	Serial	Multitcore	KBase Cloud
Config	1 core (1 node)	44 core (1 node)	118 cores (15 nodes)
Bowtie2	45 h*	1h 10m	23 m
Sort	2 hr	2 hr	N/A
Samtools	2 hr	2 hr	12 m
End-to-End Speedup	50h* 1x	5h 10m 9.6x	35 m 86x

*estimated time





Maize Population Analysis

Align and call SNPs from 131 maize samples ITB fastq / 408Gbp input data

	Serial	KBase cloud (small)	KBase Cloud (large)
Config	1 core (1 node)	210 cores (15 nodes)	854 cores (61 nodes)
Bowtie2	1311 hr*	19.5 hr	5 hr
Sort	58 hr*	N/A	N/A
Samtools	58 hr*	3.5 hr	1.5 hr
End-to-End Speedup	1427 hr* 1x	23 hr 62x	6.5 hr 219x

*estimated time





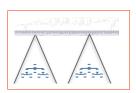
Networks: Cross-cut example

I. Networks-based knowledge discovery

Networks-based ontologies









Gene-ontologies matcher



Algorithms and UI tools to search and analyze best matched network components for a user specified gene set

II. Facilitate building predictive models

Networks-based reliable orthologs

Plant genomes

co-expression based functional orthologs (Mutwil et al. Plant Cell 2011)

Microbial genomes

co-localization based reliable orthologs

III. Infrastructure for scientific social networks

Networks of scientific communities and projects

Support narrative interface. Social networks connecting users and joint projects

Networks of algorithms similarity



Allows KBase to diversify its menu of algorithms and avoid algorithms producing nearly identical results

Networks quality control

Assign quality measures to KBase networks to allow healthy competition between algorithms and teams





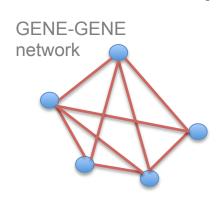
Datasets and Networks API

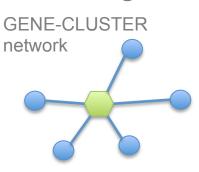
I. Datasets: collected, processed, classified

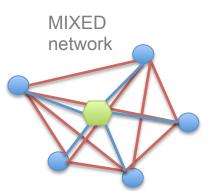
KBase domain	Dataset sources	Datasets
Microbes	7	5099
Plants	6	46
Communities	1	1

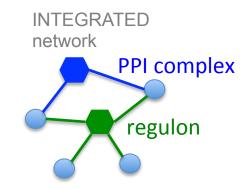
Network types			
REGULATORY_NETWORK	CO_FITNESS		
PROT_PROT_INTERACTION	CO_EXPRESSION		
METABOLIC_SUBSYSTEM	FUNCTIONAL_ABUNDANCE		
FUNCTIONAL_ASSOCIATION	PHYLOTYPE_ABUNDANCE		

II. Networks API: provide heterogeneous networks in unified format









Networks build methods

Network buildFirstNeighborNetwork(
list<string> datasetIds,
list<string> entityIds,
list<EdgeType> edgeTypes)

Network buildInternalNetwork(
list<string> datasetIds,
list<string> geneIds,
list<EdgeType> edgeTypes)

Datasets management methods

list<Dataset> allDatasets()
list<DatasetSource> allDatasetSources()
list<NetworkType> allNetworkTypes()





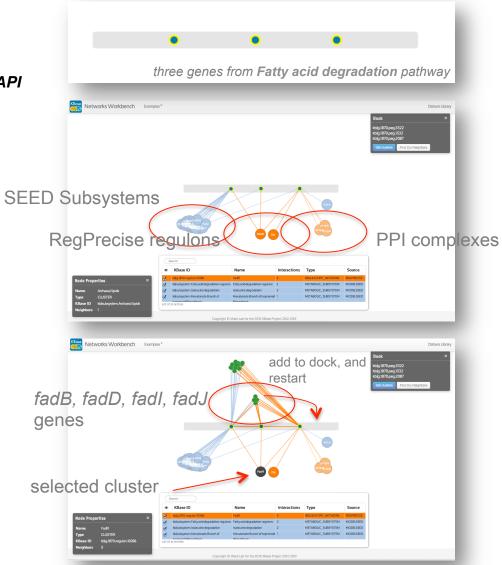
Networks Workbench

Iterative exploration and building network components

powered by the developed Networks API

Gene clusters associated with genes from dock panel

Putative members of the same network component (docked genes)







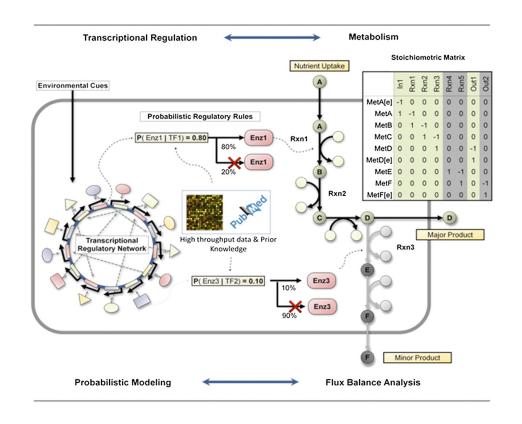
Working with collaborators early

ENSURING IMPACT





Using KBase framework to enable PROM

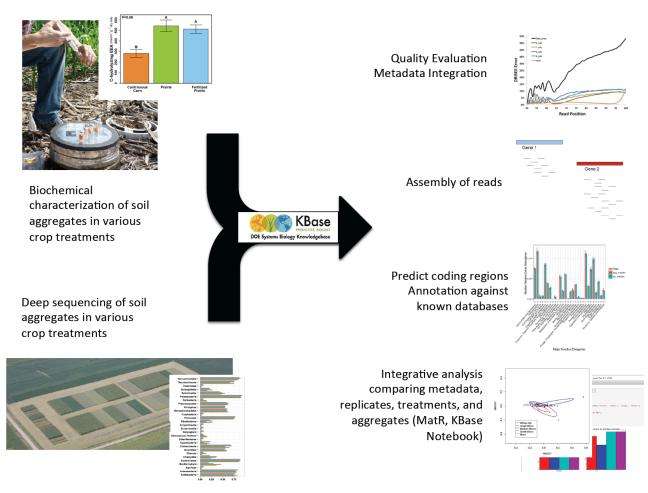


- Nathan Price's probabilistic regulation of metabolism (PROM) integrates metabolic models and functional data to make better predictions of growth given genetic or transcription variation.
- Difficult to access and for people to use.
- Previously applied to just two organisms.
- Now a KBase service that can be applied to any genome for which there is expression or variation data.
- Testing on Shewanella oneidensis MR-1 with transcription, TF knockout and growth/fitness data available in KBase.





KBase Microbial Communities Analysis Tools to Discover Niche Selection in Crop Soil Aggregates



Kirsten Hofmockel, Iowa State, used KBase services to analyze and compare metagenomes from different sized soil aggregates across different crop treatments.

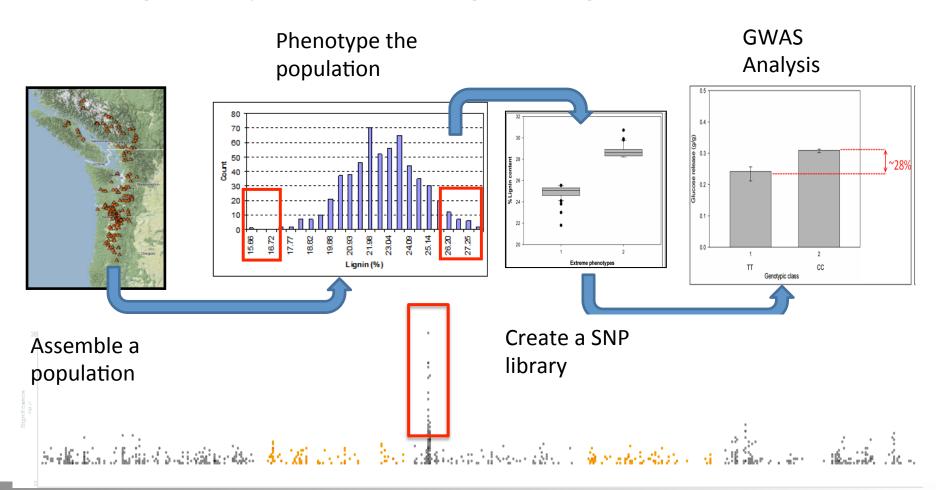




Work with Tuskan (ORNL) & DiFazio (WVU) Identifies important SNPs

Variation in Lignin Composition and Content

Extreme variation contained in native populations of *Populus* detected in common garden experiments linked to genes using Association Genetics





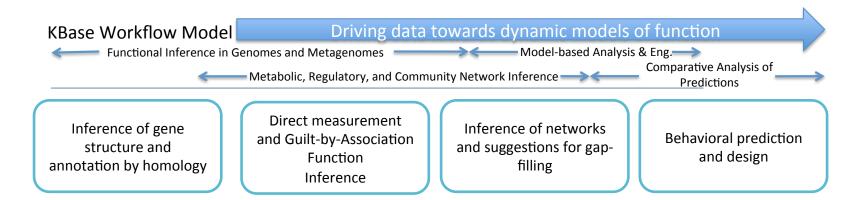


HOW ARE WE BUILDING KBASE?



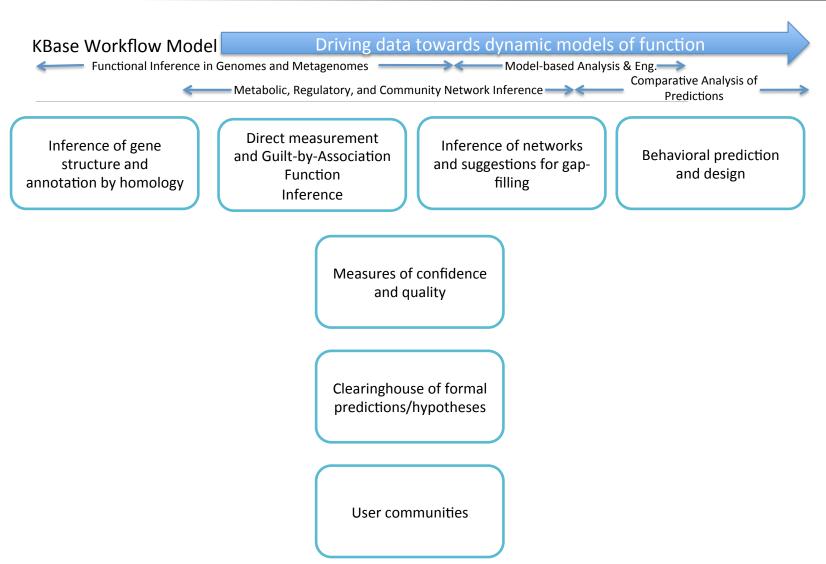


Define over research "paths"





Link design to KBase Concepts





Inference of gene structure and annotation by homology

Direct measurement and Guilt-by-Association Function Inference

Inference of networks and suggestions for gap-filling

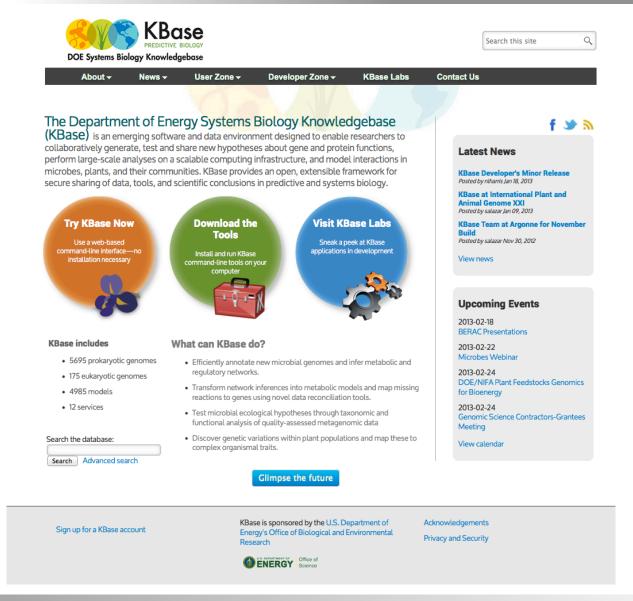
Measures of Confidence and Quality

Clearinghouse of Predictions/Hypotheses

User Communities



Three "Products" highlighted on Home Page

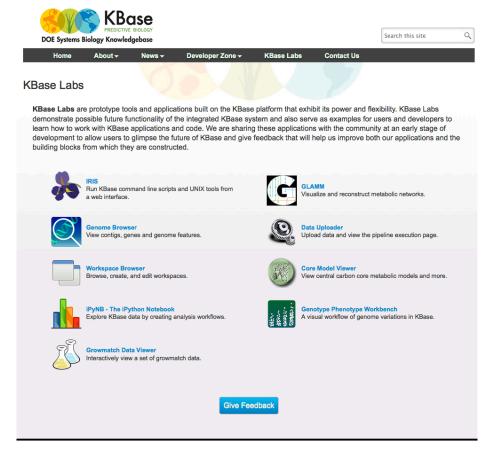








- Labs are prototypes and applications that demonstrate KBase present and possible future function.
- Early stage functionality both provides utility and a way for the community to provide feedback.





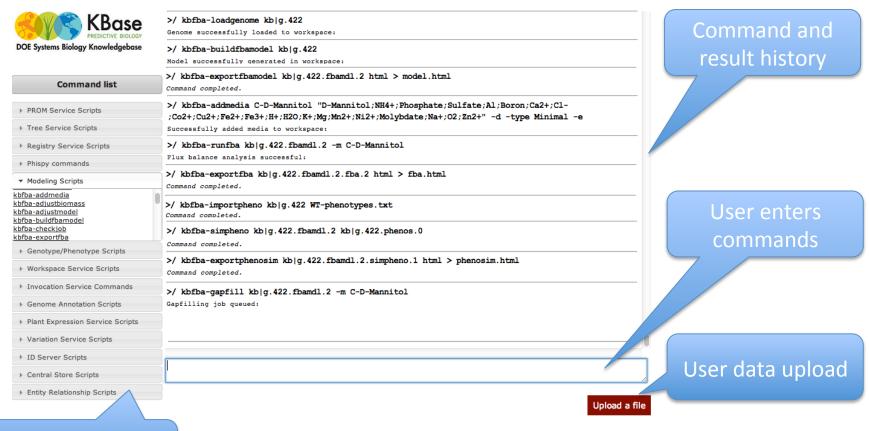
KBase is sponsored by the U.S. Department of Energy's Office of Biological and Environmental Research.





IRIS: Command-Line On the Web

Metabolic workflow in IRIS



Directory of services

IRIS is a web-based terminal to give you access to the full KBase command line without the need to install anything!





Command Line

- Command-line environment for programmers
- Available via downloadable Macintosh DMG or Ubuntu (linux) image
- Installs clean environment for KBase application development

Populus reads to SNPs in Five Easy Steps

- Identify reference genome
 \$ all_entities_Genome -f scientific_name | grep -i 'Populus'
- Upload Reads to KBase cloud
 \$ jk_fs_put_pe populus.1.fq.gz populus.2.fq.gz populus
- Align Reads with Bowtie2
 \$ jk_compute_bowtie -in=populus.pe -org=populus -out=populus_align
- 4. Call SNPs with SAMTools\$ jk_compute_samtools_snp -in=populus_align -org=populus -out=populus_snps
- 5. Merge and Download VCF files \$ jk_compute_vcf_merge -in=populus_snps --alignments=populus_align -out=populus.vcf \$ jk_fs_get populus.vcf

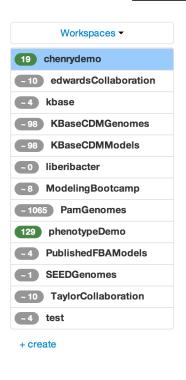




Prototype collaborative workspaces

View Objects Produced by Analysis in an Online Collaborative Workspace





10 record	s per page	Search:				
Workspace *	ID \$	Type ‡	Command \$	Owner ‡	Modified	\$
chenrydemo	kb g.422.fbamdl.2.fba.3 (0)	FBA	runfba	chenry	2013-02-19T01:58:45	
chenrydemo	kb g.422.fbamdl.2.fba.0 (0)	FBA	runfba	chenry	2013-02-19T01:58:45	
chenrydemo	kb g.2793.fbamdl.0.fba.4 (0)	FBA	runfba	chenry	2013-02-19T01:58:45	
chenrydemo	kb g.422.fbamdl.2.fba.2 (0)	FBA	runfba	chenry	2013-02-19T01:58:45	
chenrydemo	kb g.2793.fbamdl.0.fba.2 (0)	FBA	runfba	chenry	2013-02-19T01:58:45	
chenrydemo	kb g.2793.fbamdl.0.fba.0 (0)	FBA	runfba	chenry	2013-02-19T01:58:45	
chenrydemo	kb g.2793.fbamdl.0.fba.3 (0)	FBA	runfba	chenry	2013-02-19T01:58:45	
chenrydemo	kb g.2793 (1)	Genome	genome_to_workspace	chenry	2013-02-19T01:58:45	
chenrydemo	83333.1 (0)	Genome	genome_to_workspace	chenry	2013-02-19T01:58:45	
chenrydemo	kb g.422 (3)	Genome	genome_to_workspace	chenry	2013-02-19T01:58:45	

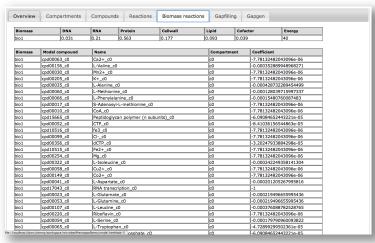
- Object model supports provenance, meaning all previous versions of the objects can be retrieved
- Workspace browser provides direct links to view any object contained in the workspace



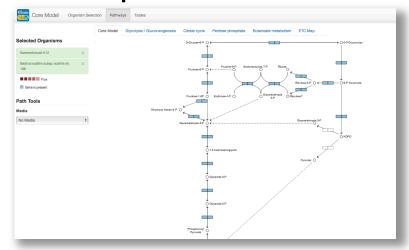


Visualizing Metabolic Models and FBA in KBase

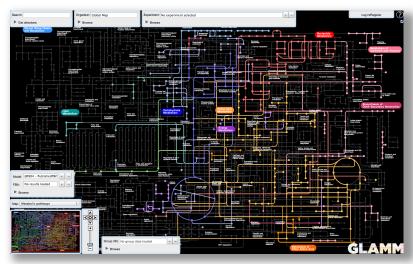
All views may be used for all public and private models and FBA solutions



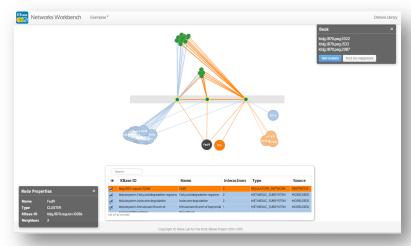
Simple Tabular Views



Comparative Model Viewer



Interactive metabolic maps and models

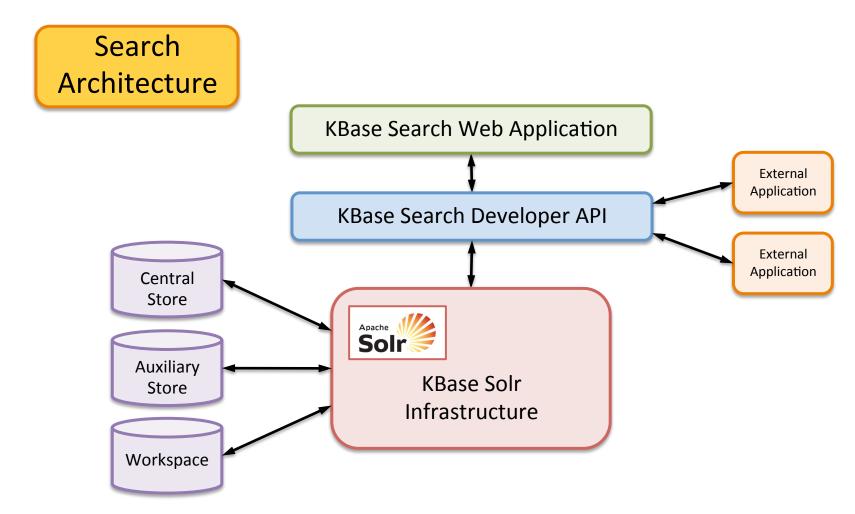


Network Analysis Workbench





Search Prototype



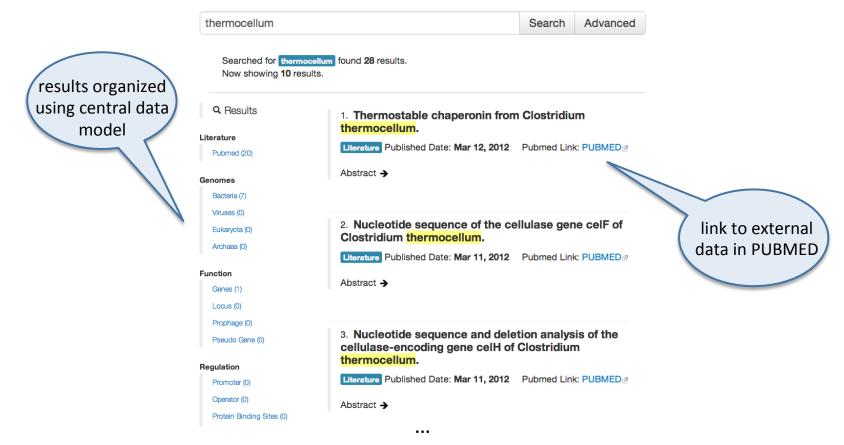




Search with keyword: thermocellum

clostridium Search Advanced

KBase Search









KBase Search

thermocellum Search Advanced Bacteria Clostridium thermocellum ATCC 27405 **RNA Features** Contigs Genome Size genome 3843301 Protein Encoding Genes GC Content Complete details 38.9865899132022 links to Subsystem Contigs Genes RNAs features Subsystem **Function In Cell** Version Restriction-Modification System 2.x Glutathione-regulated potassium-efflux system and associated functions 9.71 1.111 Queuosine-Archaeosine Biosynthesis Experimental tye 4 Methylglyoxal Metabolism 9.0 Ribospme LSU Symbiont Synthesis of osmoregulated periplasmic glucans 1.x

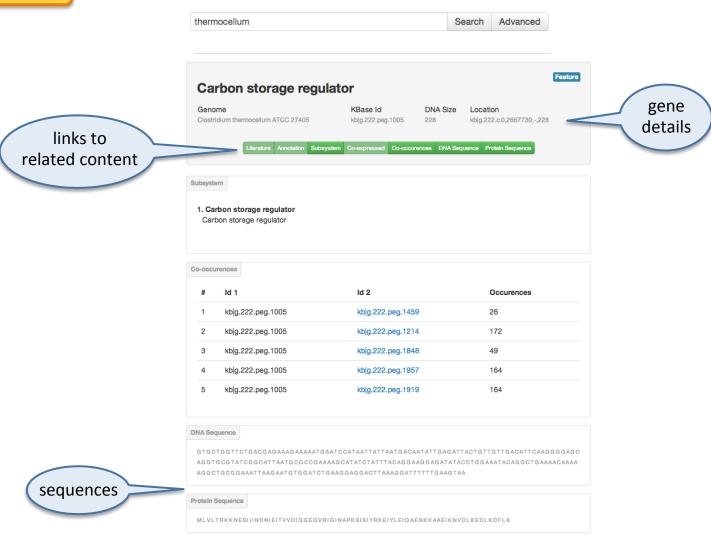
...





Gene page

KBase Search







Initial Platform Modules

	IRIS	Search		Core Model Viewer		/er	iPy Notebook	
GUI Components	Workspace Browser			Genome Browser		Genotype Phenotype Workbench		
	Read QC Serv	FBA Modeling Service Network Service				ervice		
Services	Plant Expression Service Genotype Phenotype Service					rvice		
	Similarity Service		Prophage Finder		der	Ontology Service		
	Metagenomics API		Annotation Service		PROM Service			
	Metagenomics R Tools			Tree Service		Assembly Service		
	Experiments Service		Translation Service		ervice	Protein Info Service		
Infrastructure Services	Authorization	CI	uster Service ID		ID Service	Service 1		Compiler
	Authentication	E	Entity Relationship Service			Service Registry		
Data Stores	Auxiliary Store	liary Store Repositories User Workspa			Workspac	ace Central Store		
	Shock		MongoDB			Mysq		
Language Support	Perl Python Jav		vascript Java		a	Torque Hadoop		Hadoop
Cloud Virtualization	OpenStack Development and Scaling KVM Production Endpoints							





Initial KBase Services

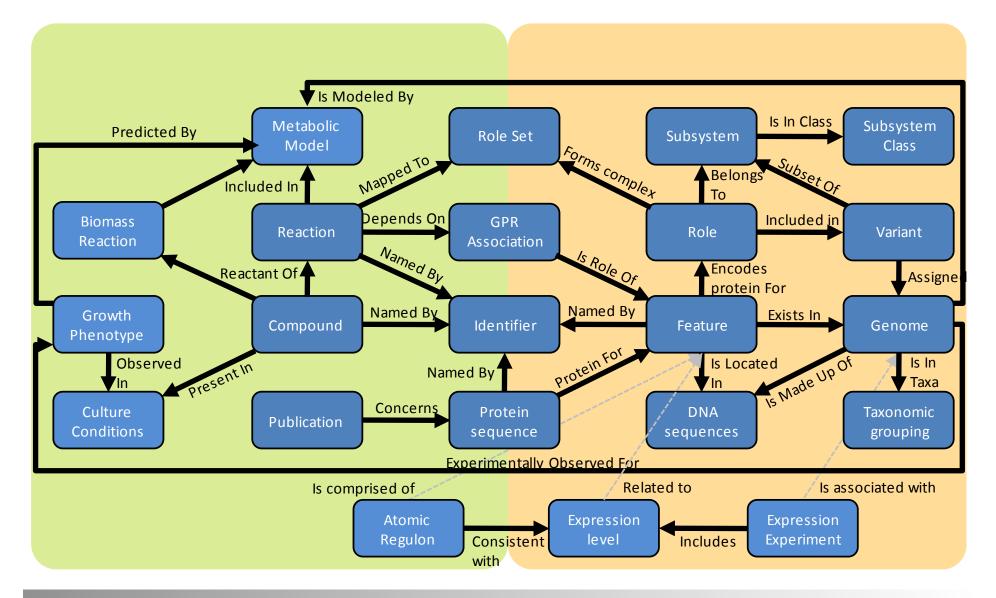
- IRIS
- KBase Notebook
- Auxiliary Store Service
- Communities API
- Metagenomics Analysis Tools R
- QC Service
- Annotation Service
- Central Store
- Core Model Viewer
- Experiment data
- FBA Modeling
- Metabolic Map Viewer
- Microbes Model Builder
- Phispy
- Probabilistic Annotation
- Protein Info service
- Regulation Service
- Similarity Service

- Translation Service
- Workspace Service
- KB Model Seed
- Tree Service
- Assembly Service
- Authorization Service
- Network Service
- Genotype Phenotype Service
- Genotyping Service
- Ontology Service Plant
- Expression Service
- Authentication and Authorization Client
- Cluster Service
- ERDB service
- File Type Service
- ID Service
- Registry
- Type Compiler





KBase Central Data Model



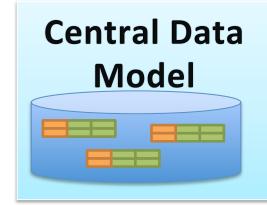




The KBase Data Stores

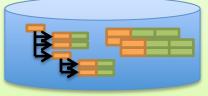
Data Stores: Storing a diverse range of biological data requires multiple approaches:

- Highly structured data in relational databases
- Frequently changing user data
- Large bulk data



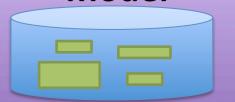
Petabytes of Raw Data

User Data Model



Flexible Storage For Workspaces

Auxiliary Data Model

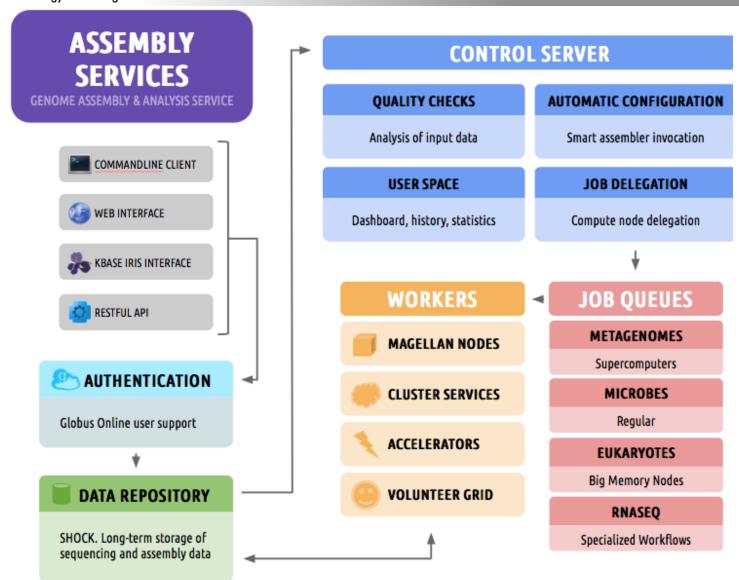


Structured Storage For Curated Data





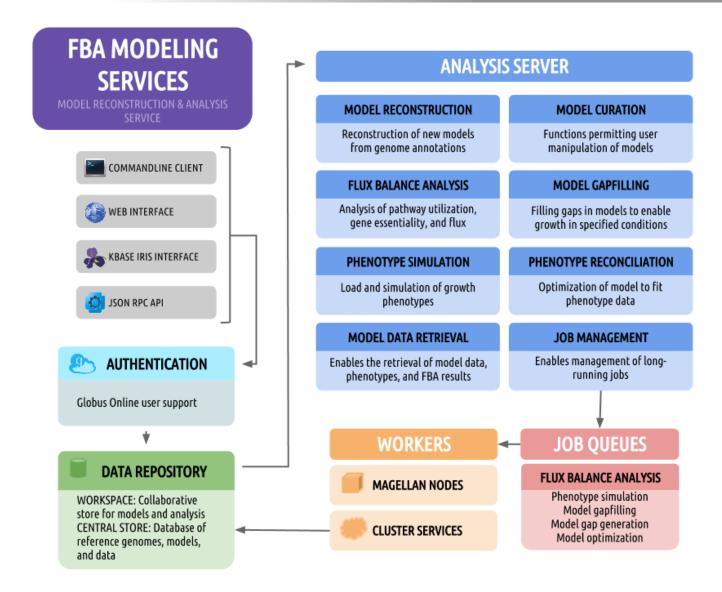
The KBase Assembly Service







Flux Balance Analysis Modeling Services









Helping users and developers manage complexity

Website and Outreach





Training

KBase Training Resources

Several types of training are being offered, either as in-person sessions or as web-based resources:

- User Manuals are online procedural documents describing each of the services with detailed information about functionality and usage.
- Tutorials are both online training resources and in-person sessions* focused on using specific
 aspects of KBase. Online resources are in the form of written walk-throughs and video tutorials.
 In-person tutorials will typically be 2-3 days, and may be immediately followed by a 1-day workshop as
 part of the same agenda. In-person tutorials are bimonthly.
- Workshops are in-person sessions* focused on scientific problems. We will guide you through the
 use of KBase to accomplish tasks that are of interest to you. Currently, workshops will be single-day
 sessions that are paired with relevant tutorials (i.e., offered at the end of a tutorial session). Later in
 the project, workshops will be stand-alone, multiple-day events held annually.
- Bootcamps are in-person sessions focused on developing computational tools in KBase. Join our developers and help build KBase.

plus ... Monthly webinars





When and Where

Scheduled KBase Events can be found at http://kbase.us

Calendar



Upcoming Training Sessions

Bootcamps:

February 12-13, 2013: Full March 6-7, 2013: Open April 24-25, 2013: Open

Tutorials:

February 11-13, 2013: Full March 11-13, 2013: Full May 6-8, 2013: Open, topics include IRIS for Microbes, IRIS for Plants, and matR for Communities July 15-17, 2013: Open, topics TBD

Workshops:

Requires concurrent registration in a Tutorial Session. Feb 14, 2013: Full March 14, 2013: Full May 9, 2013: Open, topics TBD July 18, 2013: Open, topics TBD

Contact us at outreach@kbase.us to register for a session.

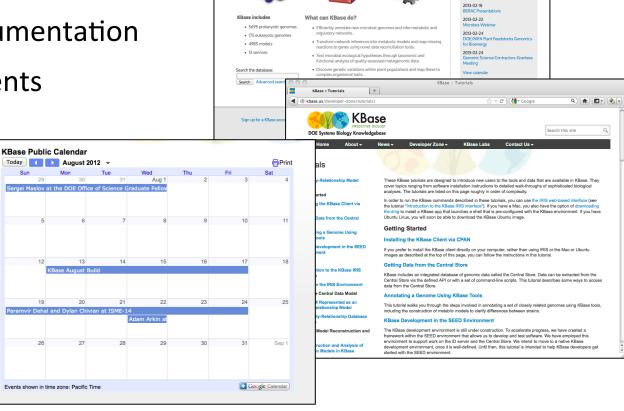


Online Resources

f 🥦 🔊

- User manuals and tutorials
- Video tutorials (coming soon)
- Developer documentation
- Calendar of events
- FAQs
- Press

help@kbase.us



KBase

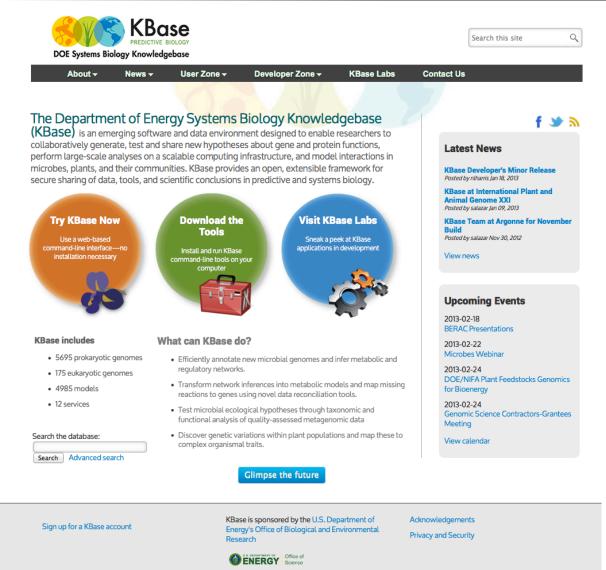
The Department of Energy Systems Biology Knowledgebase

(KBase) is an emerging software and data environment designed to enable researchers to collaboratively generals, test and share new hypotheses about gene and protein functions, perform large-scale analyses on a scalable computing infrastructure, and model interactions in microbes, plants, and their communities. KBase provides an open, extensible framework for secure sharing of data, tooks, and scientific conclusions in predictive and systems biology.





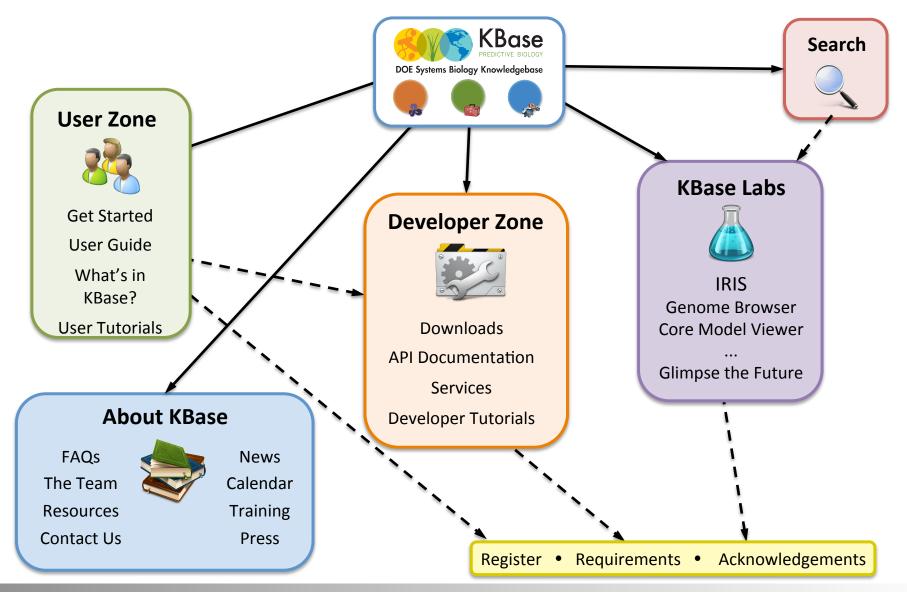
New Site for Easy Navigation







Sitemap for revamped kbase.us website







Extensive Tutorials and Documentation



Search this site

Home About → News →

Developer Zone ▼

KBase Labs

Contact Us

Tutorials

CDM Entity-Relationship Model Browser

Getting Started

Installing the KBase Client via CPAN

Getting Data from the Central Store

Annotating a Genome Using KBase Tools

KBase Development in the SEED Environment

Iris

Introduction to the KBase IRIS interface

RAST2 in the IRIS Environment

The KBase Central Data Model

The CDM Represented as an Entity-Relationship Model

The Entity-Relationship Database

Metabolic Model Reconstruction and Analysis

Reconstruction and Analysis of Metabolic Models in KBase

Command Line Scripts

Accessing Central Store Data

Getting What You Need from the

These KBase tutorials are designed to introduce new users to the tools and data that are available in KBase. They cover topics ranging from software installation instructions to detailed walk-throughs of sophisticated biological analyses. The tutorials are listed on this page roughly in order of complexity.

In order to run the KBase commands described in these tutorials, you can use the IRIS web-based interface (see the tutorial "Introduction to the KBase IRIS interface"). If you have a Mac, you also have the option of downloading the dmg to install a KBase app that launches a shell that is pre-configured with the KBase environment. If you have Ubuntu Linux, you will soon be able to download the KBase Ubuntu image.

Getting Started

Installing the KBase Client via CPAN

If you prefer to install the KBase client directly on your computer, rather than using IRIS or the Mac or Ubuntu images as described at the top of this page, you can follow the instructions in this tutorial.

Getting Data from the Central Store

KBase includes an integrated database of genomic data called the Central Store. Data can be extracted from the Central Store via the defined API or with a set of command-line scripts. This tutorial describes some ways to access data from the Central Store.

Annotating a Genome Using KBase Tools

This tutorial walks you through the steps involved in annotating a set of closely related genomes using KBase tools, including the construction of metablic models to clarify differences between strains.

KBase Development in the SEED Environment

The KBase development environment is still under construction. To accelerate progress, we have created a framework within the SEED environment that allows us to develop and test software. We have employed this environment to support work on the ID server and the Central Store. We intend to move to a native KBase development environment, once it is well-defined. Until then, this tutorial is intended to help KBase developers get started with the SEED environment.

IRIS: a Browser-based Framework for Interacting with KBase

Introduction to the KBase IRIS interface





Extensive Tutorials and Documentation



Search this site Q

Home

About **▼**

News **▼**

Developer Zone ▼

KBase Labs

Contact Us

API and Command-Line Documentation

CDM Command Line Scripts

CDM API

CDMI Entity-Relationship Command Line Scripts

CDMI Entity-Relationship API

ID Server Command Line Scripts

ID Server API

Workspace Service

Plant Expression Service

Tree Service

Ontology Service

Protein Info Service

Similarity Service

Communities API

QC Service

Authorization Client

Genome Annotation Service

Translation Service

Networks Service

Reference Documentation

Each of the services provided by the KBase project includes developer reference documentation. The list of currently available reference documents is shown on the left side of this page.

CDM Command Line Scripts

The CDM command line scripts allow users to access data in the Central Store. These scripts generally implement well trodden paths. These are commands that are useful under many circumstances and provide the basic functionality required for common analyses.

CDM API

The Central Data Model API allows users to query instances of the CDM. These include the Central Store which is the primary repository of genomic and modeling data, and Tiny Stores, which support per-user storage of genomic and modeling data.

CDMI Entity-Relationship Command Line Scripts

The CDMI Entity-Relationship command line scripts enable direct access to entities and relationships in the Central Store. Accessing relationships allows an user to easily navigate between entities in the central store, providing the ability to join data represented in more than one entity.

CDMI Entity-Relationship API

The CDMI Entity-Relationship API provides access to all entities and relationships in the CDM entity-relationship model. It is the API on which the CDM Entity-Relationship command scripts are built.

ID Server Command Line Scripts

The ID Server command line scripts allow ID allocation and lookup services. This is the core service for generating



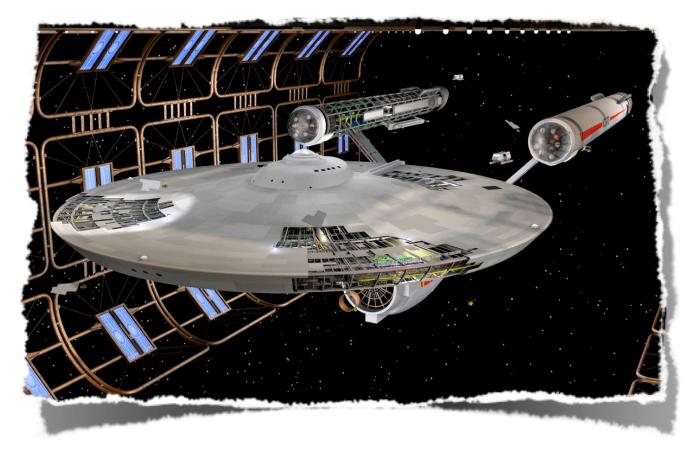


MOAs and Collaborations

- Coordination and shared milestones with the BRCs
- Infrastructure collaborations with JGI, EMSL, NERC.
- Scientific collaborations with ENIGMA, PMI, and other SFAs
- MOAs with NSF NSF for iPLANT and pending for USDA
- Preparation for collaboration and support for future DOE calls
- Needs survey, bootcamps, and scientific discussions with >70 community scientists.







What next?

Building a starship in deep space?





Into the future

- The data model must evolve to support the modeling mission
- A framework for turning bioinformatics algorithms' output into models needs further development
- Theory for integrative, cross-scale predictive biology under development
- Much better ontologies for nearly everything
- Building the social tools.

- Need to improve data import, quality assessment and metadata
- Efficient incorporation of new third party algorithms and support with scalable computing.
- Growing a strong external development community while maintaining quality, stability and vision.
- Launching the KBase Foundation to ease licensing and growth of KBase user participation.



A more concrete view of the "Narrative" interface





Narrative Desiderata

Users can share knowledge at at multiple levels of granularity

- Cut and paste parts of narratives to reuse workflows
- Cross-citation and branching of narratives

Project management

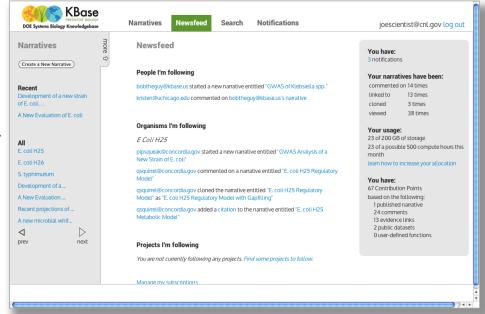
- Creation of teams allows management of projects
- Electronic lab notebook for computational researchers
- Projects can track progress

Possible publication model

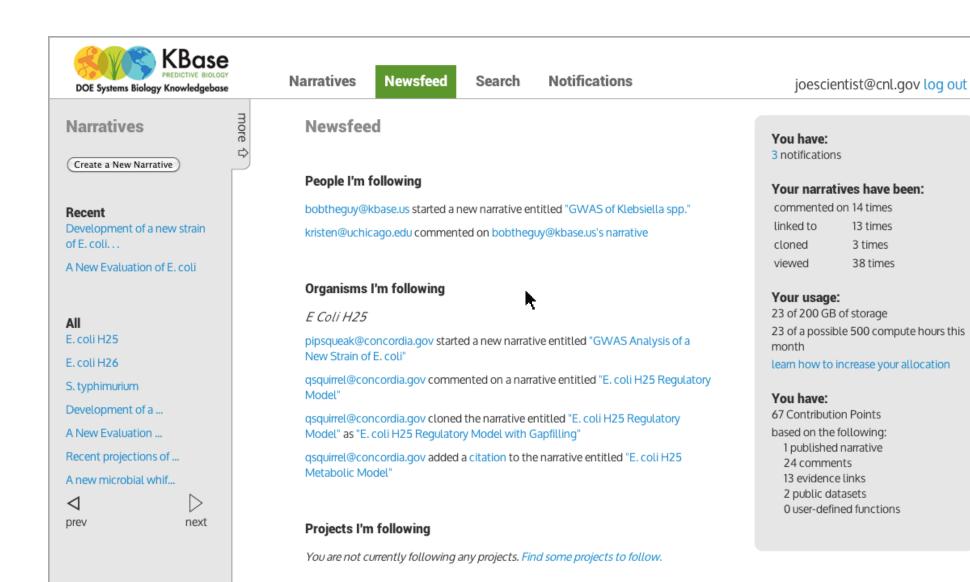
- Finalized Narratives are reviewed, assigned DOI numbers, and accepted in an appropriate journal
- Citation metrics

Metrics of Research Efficiency

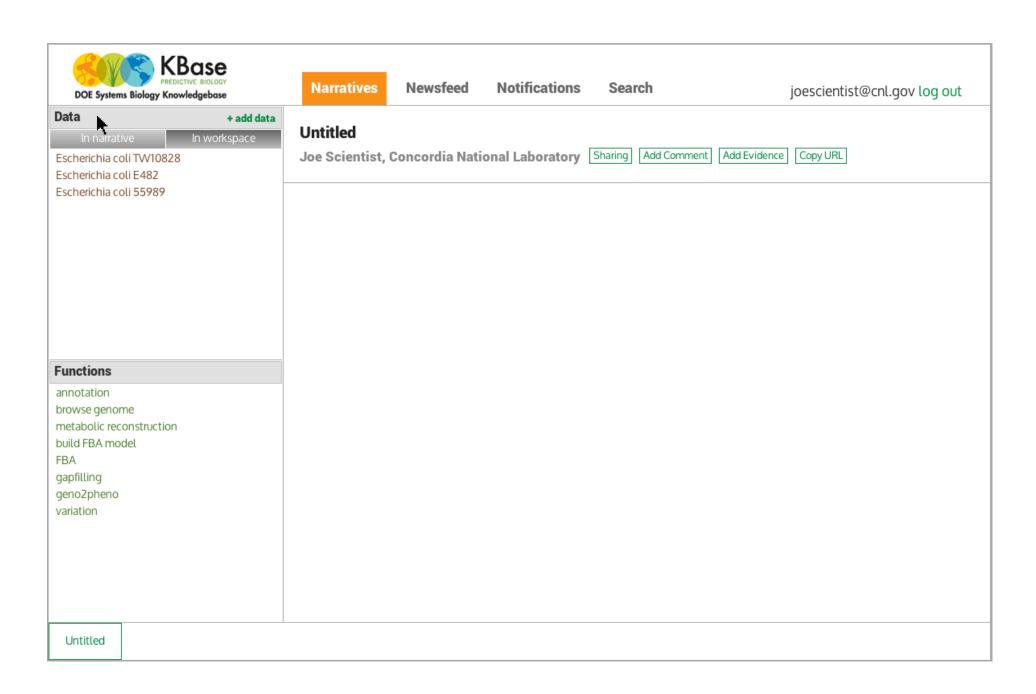
- Times to completion of narratives
- Times from hypothesis to confirming data/narratives
- User, data, and algorithm ratings by how many times the products appear in or are cited by narratives.
 - Can be aggregated by user, team, location, agency
 - People networks can be inferred by looking at team, citation, and comment structures.

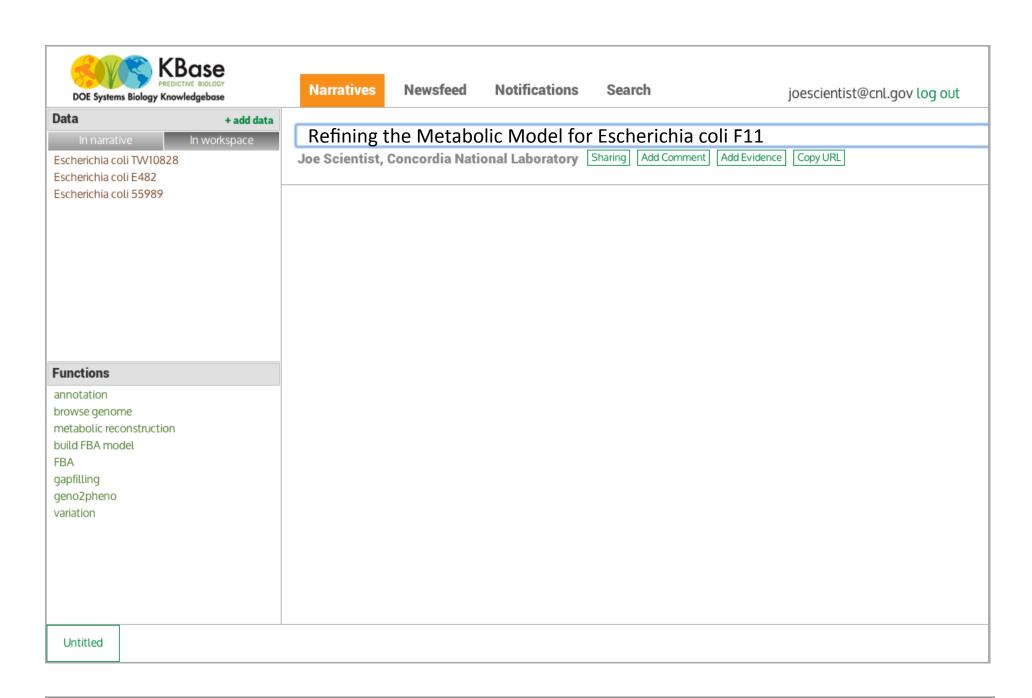


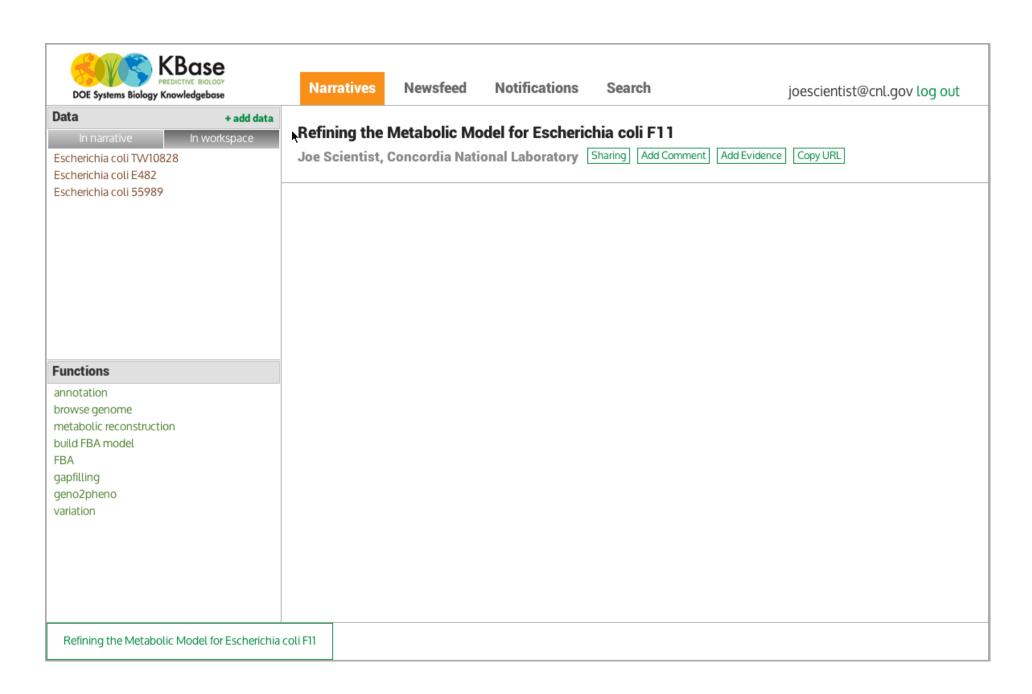




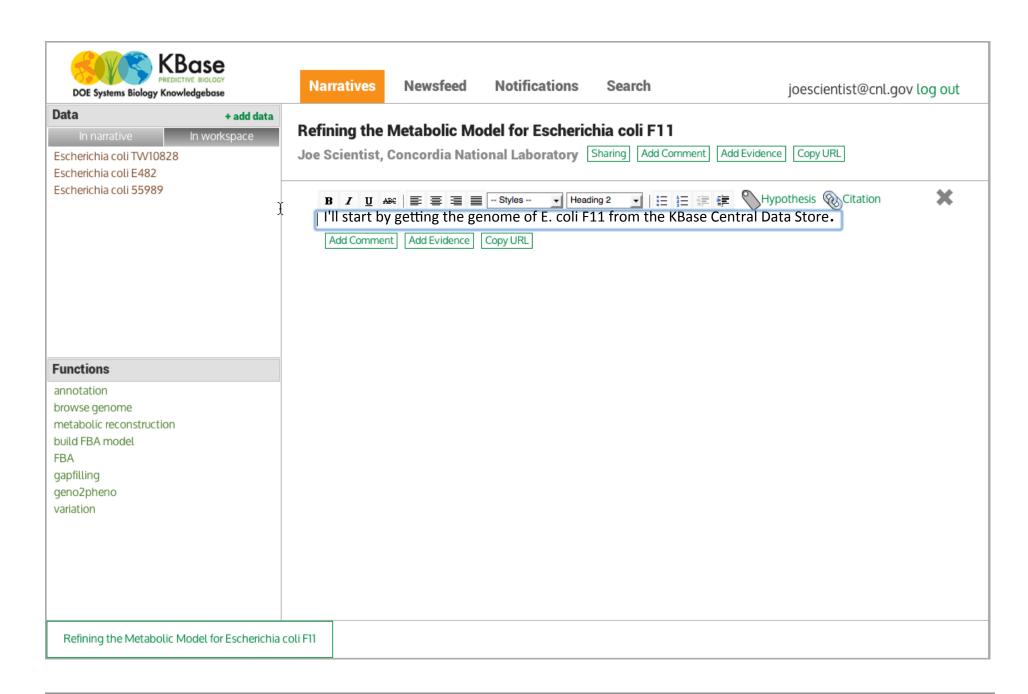
Manage my subscriptions

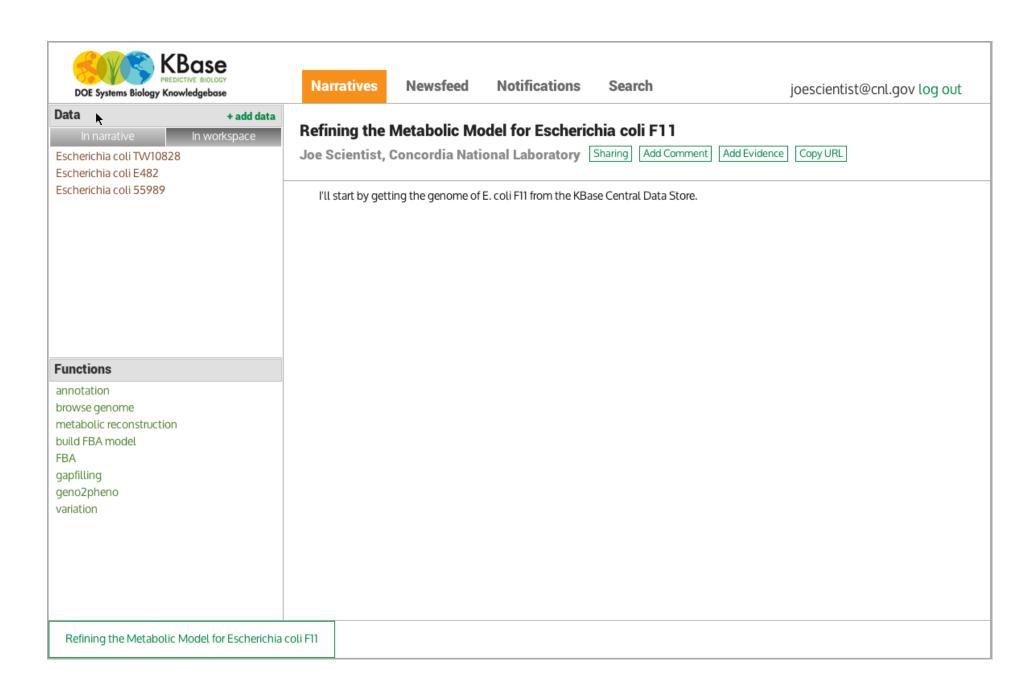


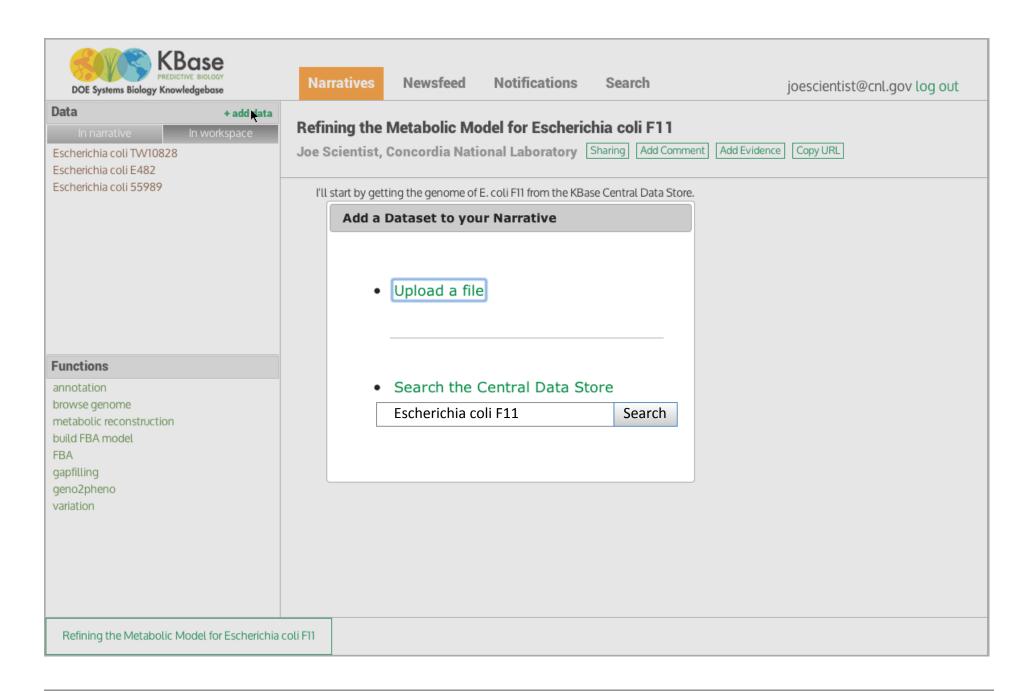


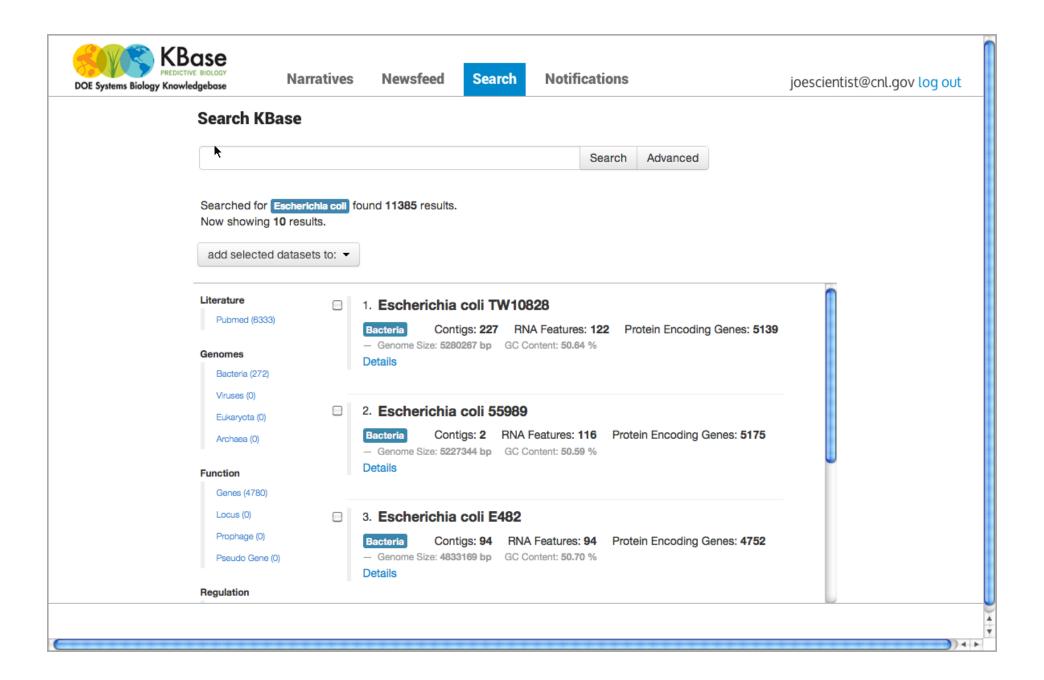


DOE Systems Biology Knowledge	1SE BIOLOGY gebase	Narratives	Newsfeed	Notifications	Search	joescientist@cnl.gov log out
In narrative In Escherichia coli TW10828 Escherichia coli E482 Escherichia coli 55989	+ add data workspace		Concordia Nati	odel for Escheri		t Add Evidence Copy URL
Functions annotation browse genome metabolic reconstruction build FBA model FBA gapfilling geno2pheno variation						
Refining the Metabolic Mod	lel for Escherichia o	coli F11				











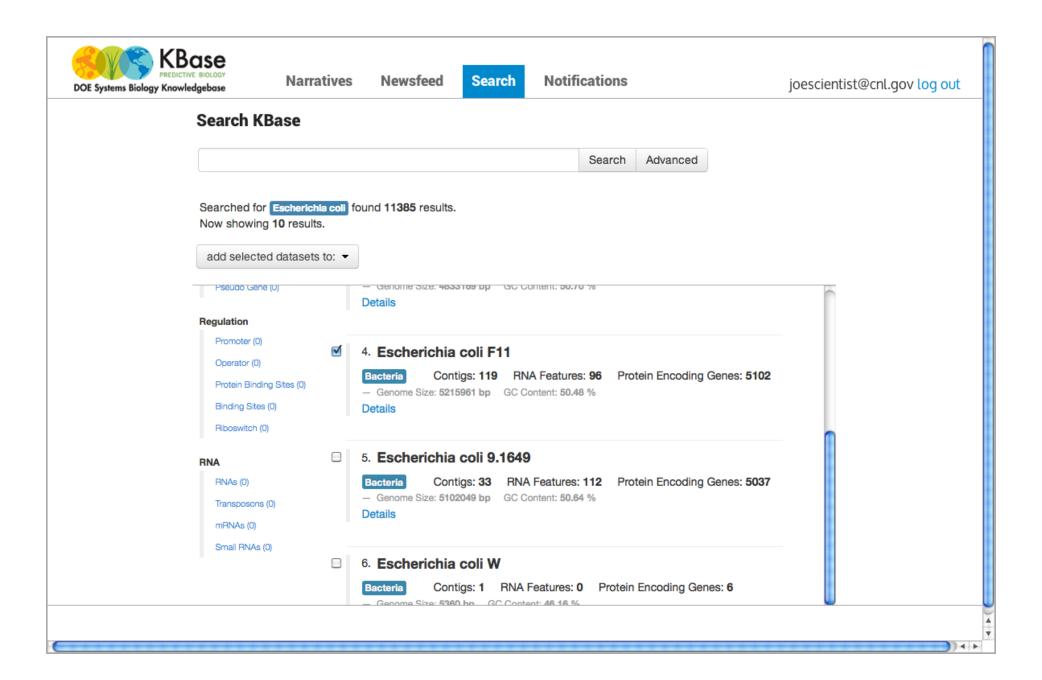
Newsfeed

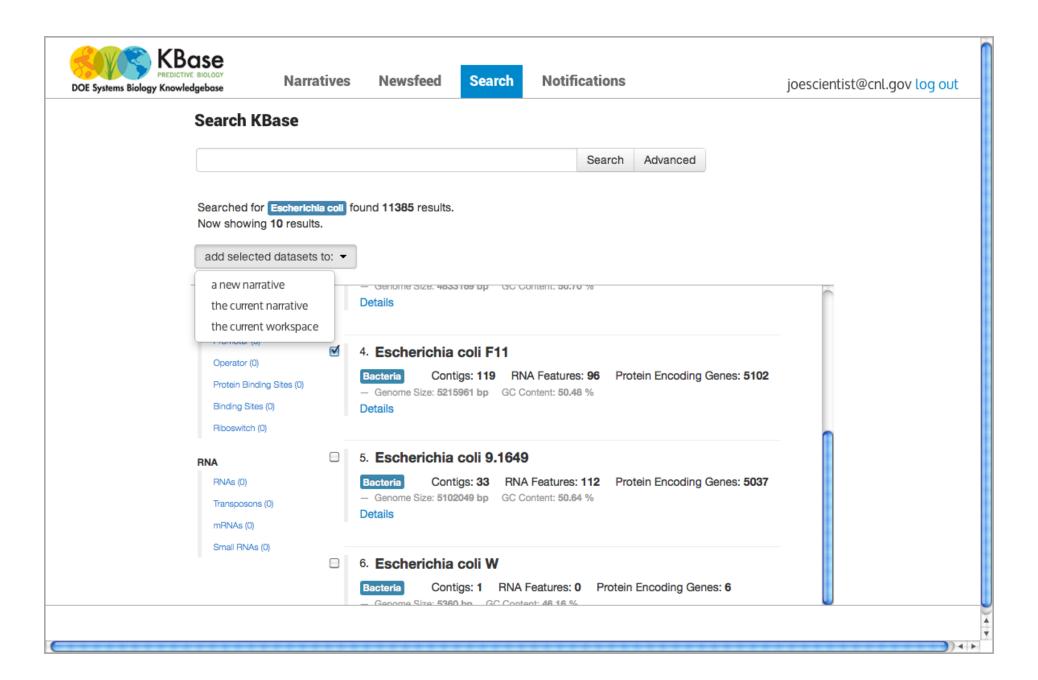
Search

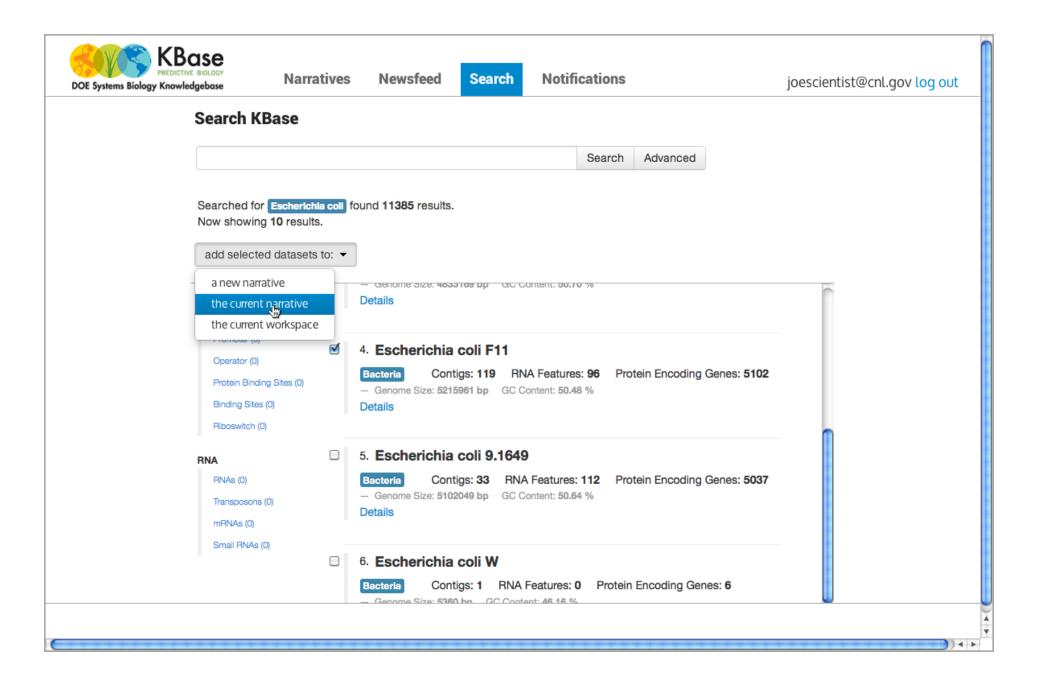
Notifications

joescientist@cnl.gov log out

Search KBase Advanced Search Searched for Escherichia coli found 11385 results. Now showing 10 results. add selected datasets to: ▼ Pseudo Gene (U) Genome Size, 4033 ros pp GC Content, 30.70 % Details Regulation Promoter (0) 4. Escherichia coli F11 Operator (0) Contigs: 119 RNA Features: 96 Protein Encoding Genes: 5102 Bacteria Protein Binding Sites (0) Genome Size: 5215961 bp GC Content: 50.48 % Binding Sites (0) Details Riboswitch (0) 5. Escherichia coli 9.1649 RNA Bacteria Contigs: 33 RNA Features: 112 Protein Encoding Genes: 5037 RNAs (0) Genome Size: 5102049 bp GC Content: 50.64 % Transposons (0) Details mRNAs (0) Small RNAs (0) 6. Escherichia coli W Contigs: 1 RNA Features: 0 Protein Encoding Genes: 6 Bacteria Genome Size: 5360 hn GC Content: 46 16 %









Newsfeed Notifications

I'll start by getting the genome of E. coli F11 from the KBase Central Data Store.

Search

joescientist@cnl.gov log out

Copy URL

+ add data Refining the Metabolic Model for Escherichia coli F11

×

In workspace

Escherichia coli TW10828 Escherichia coli E482 Escherichia coli 55989

Data

Escherichia coli F11 Genome, annotated

Escherichia coli F11 Genome, annotated

Joe Scientist, Concordia National Laboratory Sharing

Domain: Bacteria

Taxon: gamma-proteobacteria

KBase ID; KB|g.691 Source: Joe Scientist

Version: Mar 27, 2013 08:13:00 PST

Complete genome

Contigs: 2

Add Comment

Base pairs: 5,280,267

PEGs: 232

GC Content: 50.64%

Add Evidence

Functions

annotation browse genome

metabolic reconstruction

build FBA model

FBA

gapfilling

geno2pheno

variation



Newsfeed Notifications Search

joescientist@cnl.gov log out

Data

+ add data In workspace

Escherichia coli TW10828 Escherichia coli E482

Escherichia coli 55989

Escherichia coli F11 Genome, annotated

Refining the Metabolic Model for Escherichia coli F11

Joe Scientist, Concordia National Laboratory Sharing

Add Comment

Add Evidence

Copy URL

I'll start by getting the genome of E. coli F11 from the KBase Central Data Store.

Escherichia coli F11 Genome, annotated

Domain: Bacteria

Taxon: gamma-proteobacteria

KBase ID: KB|q.691 Source: Joe Scientist

Version: Mar 27, 2013 08:13:00 PST

Complete genome

Contigs: 2

Base pairs: 5,280,267

PEGs: 232

GC Content: 50.64%

Functions

annotation

browse genome

metabolic reconstruction

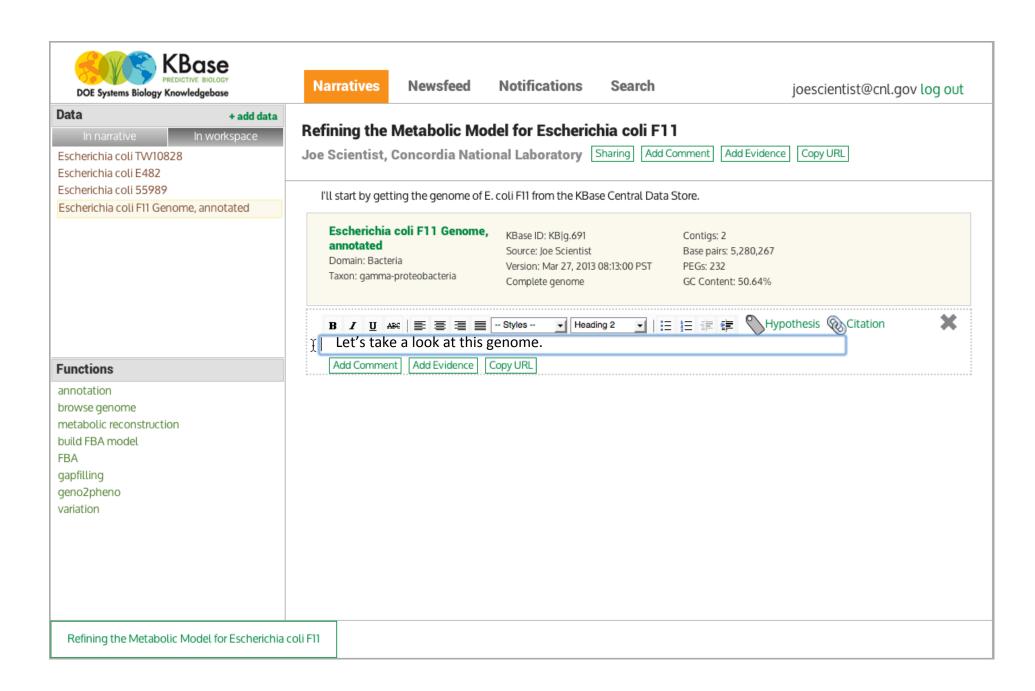
build FBA model

FBA

gapfilling

geno2pheno

variation





Newsfeed Notifications Search

joescientist@cnl.gov log out

Data

+ add data

In workspace

Escherichia coli TW10828

Escherichia coli E482

Escherichia coli 55989

Escherichia coli F11 Genome, annotated

Refining the Metabolic Model for Escherichia coli F11

Joe Scientist, Concordia National Laboratory Sharing

Add Comment

Add Evidence

Copy URL

I'll start by getting the genome of E. coli F11 from the KBase Central Data Store.

Escherichia coli F11 Genome, annotated

Domain: Bacteria

Taxon: gamma-proteobacteria

KBase ID: KB|q.691 Source: Joe Scientist

Version: Mar 27, 2013 08:13:00 PST

Complete genome

Contigs: 2

Base pairs: 5,280,267

PEGs: 232

GC Content: 50.64%

Let's take a look at this genome.

Functions

annotation browse genome metabolic reconstruction

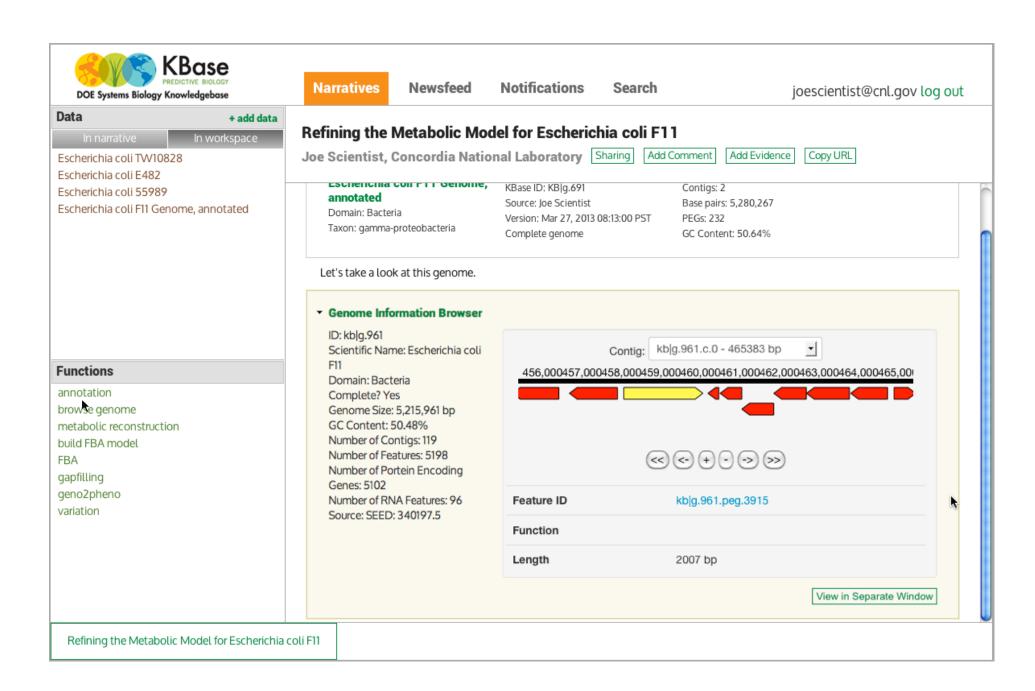
build FBA model

FBA

gapfilling

geno2pheno

variation





Newsfeed Notifications Search

joescientist@cnl.gov log out

Data

+ add data

In workspace

Escherichia coli TW10828 Escherichia coli E482 Escherichia coli 55989

Escherichia coli F11 Genome, annotated

Refining the Metabolic Model for Escherichia coli F11

Joe Scientist, Concordia National Laboratory Sharing

Add Comment

Add Evidence

Copy URL

I'll start by getting the genome of E. coli F11 from the KBase Central Data Store.

Escherichia coli F11 Genome, annotated

Domain: Bacteria

Taxon: gamma-proteobacteria

KBase ID: KB|q.691 Source: Joe Scientist

Version: Mar 27, 2013 08:13:00 PST

Complete genome

Contigs: 2

PEGs: 232

Base pairs: 5,280,267

GC Content: 50.64%

Let's take a look at this genome.

▼ Genome Information Browser

Functions

annotation

browse genome

metabolic reconstruction

build FBA model

FBA

gapfilling

geno2pheno

variation



Newsfeed Notifications Search

joescientist@cnl.gov log out

Data

+ add data

In workspace

Escherichia coli TW10828 Escherichia coli E482 Escherichia coli 55989

Escherichia coli F11 Genome, annotated

Refining the Metabolic Model for Escherichia coli F11

Joe Scientist, Concordia National Laboratory Sharing

Add Comment

Add Evidence

Copy URL

I'll start by getting the genome of E. coli F11 from the KBase Central Data Store.

Escherichia coli F11 Genome, annotated

Domain: Bacteria

Taxon: gamma-proteobacteria

KBase ID: KB|q.691 Source: Joe Scientist

Version: Mar 27, 2013 08:13:00 PST

Complete genome

Contigs: 2

Base pairs: 5,280,267 PEGs: 232

GC Content: 50.64%

Let's take a look at this genome.

▼ Genome Information Browser

Now I'm going to run a metabolic reconstruction on this genome. Let's see how the initial one comes out. This is the first time I've done this for this particular strain, so it will be interesting to see which roles are found.

Functions

annotation

browse genome

metabolic reconstruction

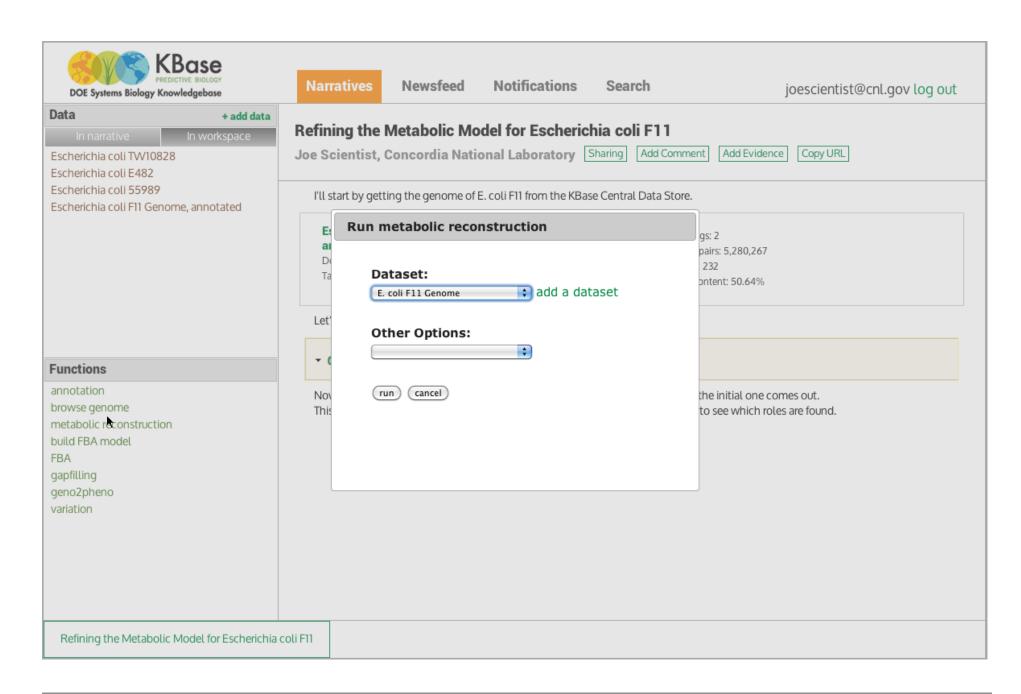
build FBA model

FBA

gapfilling

geno2pheno

variation





Notifications

Search

joescientist@cnl.gov log out

Data

+ add data

In workspace

Escherichia coli TW10828 Escherichia coli E482

Escherichia coli 55989

Escherichia coli F11 Genome, annotated

Escherichia coli F11 Metabolic Reconstruction

Refining the Metabolic Model for Escherichia coli F11

Joe Scientist, Concordia National Laboratory Sharing

Newsfeed

Add Comment

Add Evidence

Copy URL

Till start by getting the genome of E. coll FIT from the KBase Central Data Store.

Escherichia coli F11 Genome. annotated

Domain: Bacteria

Taxon: gamma-proteobacteria

KBase ID: KB|q.691 Source: loe Scientist

Version: Mar 27, 2013 08:13:00 PST

Complete genome

Contigs: 2

Base pairs: 5,280,267

PEGs: 232

GC Content: 50.64%

Let's take a look at this genome.

▼ Genome Information Browser

Now I'm going to run a metabolic reconstruction on this genome. Let's see how the initial one comes out. This is the first time I've done this for this particular strain, so it will be interesting to see which roles are found.

Run Metabolic Reconstruction on E. coli F11 Genome

Started: 9/27/2012 4:15:32pm Finished: 9/27/2012 4.15:33pm

FBA

gapfilling

Functions

annotation

browse genome

build FBA model

metabolic reconstruction

geno2pheno

variation

Escherichia coli F11 Metabolic Reconstruction

Source: calculated

Version: Mar 27, 2013 08:13:00 PST

Roles: 29,294



Notifications

joescientist@cnl.gov log out

Data

+ add data

In workspace

Escherichia coli TW10828 Escherichia coli E482

Escherichia coli 55989

Escherichia coli F11 Genome, annotated

Escherichia coli F11 Metabolic Reconstruction

Refining the Metabolic Model for Escherichia coli F11

Joe Scientist, Concordia National Laboratory Sharing

Newsfeed

Search

Add Comment

Add Evidence

Copy URL

Escherichia coli F11 Genome. annotated

Domain: Bacteria

Taxon: gamma-proteobacteria

KBase ID: KB|q.691

Base pairs: 5,280,267 Source: Joe Scientist

Version: Mar 27, 2013 08:13:00 PST PEGs: 232

Complete genome

GC Content: 50.64%

Contigs: 2

Let's take a look at this genome.

▼ Genome Information Browser

Now I'm going to run a metabolic reconstruction on this genome. Let's see how the initial one comes out. This is the first time I've done this for this particular strain, so it will be interesting to see which roles are found.

Version: Mar 27, 2013 08:13:00 PST

Run Metabolic Reconstruction on E. coli F11 Genome

Started: 9/27/2012 4:15:32pm Finished: 9/27/2012 4.15:33pm

Escherichia coli F11 Metabolic Reconstruction

Source: calculated

Roles: 29,294

1 Comment

Add Comment

Add Evidence

Copy URL

Functions annotation

browse genome

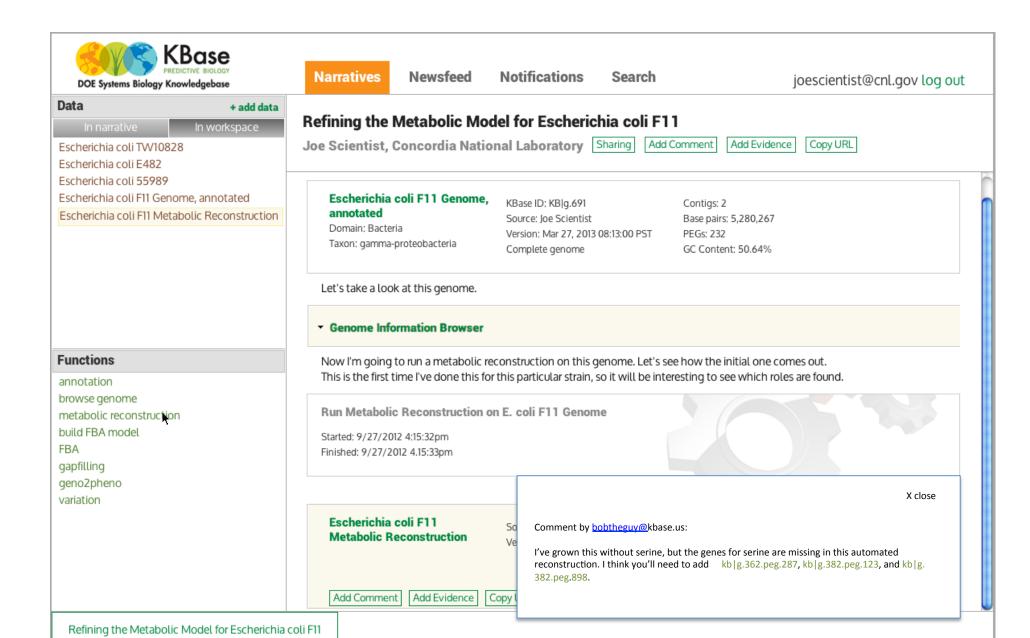
metabolic reconstruction

build FBA model

FBA

gapfilling

geno2pheno variation





Newsfeed Notifications Search

joescientist@cnl.gov log out

Data

+ add data

In workspace

Escherichia coli TW10828 Escherichia coli E482

Escherichia coli 55989

Functions

annotation browse genome

FBA

gapfilling geno2pheno variation

metabolic reconstruction build FBA model

Escherichia coli F11 Genome, annotated

Escherichia coli F11 Metabolic Reconstruction

Refining the Metabolic Model for Escherichia coli F11

Joe Scientist, Concordia National Laboratory Sharing

Add Comment

Add Evidence

Copy URL

Escherichia coli F11 Genome. annotated

Domain: Bacteria

Taxon: gamma-proteobacteria

KBase ID: KB|q.691

Source: Joe Scientist Version: Mar 27, 2013 08:13:00 PST

Complete genome

PEGs: 232

GC Content: 50.64%

Base pairs: 5,280,267

Contigs: 2

Let's take a look at this genome.

▼ Genome Information Browser

Now I'm going to run a metabolic reconstruction on this genome. Let's see how the initial one comes out. This is the first time I've done this for this particular strain, so it will be interesting to see which roles are found.

Run Metabolic Reconstruction on E. coli F11 Genome

Started: 9/27/2012 4:15:32pm Finished: 9/27/2012 4.15:33pm

Escherichia coli F11 Metabolic Reconstruction

Source: calculated

Version: Mar 27, 2013 08:13:00 PST

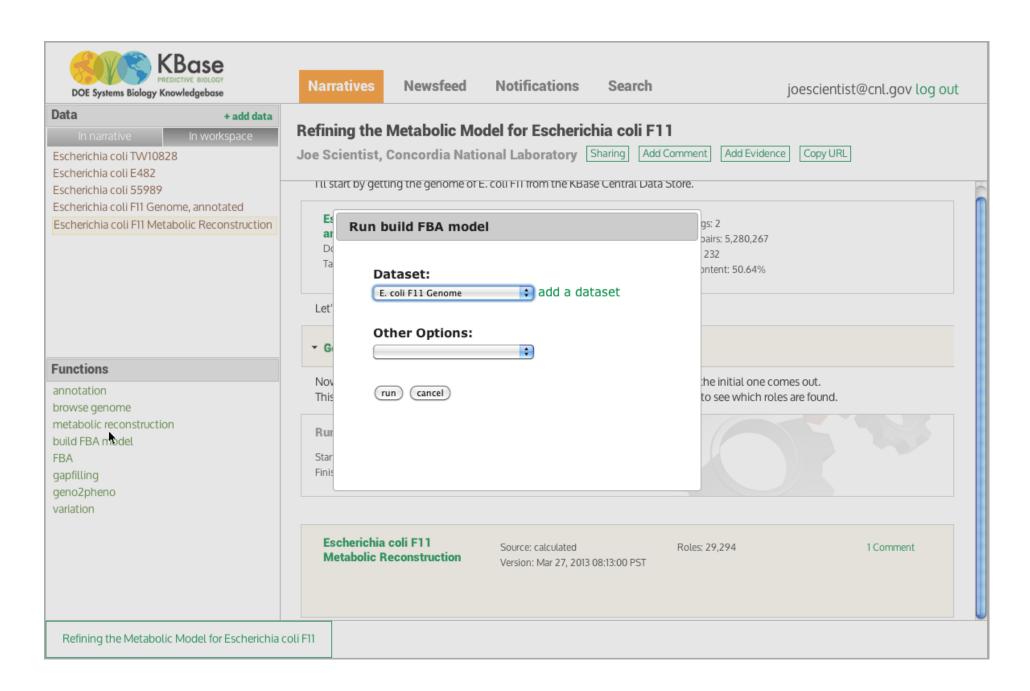
Roles: 29,294

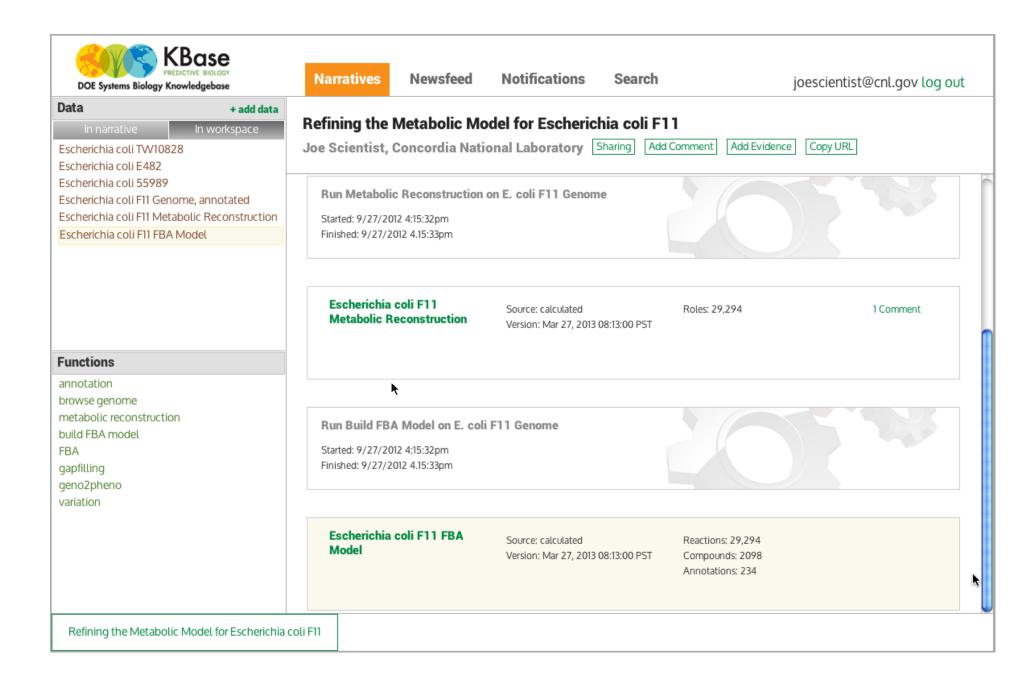
1 Comment

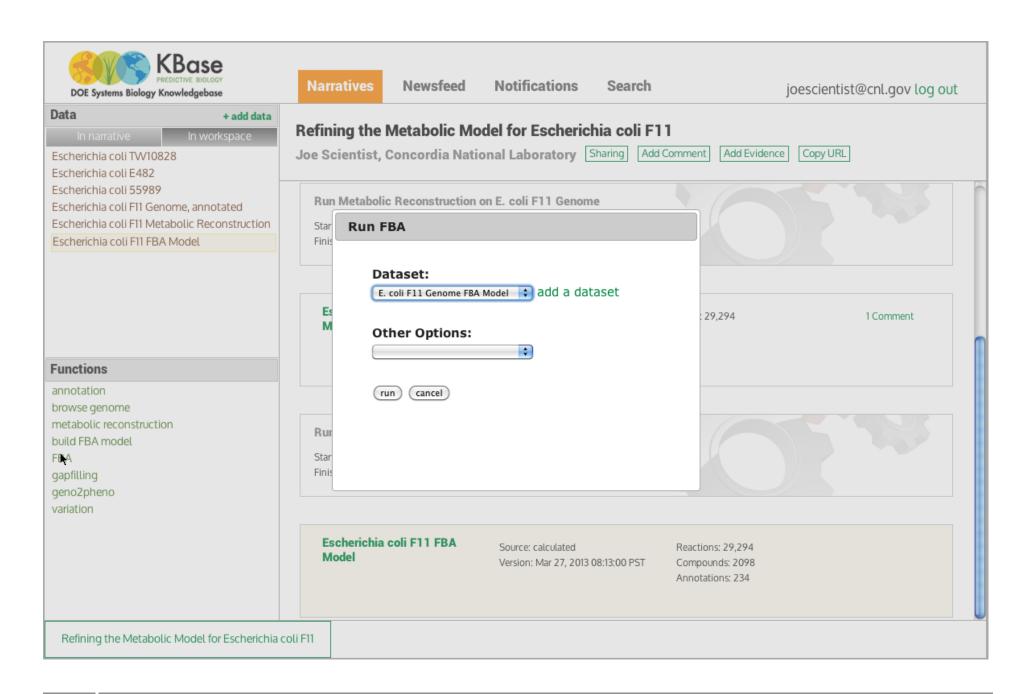
Add Comment

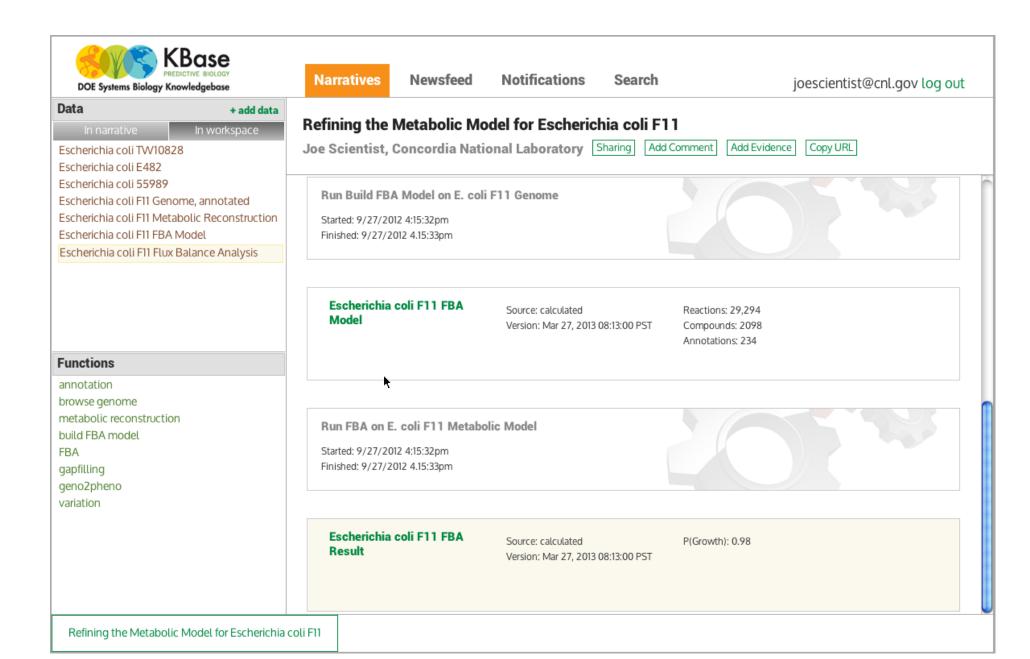
Add Evidence

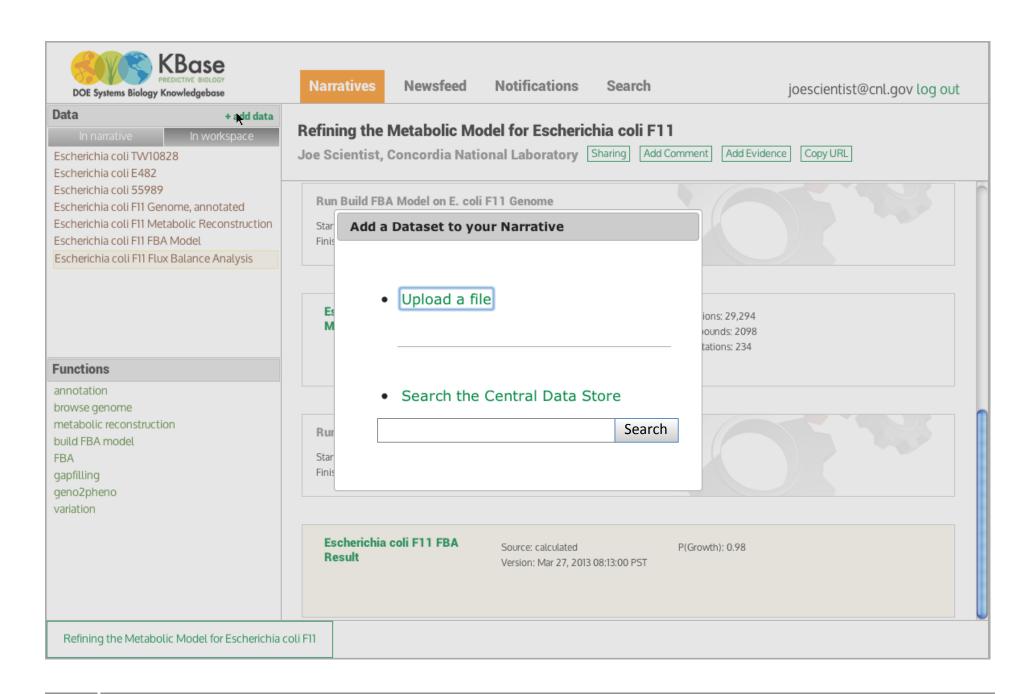
Copy URL

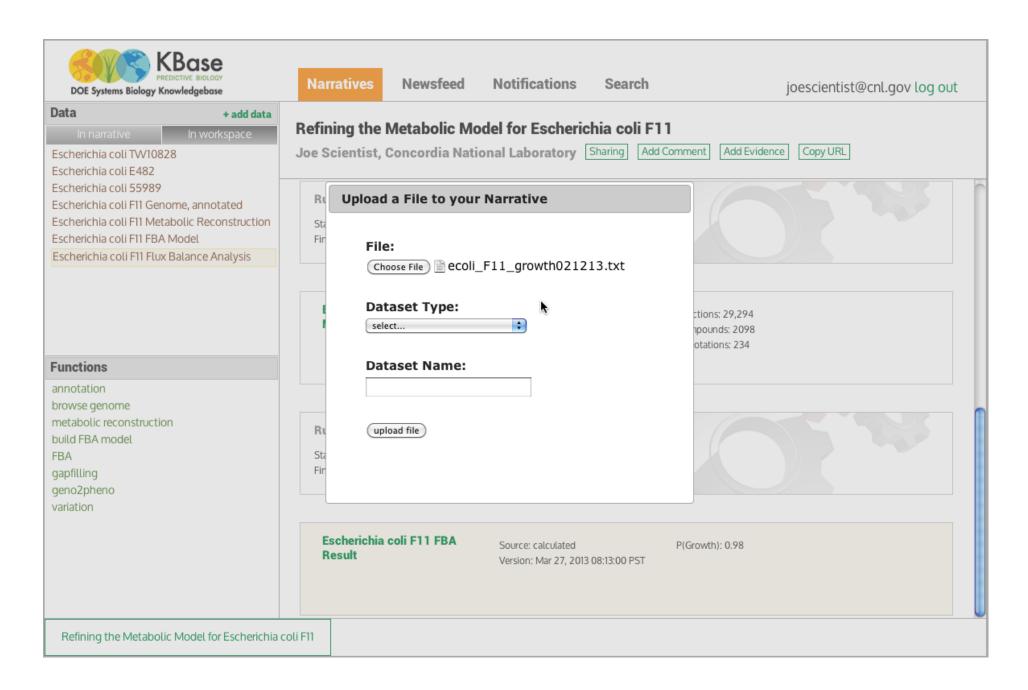


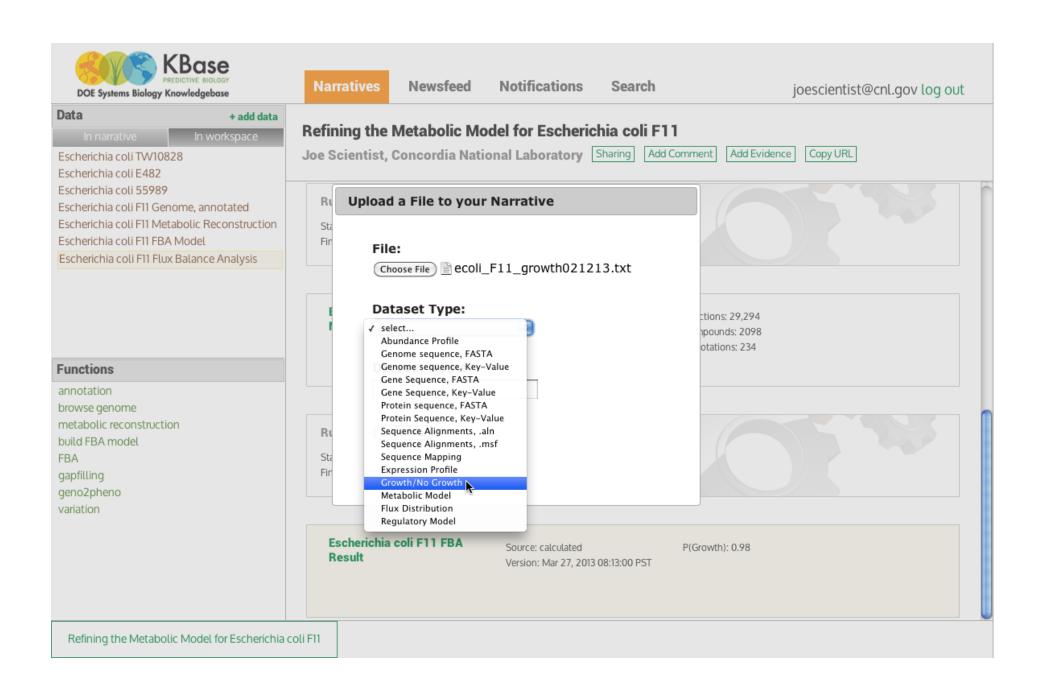


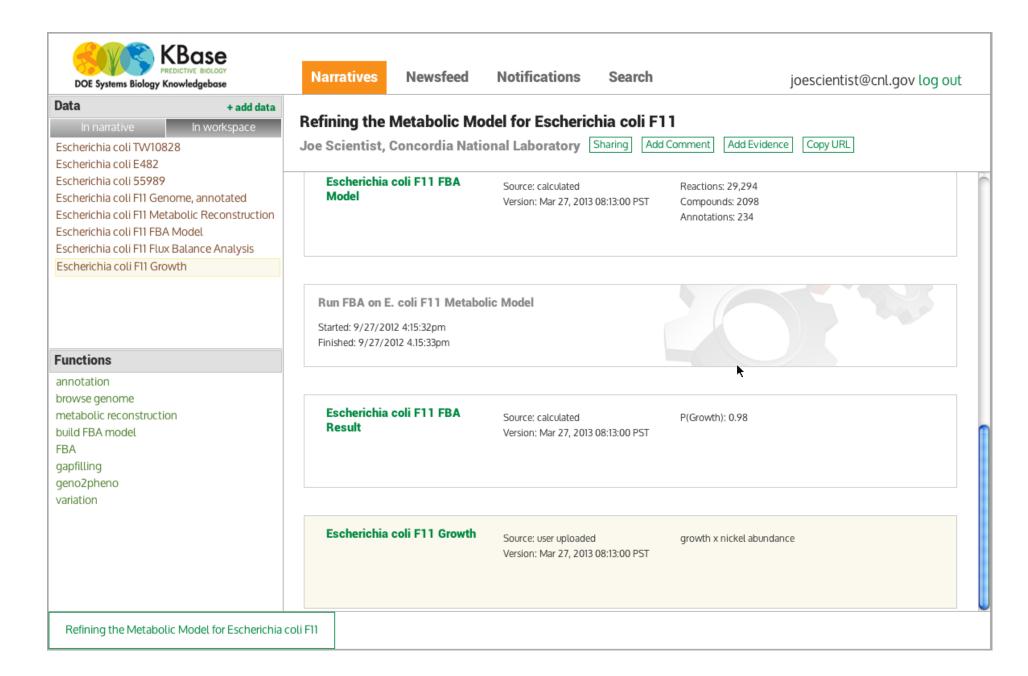


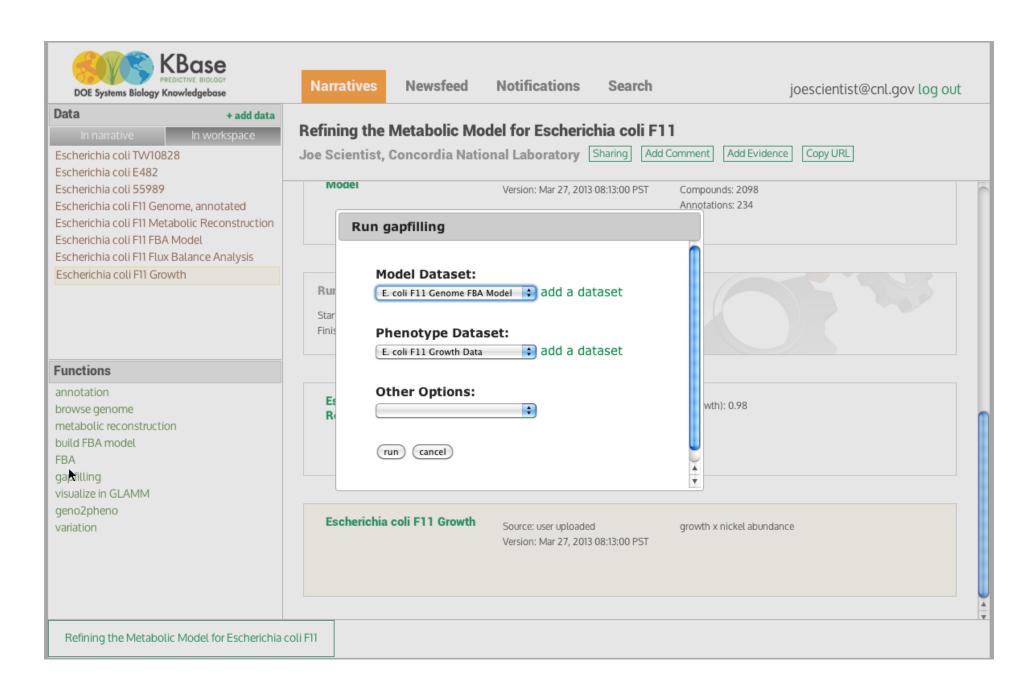


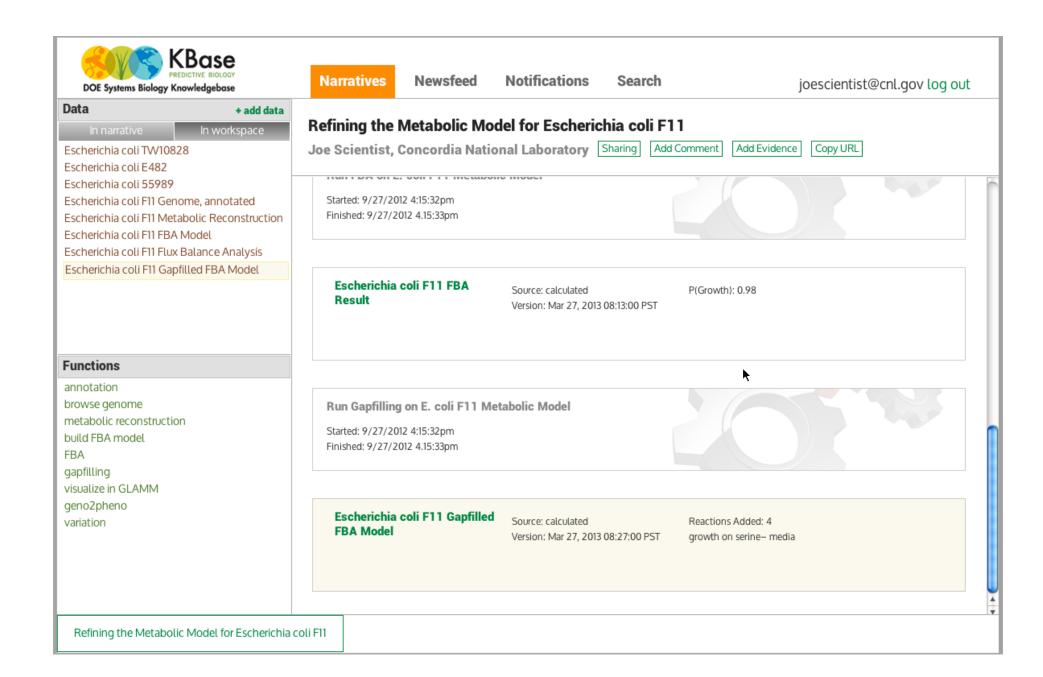














Data + a

+ add data

In narrative

In workspace

Escherichia coli TW10828

Escherichia coli E482

Escherichia coli 55989

Escherichia coli F11 Genome, annotated

Escherichia coli F11 Metabolic Reconstruction

Escherichia coli F11 FBA Model

Escherichia coli F11 Flux Balance Analysis

Escherichia coli F11 Growth

Escherichia coli F11 Gapfilled FBA Model

Functions

annotation

browse genome

metabolic reconstruction

build FBA model

FBA

gapfilling

visualize in GLAMM

geno2pheno

variation

Narratives

Newsfeed

Notifications

Search

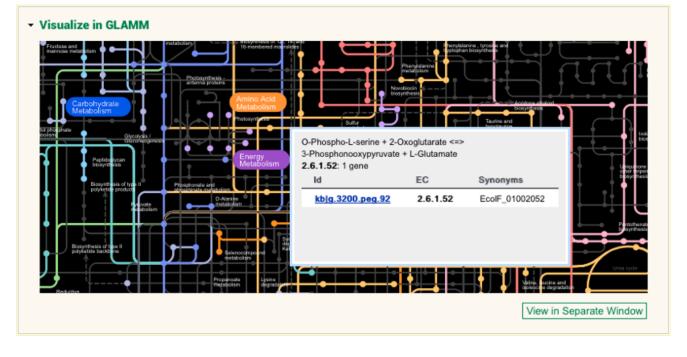
joescientist@cnl.gov log out

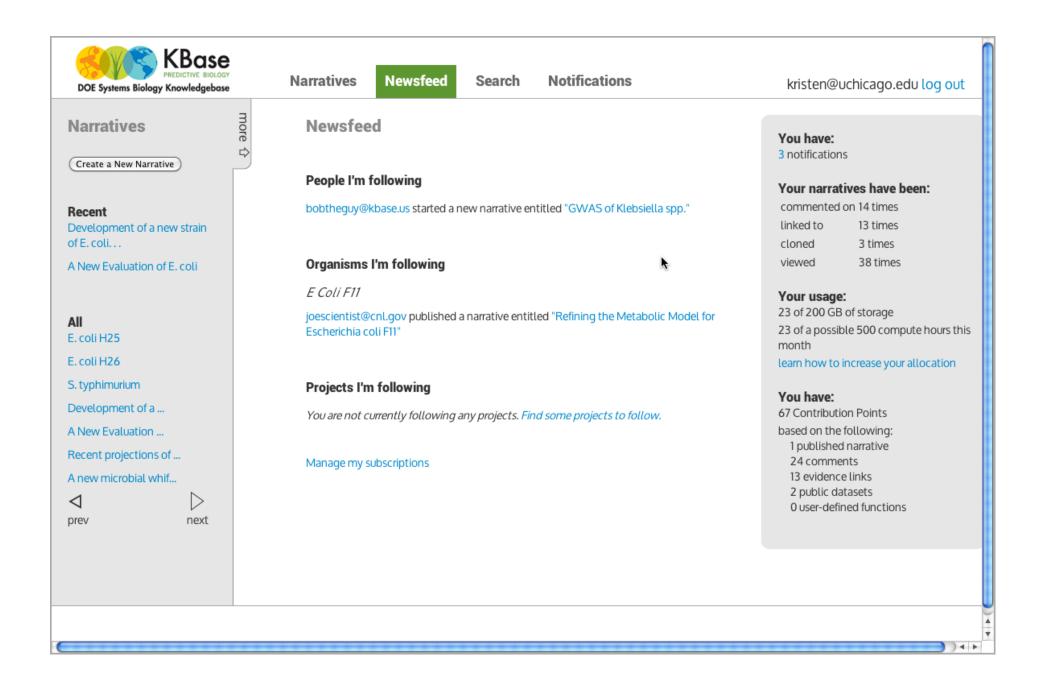
Refining the Metabolic Model for Escherichia coli F11

Joe Scientist, Concordia National Laboratory | Sharing | Add Comment | Add Evidence | Copy URL

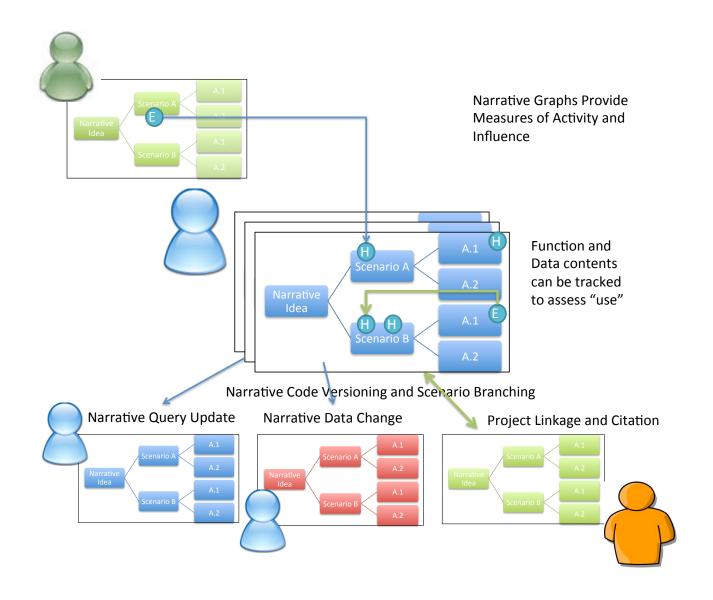
version; mar z7, z013 08;27;00 PST

growin on serine- media





Concept: Interactive community knowledge



Into the future

- The data model must evolve to support the modeling mission
- A framework for turning bioinformatics algorithms' output into models needs further development
- Theory for integrative, cross-scale predictive biology under development
- Much better ontologies for nearly everything
- Building the social tools.

- Need to improve data import, quality assessment and metadata
- Efficient incorporation of new third party algorithms and support with scalable compute.
- Growing a strong external development community while maintaining quality, stability and vision.
- Launching the KBase Foundation to ease licensing and growth of KBase user participation.

A more concrete view of the "Narrative" interface

Thanks to our Team and DOE!

Andrin Andrews	LDNII	Management
Arkin, Adam	LBNL	Management
Baumohl, Jason	LBNL	Microbes
Best, Aaron	Hope	Microbes
Bischof, Jared	ANL	Communities (Folker)
Bowen, Ben	LBNL	Microbes
Brenner, Steven	LBNL	Microbes
Brettin, Tom	ANL	Infrastructure
Canon, Shane	LBNL	Infrastructure
Chan, Stephen	LBNL	Infrastructure
Chandonia, John-Marc	LBNL	Microbes, Networks
Chivian, Dylan	LBNL	Communities
Cholia, Shreyas	LBNL	Infrastructure
Conrad, Neal	ANL	Infrastructure
Cottingham, Bob	ORNL	Management
Davison, Brian	ORNL	Outreach
Dehal, Paramvir	LBNL	Microbes
DeJongh, Matt	Hope	Microbes
Desai, Narayan	ANL	Infrastructure
Devoid, Scott	ANL	Infrastructure
Disz, Terry	ANL	Infrastructure
Drake, Meghan	ORNL	Outreach
Fang, Gang	Yale	Plants
Fei He	BNL	Plants
Frybarger, Paul	ANL	Microbes
Gerstein, Mark	Yale	Plants
Glass, Elizabeth Marland	ANL	Outreach
Gordon, India	ANL	Adminstration
Greiner, Annette	LBL/NERSC	Infrastructure
Gurtowski, James	CSHL	Plants
Harris, Nomi	LBNL	Management
Harrison, Travis	ANL	Communities
Henderson, Matt	LBNL	Communities
Henry, Chris	ANL	Microbes
Howe, Adina	ANL	Communities
Joachimiak, Marcin	LBNL	Microbes/Communities
Keegan, Kevin	ANL	Communities
Keller, Keith	LBNL	Microbes
Kora, Guru	ORNL	Infrastructure
Kumari, Sunita	CSHL	Plants
Land, Miriam	ORNL	Infrastructure
,		

Leuze, Michael	ORNL	Infrastructure
Lochosvky, Lucas	Yale	Plants
Maslov, Sergei	BNL	Management
Meyer, Folker	ANL	Communities
Moulton, Steve	ORNL	Microbes
Mulligan, Silvia (Palomino)	ANL	Administration
Novichkov, Pavel	LBNL	Infrastructure/Microbes
Oh, Taeyun	UC Davis	Plants
Olsen, Gary	UIUC	Microbes
Olson, Bob	ANL	Infrastructure
Olson, Dan	ANL	Infrastructure
Overbeek, Ross	ANL	Microbes
Paczian, Tobias	ANL	Communities
Palumbo, Tony	ORNL	Outreach
Parrello, Bruce	ANL	Infrastructure
Pasternak, Shiran	CSHL	Plants
Poon, Sarah	LBL/NERSC	Infrastructure
Price, Gavin	LBL	Microbes
Ranjan, Priya	ORNL	Plants
Riehl, Bill	LBNL	Microbes
Ronald, Pamela	UC Davis	Plants
Salazar, Jennifer Fessler	ANL	Outreach
Schatz, Michael	CSHL	Plants
Seaver, Sam	ANL	Plants
Sharma, Manoj	LBNL	Infrastructure
Sharma, Rita	LBNL	Infrastructure
Sneddon, Michael	LBNL	Communities
Stevens, Rick	ANL	Management
Syed, Mustafa	ORNL	Infrastructure
Terry, Gwyenth	LBNL	Adminstration
Thomason, James	CSHL	Plants
Tintle, Nathan	Hope	Microbes
Trimble, Will	ANL	Communities
Tuskan, Jerry	ORNL	Plants
Wang, Daifeng	Yale	Plants
Ware, Doreen	CSHL	Plants
Weston, David	ORNL	Plants
Whitney, Cary	LBNL	Infrastructure
Wilke, Andreas	ANL	Communities
Wilkening, Jared	ANL	Communities
Xia, Fangfang	ANL	Microbes
Yoo, Shinjae	BNL	Plants
Yu, Dantong	BNL	Plants
-,	-	



Thank you!

Visit us at kbase.science.energy.gov
Contact us at outreach@kbase.us

