Exploit your Data

Galaxy

and the

GMOD Tool Suite

AMATA

conference canberra 2011

http://galaxyproject.org http://gmod.org

Agenda

Introduction

Galaxy

Worked example
Deployment Options
Community

GMOD

Software
Community

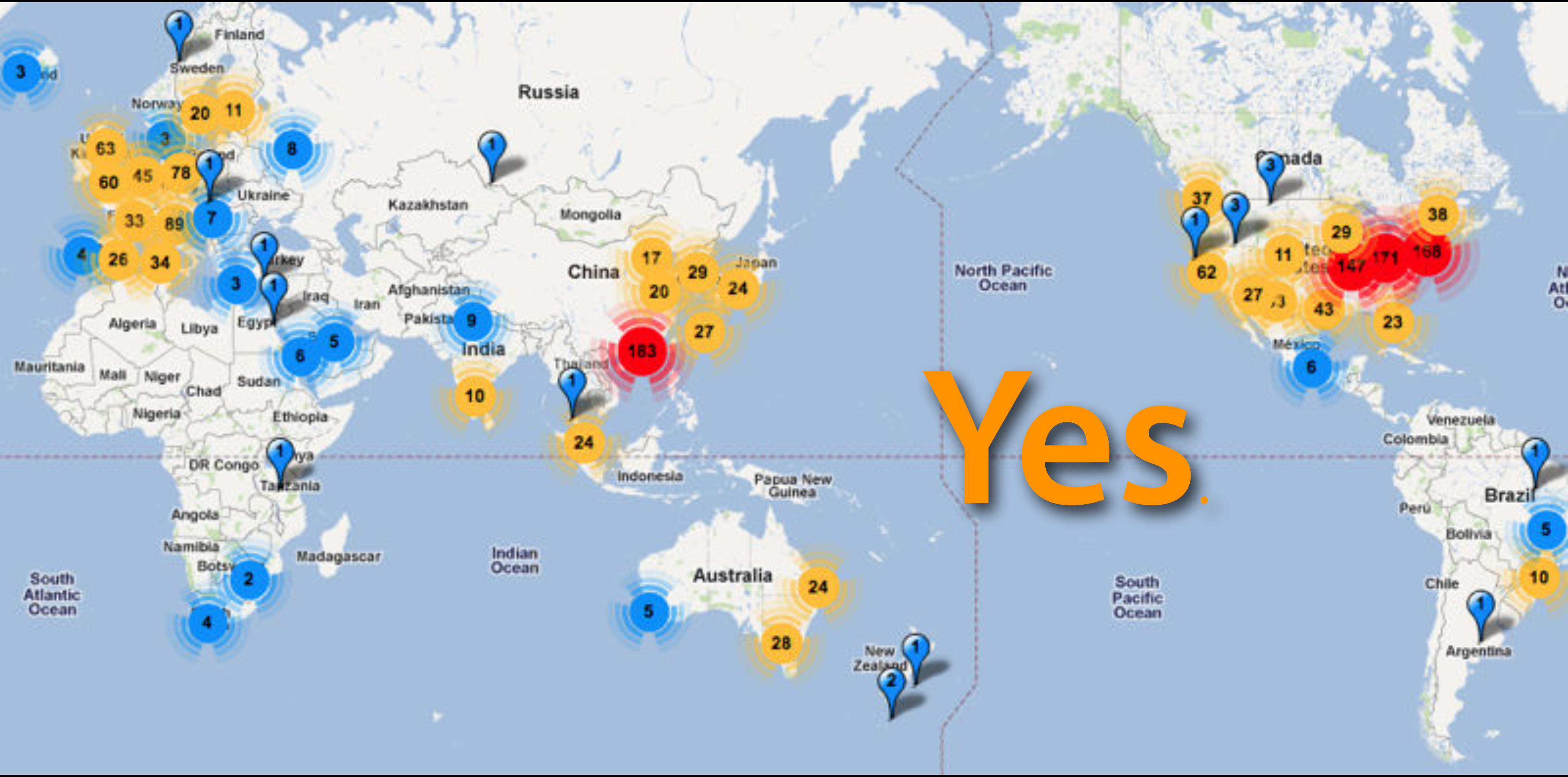
Goal for this workshop

Give you some idea what these **open source** tools **can do**, and how you might **use them** in your research.

This workshop will not cover
details of how the tools are implemented or new algorithm designs.

Are these tools timely?

Are these tools timely?



Yes.

Next Generation Genomics: World Map of High-throughput Sequencers
Nick Loman, James Hadfield

http://pathogenomics.bham.ac.uk/hts/

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Galaxy URLs to Remember

http://galaxyproject.org

http://usegalaxy.org

http://getgalaxy.org

http://usegalaxy.org/galaxy101

What is Galaxy?

- **A free (for everyone) web service** integrating a wealth of tools, compute resources, terabytes of reference data and permanent storage
- An **analysis and data integration** tool
- **Open source software** that makes integrating your own tools and data and customizing for your own site simple
- A part of **GMOD**

Galaxy aims to

Enable
accessible,
reproducible,
and
transparent
computational biomedical research.

Demo: Accessibility

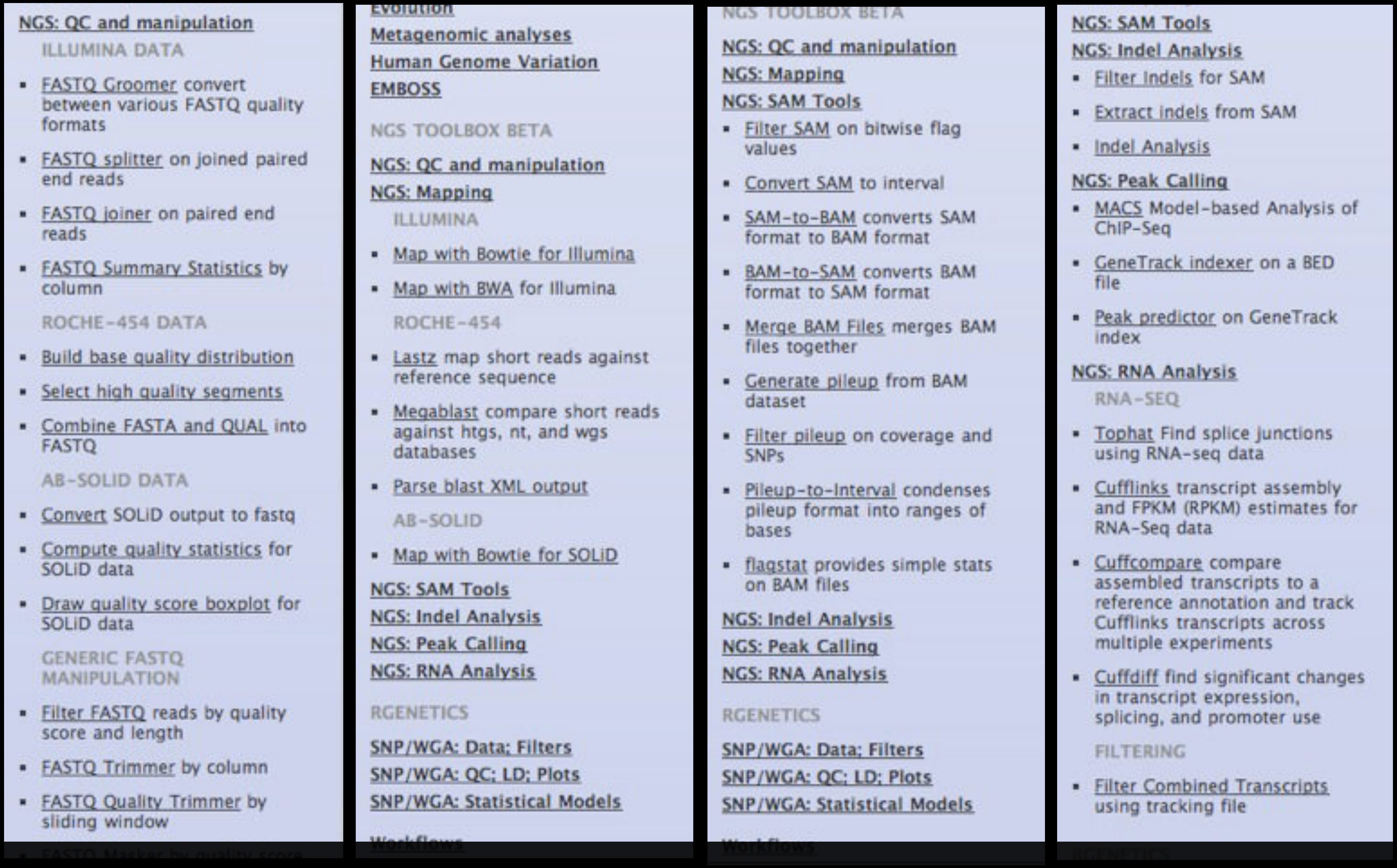
On human chromosome 22, which coding exons have the most known SNPs?

http://usegalaxy.org

Galaxy: A Rough Plan

- Get some data
  - Coding exons on chromosome 22
  - SNPs on chromosome 22
- Mess with it
  - Identify which exons have SNPs
  - Count number of SNPs in each of those exons.
  - Identify exons with most SNPs

http://usegalaxy.org/galaxy101



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computational biomedical research.

Demo: Reproducibility and Transparency

http://usegalaxy.org

Windshield splatter analysis with the Galaxy metagenomic pipeline — Genome Research

Windshield splatter analysis with the Galaxy metagenomic pipeline

Sergei Kosakovsky Pond[1,2,6,9], **Samir Wadhawan**[3,6,7], **Francesca Chiaromonte**[4], **Guruprasad Ananda**[1,3], **Wen-Yu Chung**[1,3,8], **James Taylor**[1,5,9], **Anton Nekrutenko**[1,3,9] and **The Galaxy Team**[1]

Author Affiliations

Abstract

How many species inhabit our immediate surroundings? A straightforward collection technique suitable for answering this question is known to anyone who has ever driven a car at highway speeds. The windshield of a moving vehicle is subjected to numerous insect strikes and can be used as a collection device for representative sampling. Unfortunately the analysis of biological material collected in that manner, as with most metagenomic studies, proves to be rather demanding due to the large number of required tools and considerable computational infrastructure. In this study, we use organic matter collected by a

Footnotes

[Supplemental material is available online at http://www.genome.org. All data and tools described in this manuscript can be downloaded or used directly at http://galaxyproject.org. Exact analyses and workflows used in this paper are available at http://usegalaxy.org/u/aun1/p/windshield-splatter.]

Article published online before print. Article and publication date are at http://www.genome.org/cgi/doi/10.1101/gr.094508.109.

OPEN ACCESS ARTICLE

This Article

Published in Advance October 9, 2009, doi: 10.1101/gr.094508.109

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- » Abstract ***Free***
- Full Text (PDF) ***Free***
- Supplemental Material
- All Versions of this Article:
  - gr.094508.109v1
  - 19/11/2144 ***most recent***

Current Issue

October 2010, 20 (10)

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Galaxy main site

http://usegalaxy.org

- Public web site, **anybody can use**
- Hundreds of tools
- **Persistent**
- ~500 new users per month, ~100 TB of user data, ~130,000 analysis jobs per month, every month is our busiest month ever...

But, it's a big world

Main has lots of tools, storage, processor, users, ...

- But **not all tools** - there are thousands and adding new tools is not taken lightly
- But **not infinite storage and processors** - main will continue to be maintained and enhanced, but with use limits and storage quotas

A centralized solution cannot scale to meet data analysis demands of the whole world

Scaling Galaxy

So much data:

- Encourage local Galaxy instances and Galaxy on the cloud. Support increasingly decentralized model and *improve access to existing resources*

So many tools and workflows:

- Focus on building infrastructure to allow community to integrate and share tools, workflows, and best practices

Local Galaxy Instances

http://getgalaxy.org

Galaxy is designed for local installation and customization

- Easily integrate new tools
- Easy to deploy and manage on nearly any (Unix) system
- ***Just download and run, completely self-contained!*** *

* Some assembly required.†

† But not much. ‡

‡ And help is on the way.

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http://getgalaxy.org

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Public Galaxy Servers

http://galaxyproject.org/PublicGalaxyServers

Interested in:

ChIP-chip and ChIP-seq?

- ✓ Cistrome

Statistical Analysis?

- ✓ Genomic Hyperbrowser

Sequence and tiling arrays?

- ✓ Oqtans

Text Mining?

- ✓ DBCLS Galaxy

Reasoning with ontologies?

- ✓ GO Galaxy

Internally symmetric protein structures?

- ✓ SymD

Scale up on existing resources

- Move intensive processing (tool execution) to other hosts
- Frees up the application server to serve requests and manage jobs
- Utilize existing resources
- Supports any batch scheduler that supports DRMAA (most of them)
- All levels of job running and scheduling are pluggable

CLUSTER RESOURCES™
TORQUE

GRID ENGINE

Platform Computing

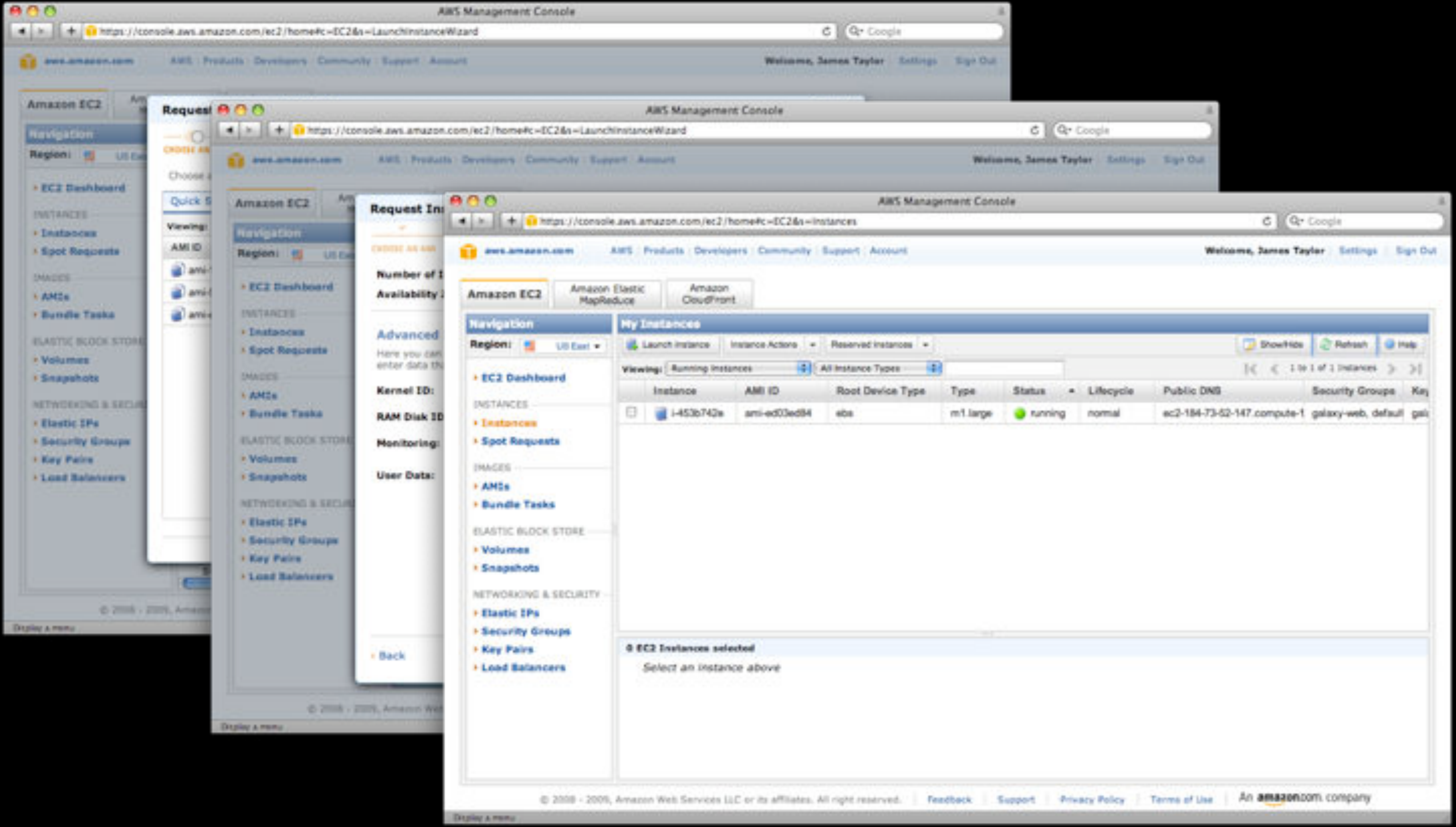
DRMAA
Distributed Resource Management Application API — www.drmaa.org

Galaxy Cloud

http://usegalaxy.org/cloud

- On-demand resource acquisition fits well with the irregular resource needs of many labs working with sequence data
- Our goal is to approach the ease of use of a “software as a service” solution while maintaining the flexibility and control of an infrastructure based solution

Using Amazon EC2: Startup in 3 steps



Viewing: Running Instances | All Instance Types

	Instance	AMI ID	Root Device Type	Type	Status	Lifecycle	Public DNS	Security Groups	Key
☐	i-453b742e	ami-ed03ed84	ebs	m1.large	● running	normal	ec2-184-73-52-147.compute-1	galaxy-web, default	gal

0 EC2 Instances selected

Select an instance above

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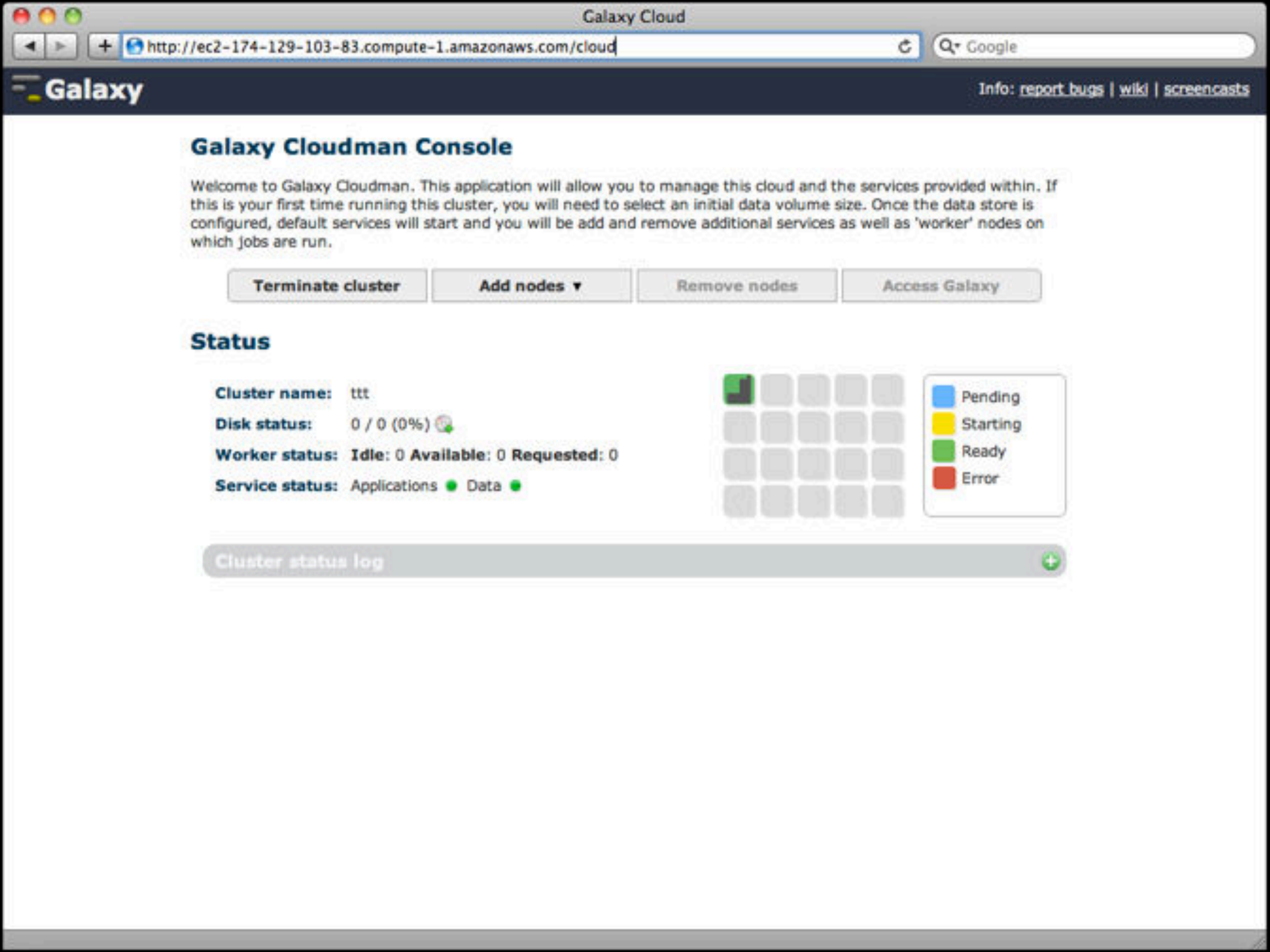


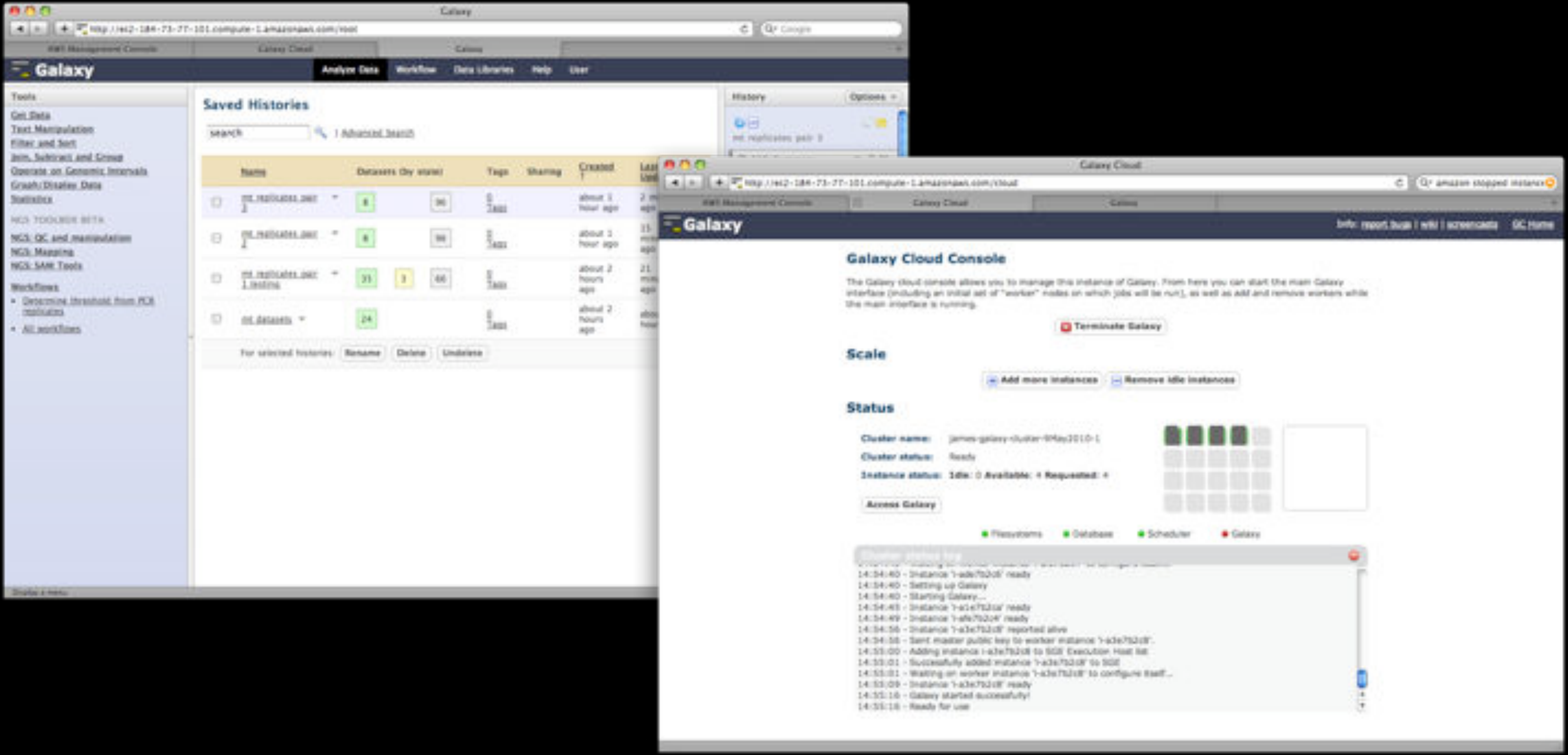
Galaxy Cloudman Console

Welcome to Galaxy Cloudman. This application will allow you to manage this cloud and the services provided within. If this is your first time running this cluster, you will need to select an initial data volume size. Once the data store is configured, default services will start and you will be add and remove additional services as well as 'worker' nodes on which jobs are run.

Status

Cluster name: ttt
Disk status: 0 / 0 (0%)
Worker status: **Idle:** 0 **Available:** 0 **Requested:** 0
Service status: Applications ● Data ●

🟦 Pending
🟨 Starting
🟩 Ready
🟥 Error



Can use like any other Galaxy instance, with additional compute nodes acquired and released (*automatically*) in response to usage

Tool installation and configuration, image creation, etc, all **completely automated and extensible**

Cloud instances include all tools available in main Galaxy *and more*

Same automation approach can be used for configuring tool dependencies for a local Galaxy

VM image with just tools available, currently at http://usegalaxy.org/vm

Why we love clouds and cloud-like things:

Reasonably cost effective and efficient
(elasticity + autoscaling definitely save money)

Analysis costs are more directly quantifiable

Infrastructure as an abstraction + standard APIs for provisioning reduces risk of vendor lock-in

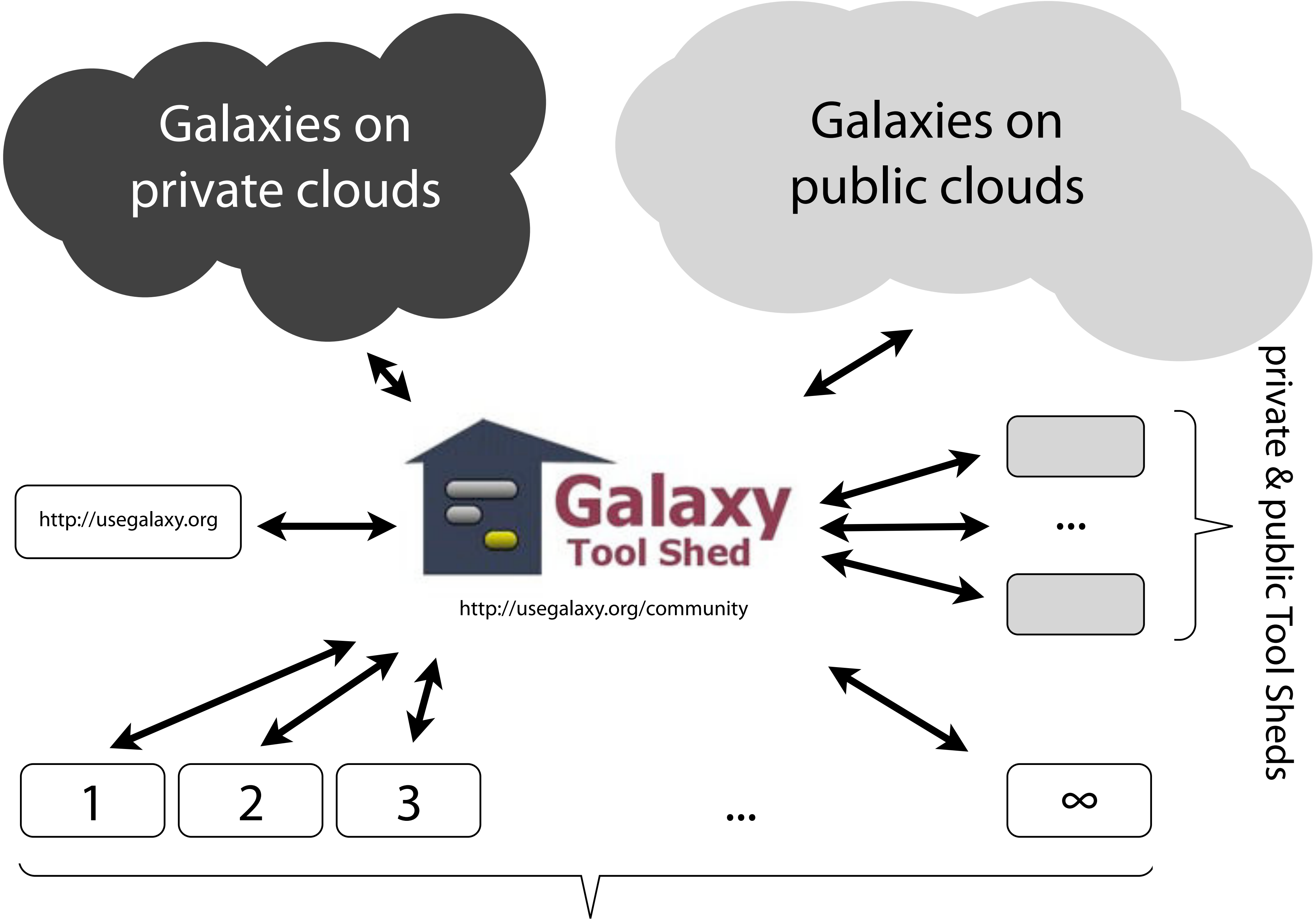
Virtualization makes *so* many things easier

Some future challenges

- Capturing and automatically deploying tool dependencies, automatic tool acquisition in Galaxy instances
- Better interfaces for highly parallel analysis (e.g. running the same workflow across 192 individuals)
- Various workflow engine improvements, partial data streaming, combined experimental/computational workflows

Galaxy Tool Shed vision

- Allow users to share “suites” containing tools, datatypes, workflows, sample data, and automated installation scripts for tool dependencies
- Integration with Galaxy instances to automate tool installation and updates



Galaxies on private clouds

Galaxies on public clouds

http://usegalaxy.org

Galaxy Tool Shed

http://usegalaxy.org/community

...

private & public Tool Sheds

1

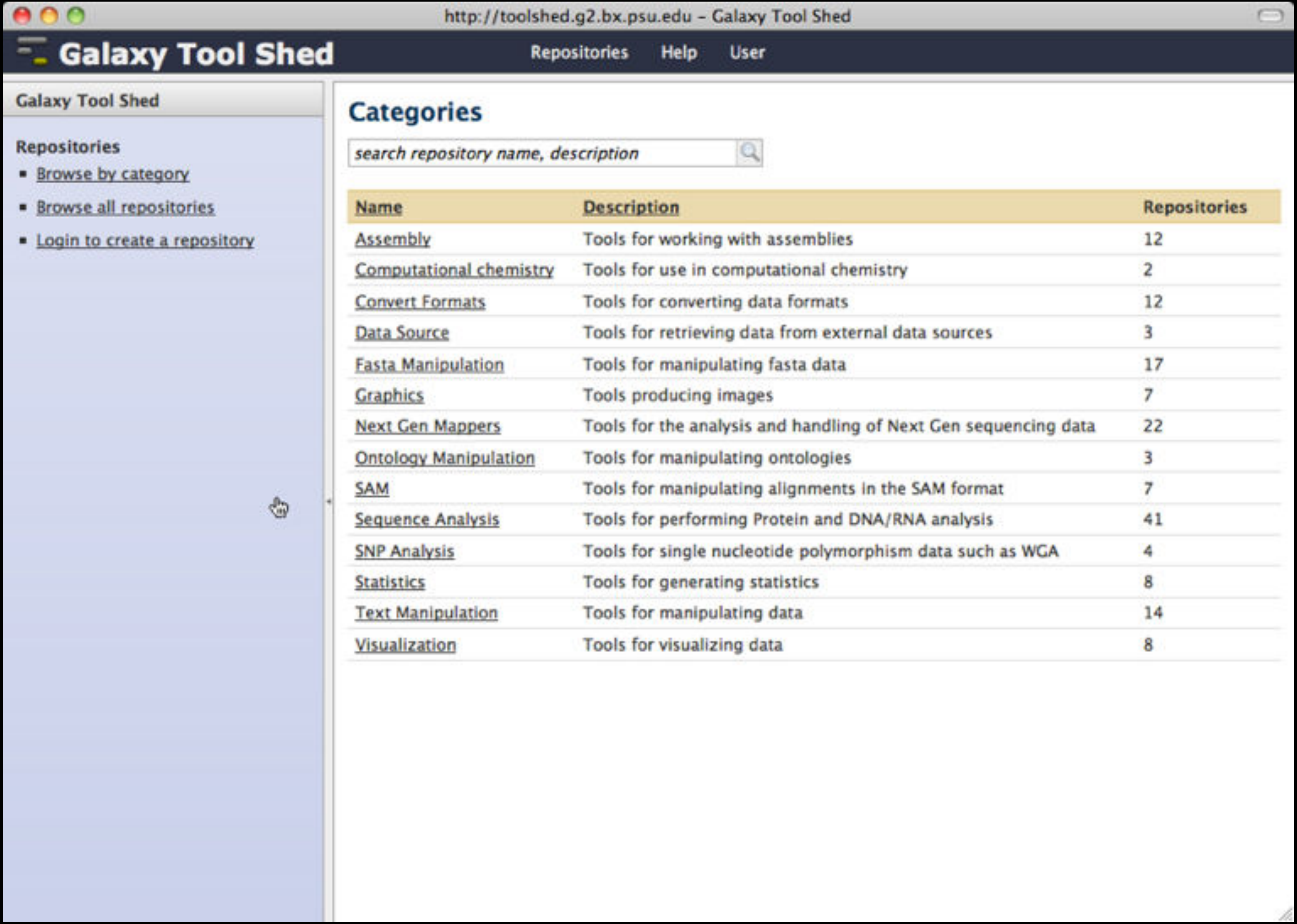
2

3

...

∞

public and private Galaxy installations

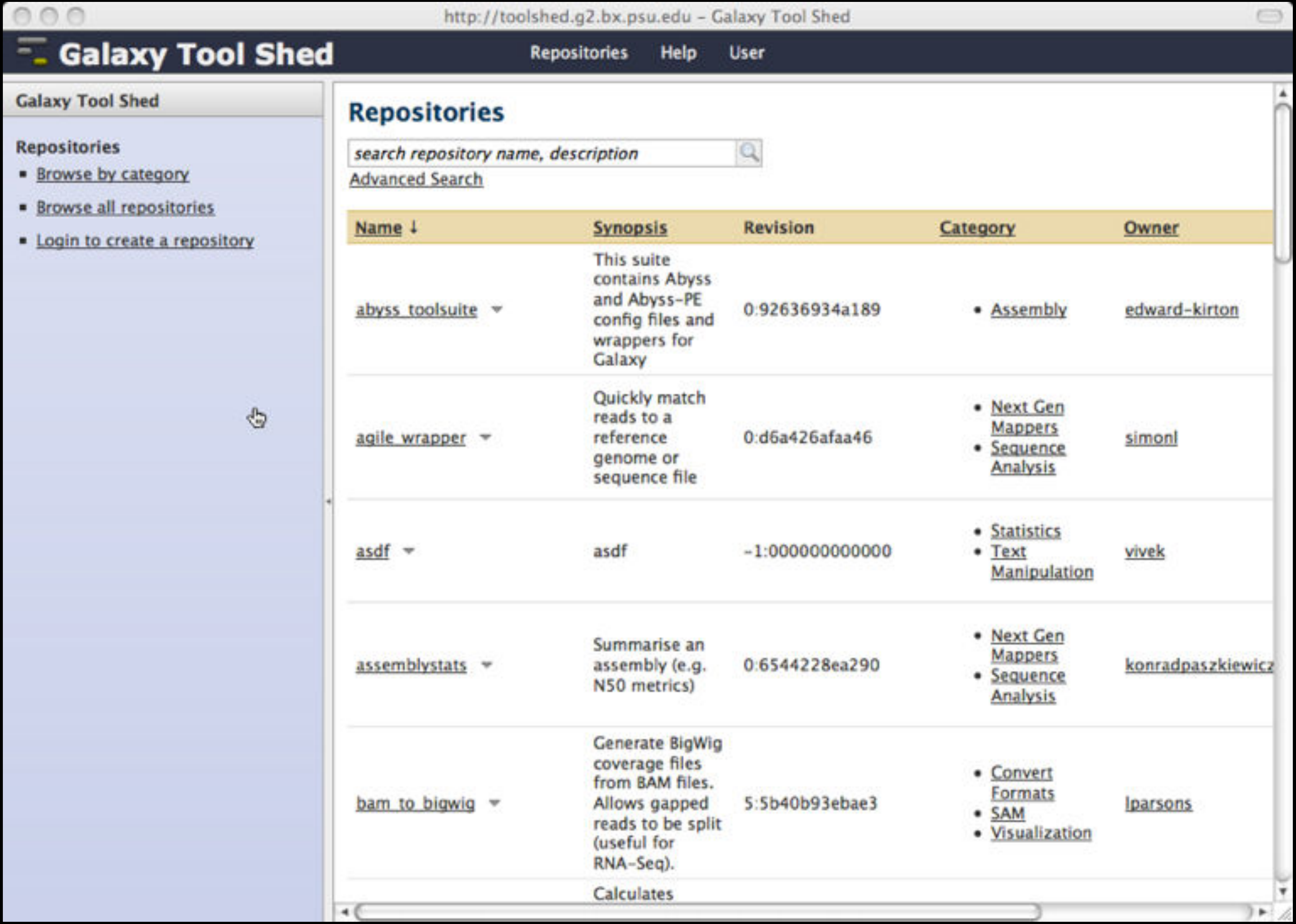


Repositories

- Browse by category
- Browse all repositories
- Login to create a repository

Categories

Name	Description	Repositories
Assembly	Tools for working with assemblies	12
Computational chemistry	Tools for use in computational chemistry	2
Convert Formats	Tools for converting data formats	12
Data Source	Tools for retrieving data from external data sources	3
Fasta Manipulation	Tools for manipulating fasta data	17
Graphics	Tools producing images	7
Next Gen Mappers	Tools for the analysis and handling of Next Gen sequencing data	22
Ontology Manipulation	Tools for manipulating ontologies	3
SAM	Tools for manipulating alignments in the SAM format	7
Sequence Analysis	Tools for performing Protein and DNA/RNA analysis	41
SNP Analysis	Tools for single nucleotide polymorphism data such as WGA	4
Statistics	Tools for generating statistics	8
Text Manipulation	Tools for manipulating data	14
Visualization	Tools for visualizing data	8



Repositories

search repository name, description

Advanced Search

Name ↓	Synopsis	Revision	Category	Owner
abyss_toolsuite	This suite contains Abyss and Abyss-PE config files and wrappers for Galaxy	0:92636934a189	- Assembly	edward-kirton
agile_wrapper	Quickly match reads to a reference genome or sequence file	0:d6a426afaa46	- Next Gen Mappers - Sequence Analysis	simonl
asdf	asdf	-1:000000000000	- Statistics - Text Manipulation	vivek
assemblystats	Summarise an assembly (e.g. N50 metrics)	0:6544228ea290	- Next Gen Mappers - Sequence Analysis	konradpaszkiewicz
bam_to_bigwig	Generate BigWig coverage files from BAM files. Allows gapped reads to be split (useful for RNA-Seq).	5:5b40b93ebae3	- Convert Formats - SAM - Visualization	lparsons
	Calculates			

Repository revision

2:bb1847435ec1 *repository tip*

Select a revision to inspect and download versions of tools from this repository.

clustalomega

Clone this repository:
hg clone http://toolshed.g2.bx.psu.edu/repos/clustalomega/clustalomega

Name:
clustalomega

Synopsis:
multiple sequence alignment program for proteins

Detailed description:
`Clustal Omega is a general purpose multiple sequence alignment program for proteins. It produces high quality alignments a`

Revision:
2:bb1847435ec1

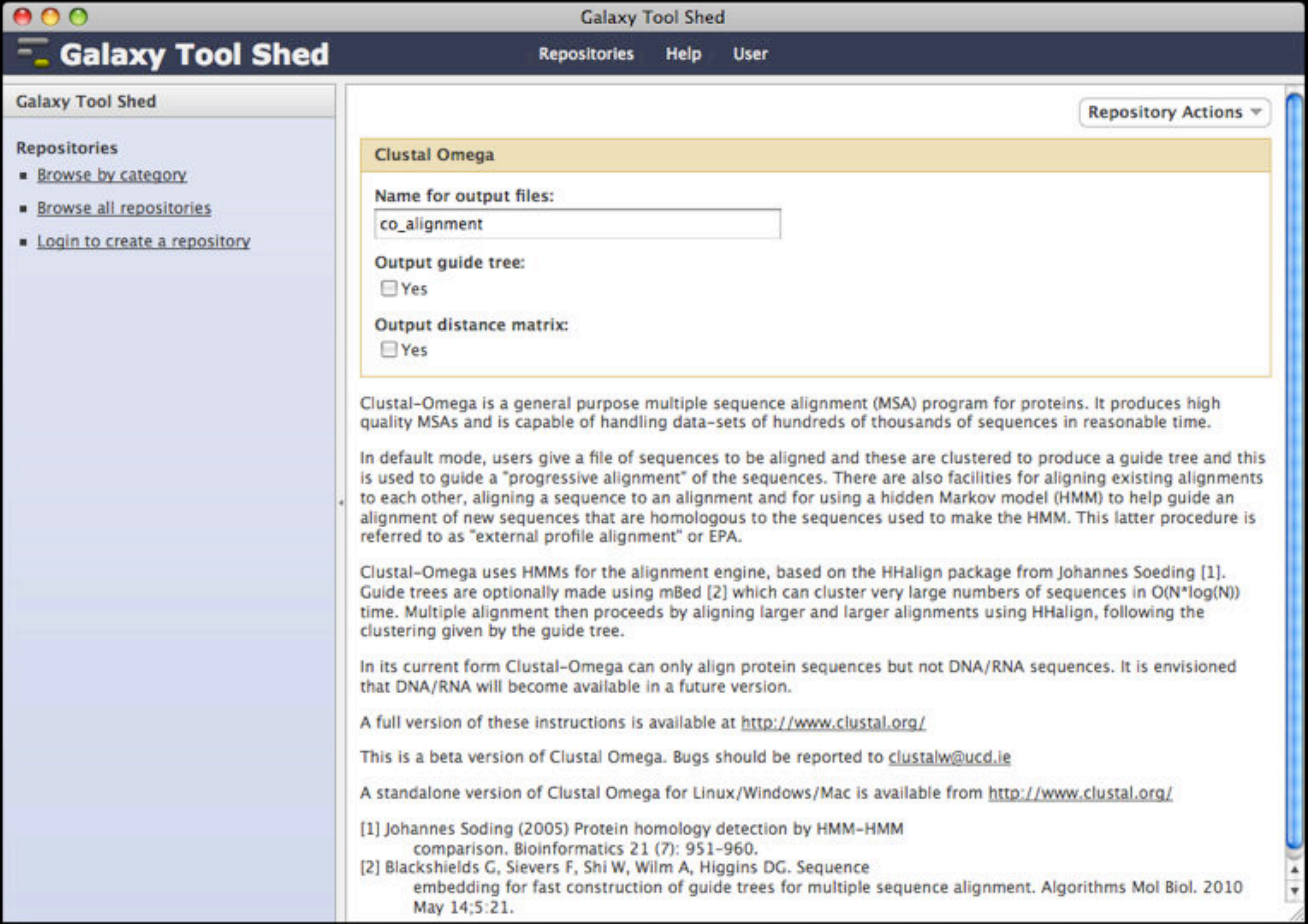
Owner:
clustalomega

Times downloaded:
39

Preview tools and inspect metadata by tool version

Tools - *click the name to preview the tool and use the pop-up menu to inspect all metadata*

name	description	version	requirements
Clustal Omega	multiple sequence alignment program for proteins	1.0.2	none



Clustal Omega

Name for output files: co_alignment

Output guide tree:
☐ Yes

Output distance matrix:
☐ Yes

Clustal-Omega is a general purpose multiple sequence alignment (MSA) program for proteins. It produces high quality MSAs and is capable of handling data-sets of hundreds of thousands of sequences in reasonable time.

In default mode, users give a file of sequences to be aligned and these are clustered to produce a guide tree and this is used to guide a "progressive alignment" of the sequences. There are also facilities for aligning existing alignments to each other, aligning a sequence to an alignment and for using a hidden Markov model (HMM) to help guide an alignment of new sequences that are homologous to the sequences used to make the HMM. This latter procedure is referred to as "external profile alignment" or EPA.

Clustal-Omega uses HMMs for the alignment engine, based on the HHalign package from Johannes Soeding [1]. Guide trees are optionally made using mBed [2] which can cluster very large numbers of sequences in O(N*log(N)) time. Multiple alignment then proceeds by aligning larger and larger alignments using HHalign, following the clustering given by the guide tree.

In its current form Clustal-Omega can only align protein sequences but not DNA/RNA sequences. It is envisioned that DNA/RNA will become available in a future version.

A full version of these instructions is available at http://www.clustal.org/

This is a beta version of Clustal Omega. Bugs should be reported to clustalw@ucd.ie

A standalone version of Clustal Omega for Linux/Windows/Mac is available from http://www.clustal.org/

[1] Johannes Soding (2005) Protein homology detection by HMM-HMM comparison. Bioinformatics 21 (7): 951-960.
[2] Blackshields G, Sievers F, Shi W, Wilm A, Higgins DG. Sequence embedding for fast construction of guide trees for multiple sequence alignment. Algorithms Mol Biol. 2010 May 14;5:21.

Galaxy Community

- Tool Shed
- Local Public Installs
- Mailing Lists (very active)
- Screencasts
- Events Calendar, News Feed
- Community Wiki
- Annual Community Meeting
  - Summer 2012 in Chicago

http://galaxyproject.org/wiki/Get%20Involved

Try it now:
http://UseGalaxy.org

Develop and deploy:
http://GetGalaxy.org

EMORY


Enis Afgan


Dannon Baker


Jeremy Goecks


Dave Clements

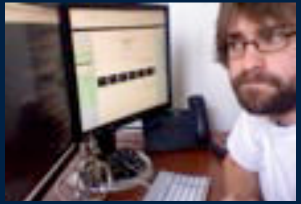

Kanwei Li


James Taylor

PENNSTATE


Guru Ananda


Dan Blankenberg


Nate Coraor


Jennifer Jackson


Greg von Kuster


Anton Nekrutenko

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http://GalaxyProject.org

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What is GMOD?

- A set of interoperable open-source **software components** for **visualizing, annotating, integrating and querying, and analyzing** biological data.
- An active **community of developers and users** asking diverse questions and facing common challenges with their biological data.

http://gmod.org

Who uses GMOD?

ParameciumDB

[[EcoliWiki]]

GeneDB

BIOCYC
Database Collection

BOVINEGENOME.ORG
THE BOVINE GENOME DATABASE

mod
ENCODE

Rice Genome Browser
Funded by the NSF

GDR

ConiferGDB

APHIDBASE

CSH

SmedGD

tair

TreeGenes
A Forest Tree Genome Database

SpBase
Strongylocentrotus purpuratus

WormBase

agresearch

SIDERE MENS EADEM MUTATO

CUGI
Clemson University Genomics Institute

CryptoDB.org
Cryptosporidium Genome Resources

Arthropod Genomics Center
Kansas State University

wFleaBase

THE CENTER FOR
GENOMICS AND
BIOINFORMATICS

dictyBase

FlyBase

MGI (MaizeGDB logo)

CGD

RGD

CSIRO

IRISA

MaizeGDB
Maize Genetics and Genomics Database

SGD

Lepido dB

CENTRE FOR
COMPARATIVE GENOMICS
Western Australia

mips
munich information center
for protein sequences

URGI

MGI

UNIVERSITY OF
CANBERRA

GRAMENE

ChromDB
The Chromatin Database

syngenta

Computational Biology
Research Group

VectorBase

Ontario Institute
for Cancer Research

Dow AgroSciences

RAP-DB

BioHealthBase
BioDefense & Public Health Database

AgBase

USDA ars

Plus hundreds, if not thousands, of others

GMOD Server Requirements

- GMOD is not a hosted solution
  - *Usually*
- Server
  - Most use Linux or other Unix variant
- GMOD System Administrator
  - Understands Linux package management, scripting, command line interfaces, relational databases, ...
  - Grad/Undergrad, half time when starting up

http://gmod.org/wiki/Computing_Requirements

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GMOD Software

Visualization

- **GBrowse** & **JBrowse** genomic browsers
- **CMap** & **GBrowse_syn** for comparative genomics

Annotation

- **MAKER** & **Apollo**

Data Integration and Querying

- **BioMart, InterMine, Chado**

Analysis

- **Galaxy, Ergatis, ISGA**

Visualization: GBrowse

- Visualize features, SNPs, quantitative data, NGS data (uses SAMtools)
- Semantic zooming
- Custom tracks, shared tracks, DAS
- Highly customisable by both admin and end-user

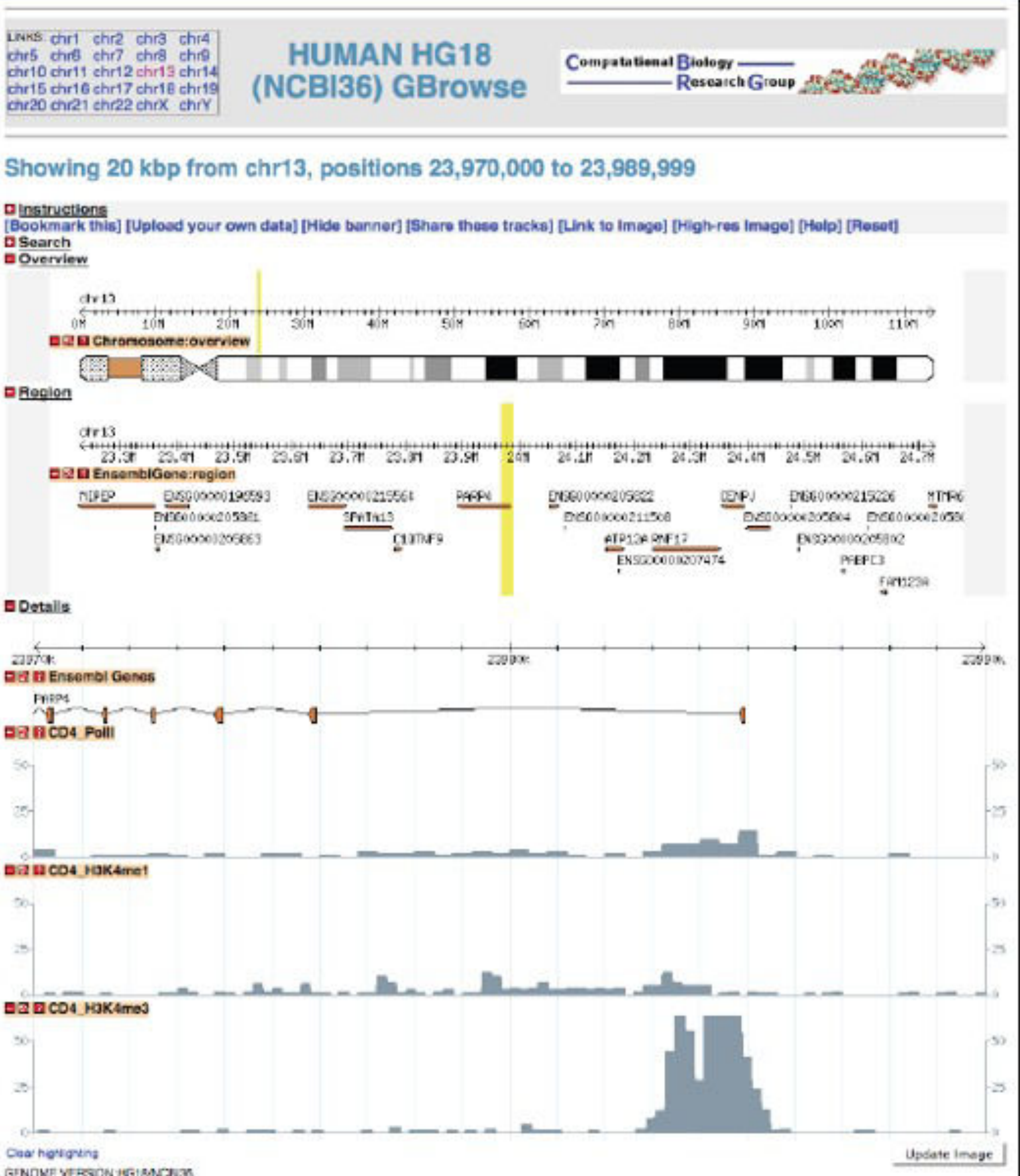
Stein, *et al.*, The Generic Genome Browser: A Building Block for a Model Organism System Database, *Genome Res.* 2002. 12: 1599-1610

GBrowse:

Genome Browser

ChIP-Seq data

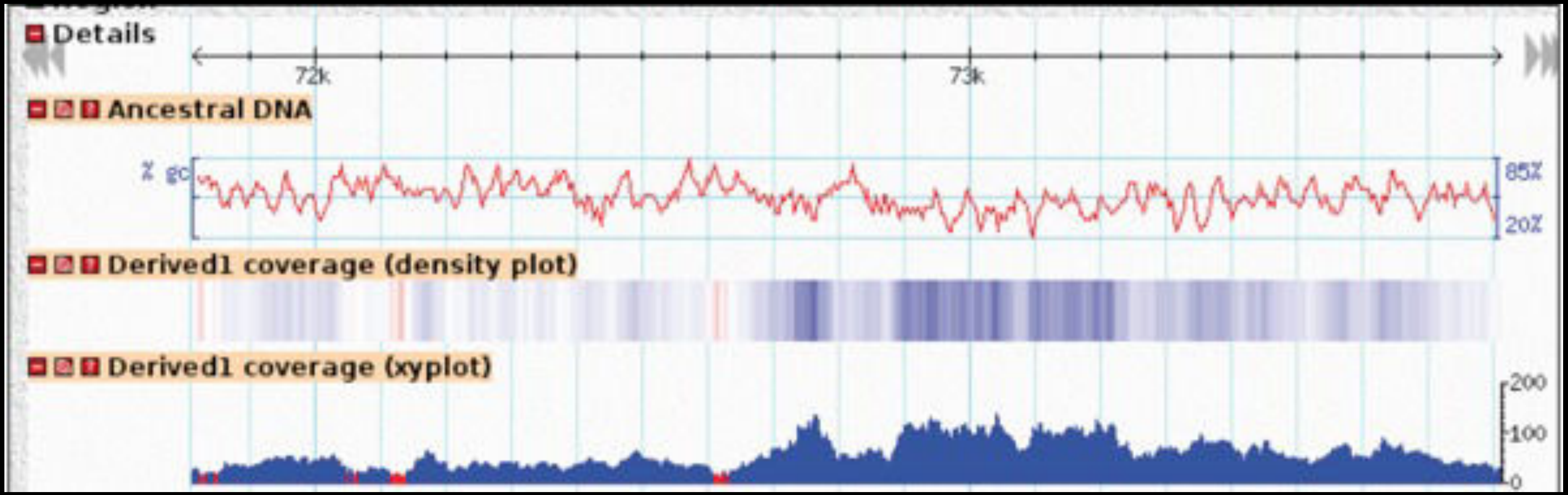
Visualization by Computational Biology Research Group @ Oxford.

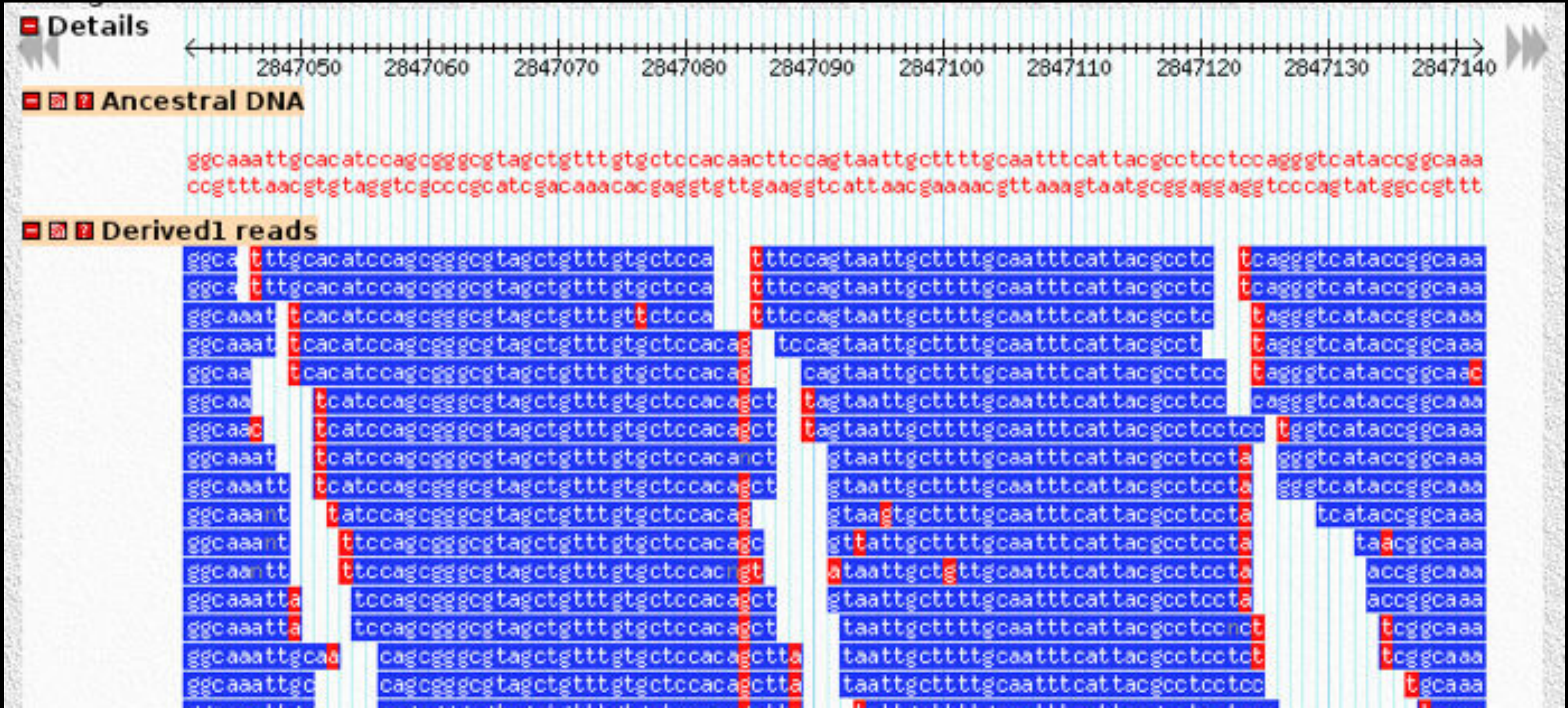


HUMAN HG18 (NCBI36) GBrowse

Showing 20 kbp from chr13, positions 23,970,000 to 23,989,999

GBrowse: Short Reads

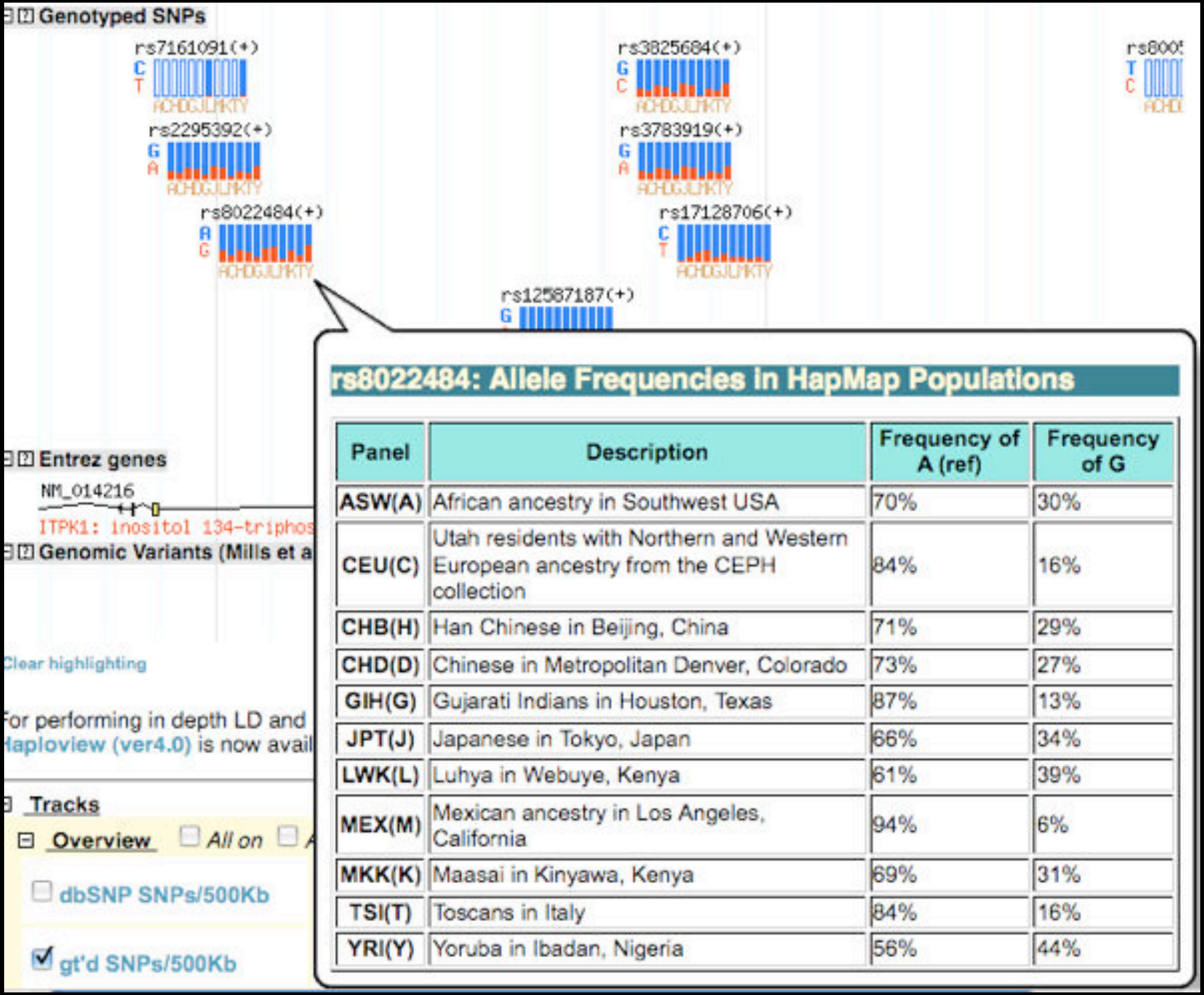




GBrowse

HapMap
Allele
Frequencies

hapmap.org

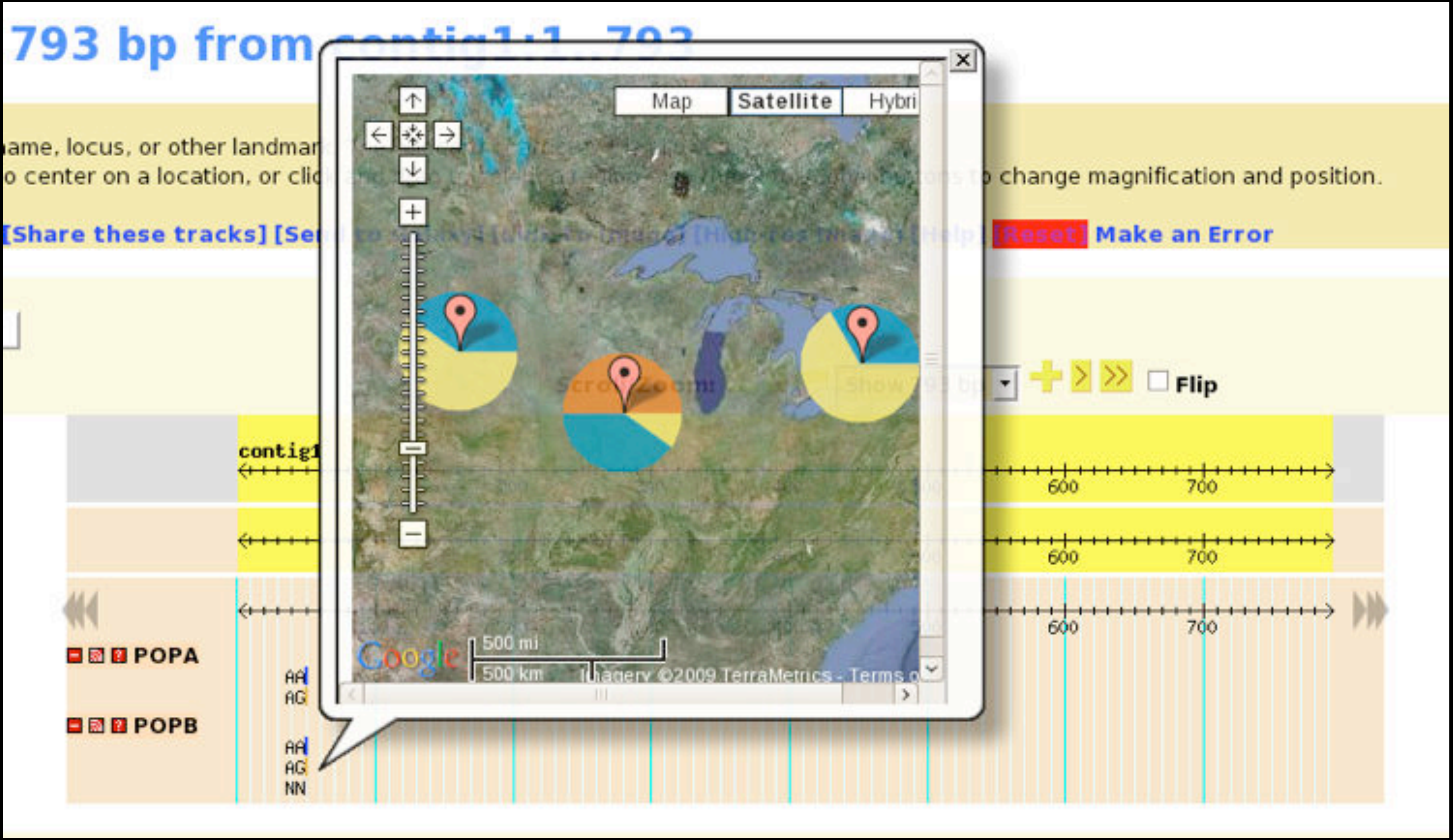


For performing in depth LD and
Haploview (ver4.0) is now avail

rs8022484: Allele Frequencies in HapMap Populations

Panel	Description	Frequency of A (ref)	Frequency of G
ASW(A)	African ancestry in Southwest USA	70%	30%
CEU(C)	Utah residents with Northern and Western European ancestry from the CEPH collection	84%	16%
CHB(H)	Han Chinese in Beijing, China	71%	29%
CHD(D)	Chinese in Metropolitan Denver, Colorado	73%	27%
GIH(G)	Gujarati Indians in Houston, Texas	87%	13%
JPT(J)	Japanese in Tokyo, Japan	66%	34%
LWK(L)	Luhya in Webuye, Kenya	61%	39%
MEX(M)	Mexican ancestry in Los Angeles, California	94%	6%
MKK(K)	Maasai in Kinyawa, Kenya	69%	31%
TSI(T)	Toscans in Italy	84%	16%
YRI(Y)	Yoruba in Ibadan, Nigeria	56%	44%

GBrowse



793 bp from contig1:1..793

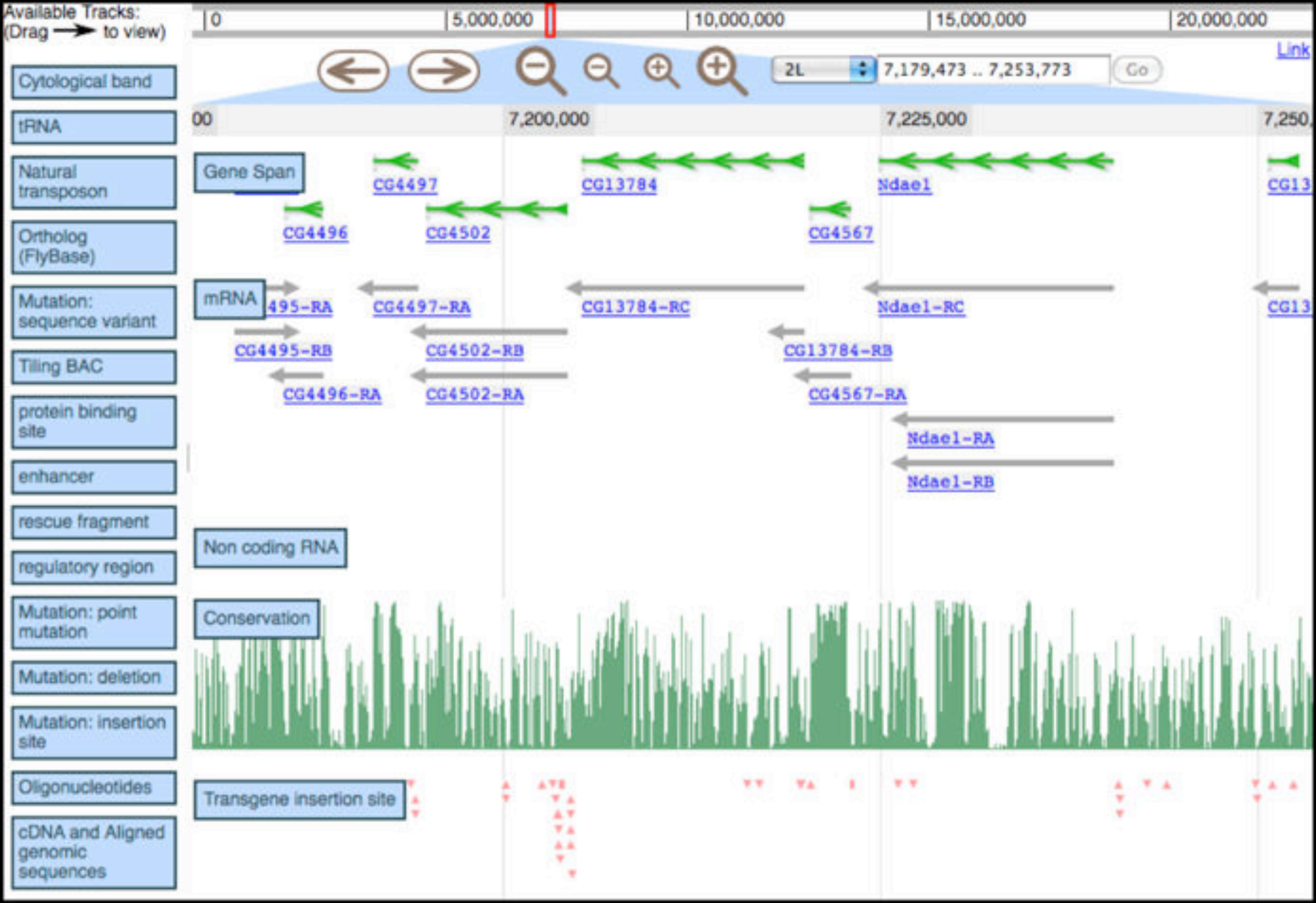
ame, locus, or other landmar

o center on a location, or clic

o change magnification and position.

Work by Yi-Hsin Erica Tsai & Ben Faga, using PhyloGeoViz

JBrowse



Skinner, *et al.*, JBrowse: A next-generation genome browser, *Genome Res*. 2009. 19: 1630-1638

GBrowse or JBrowse?

GBrowse

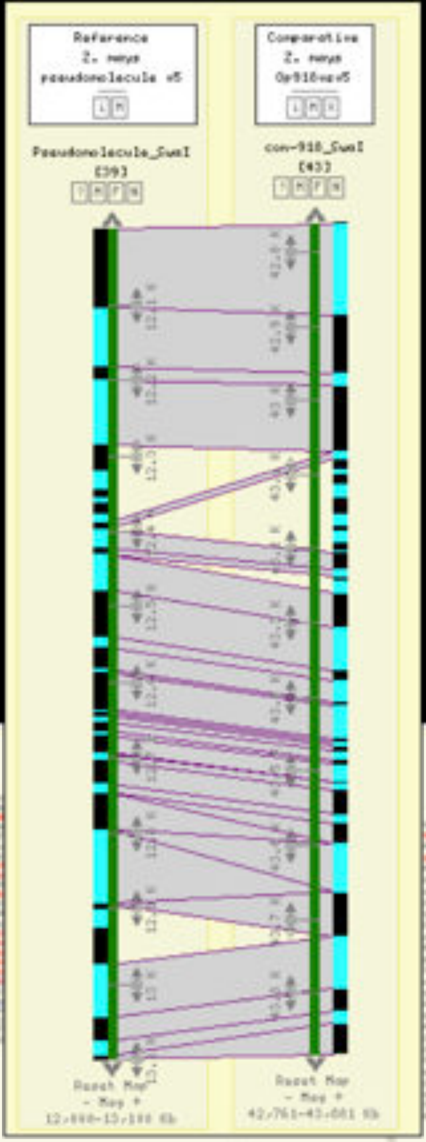
- Widely used
- Robust features & ecosystem
- Familiar interface
- Configuration is trail and error
- Requires more server
- Slower

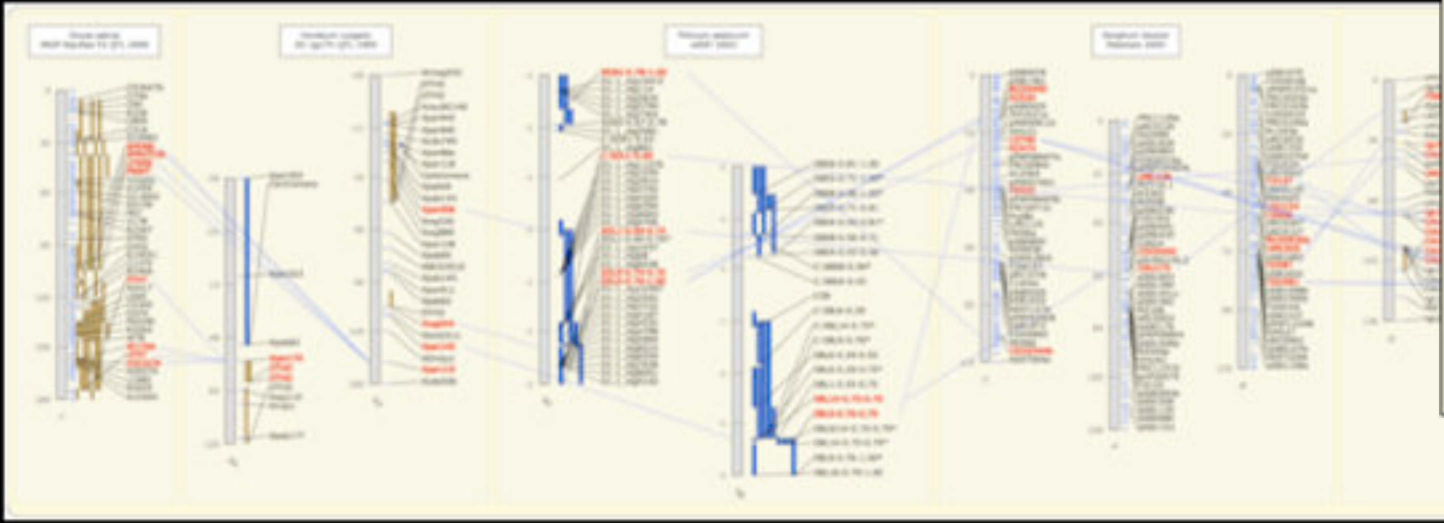
JBrowse

- Limited features
- Unfamiliar
- Lots of future development
- Configuration is simpler
- Requires less server
- Much Faster

CMap

- Comparative map viewer
- Data type agnostic. Can show linkage, physical, deletion, QTL, ...
- Anything that is points or regions on a line

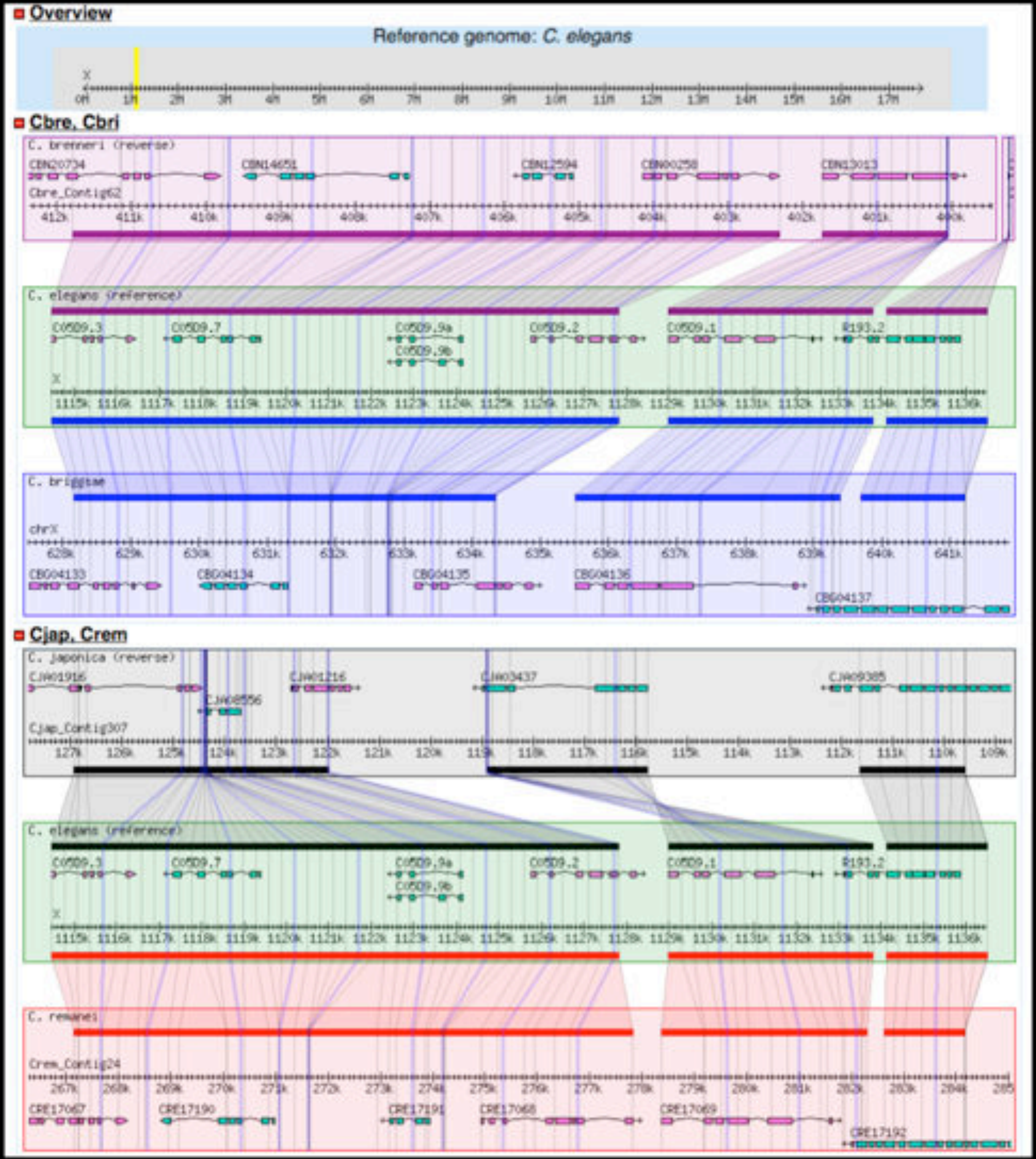




Youens-Clark, *et al.*, CMap 1.01: a comparative mapping application for the Internet, *Bioinformatics* (2009) 25 (22): 3040-3042.

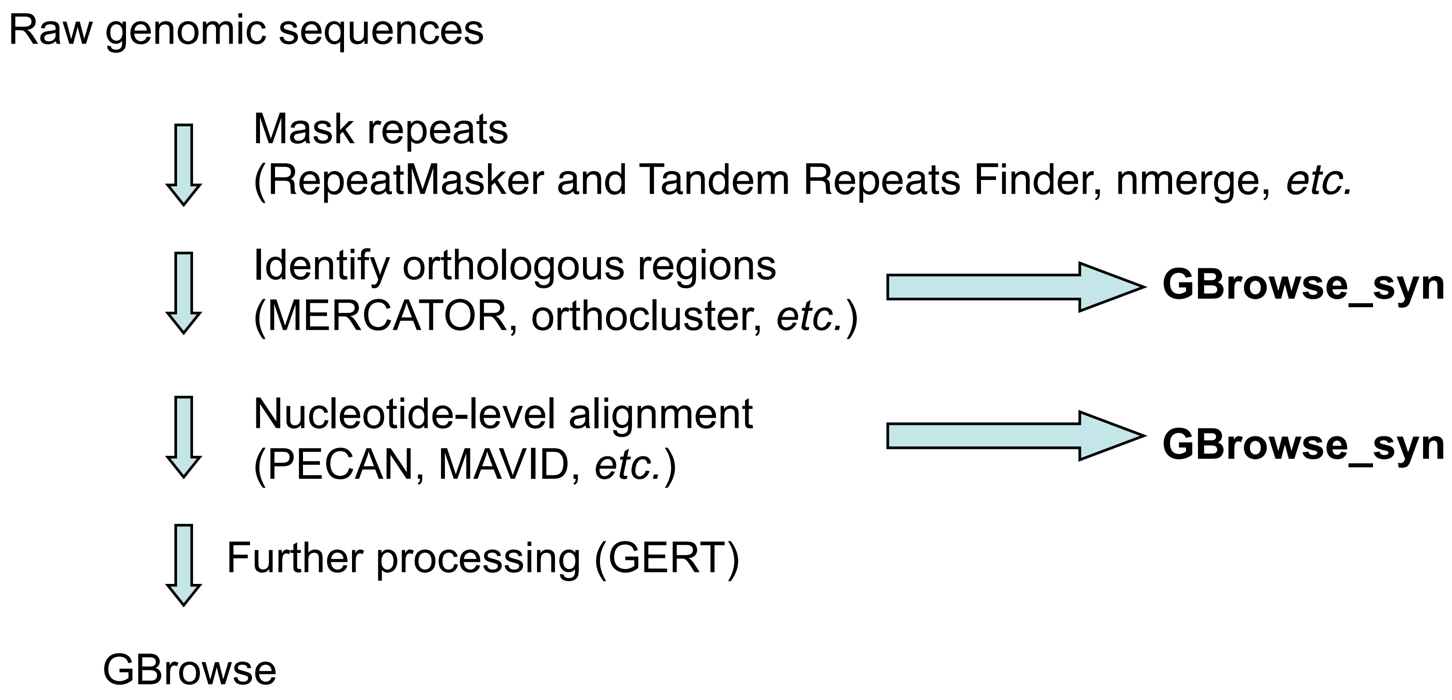
GBrowse_syn

- Comparative genomics browser
- Shows a "reference" compared to 1 or more others
- Built on GBrowse and can show any GBrowse-based annotations



McKay, *et al.*, Using the Generic Synteny Browser (GBrowse_syn), *Current Protocols in Bioinformatics*, Unit 9.12, September 2010

GBrowse_syn: Big Picture



Raw genomic sequences

Mask repeats
(RepeatMasker and Tandem Repeats Finder, nmerge, *etc.*

Identify orthologous regions
(MERCATOR, orthocluster, *etc.*)

GBrowse_syn

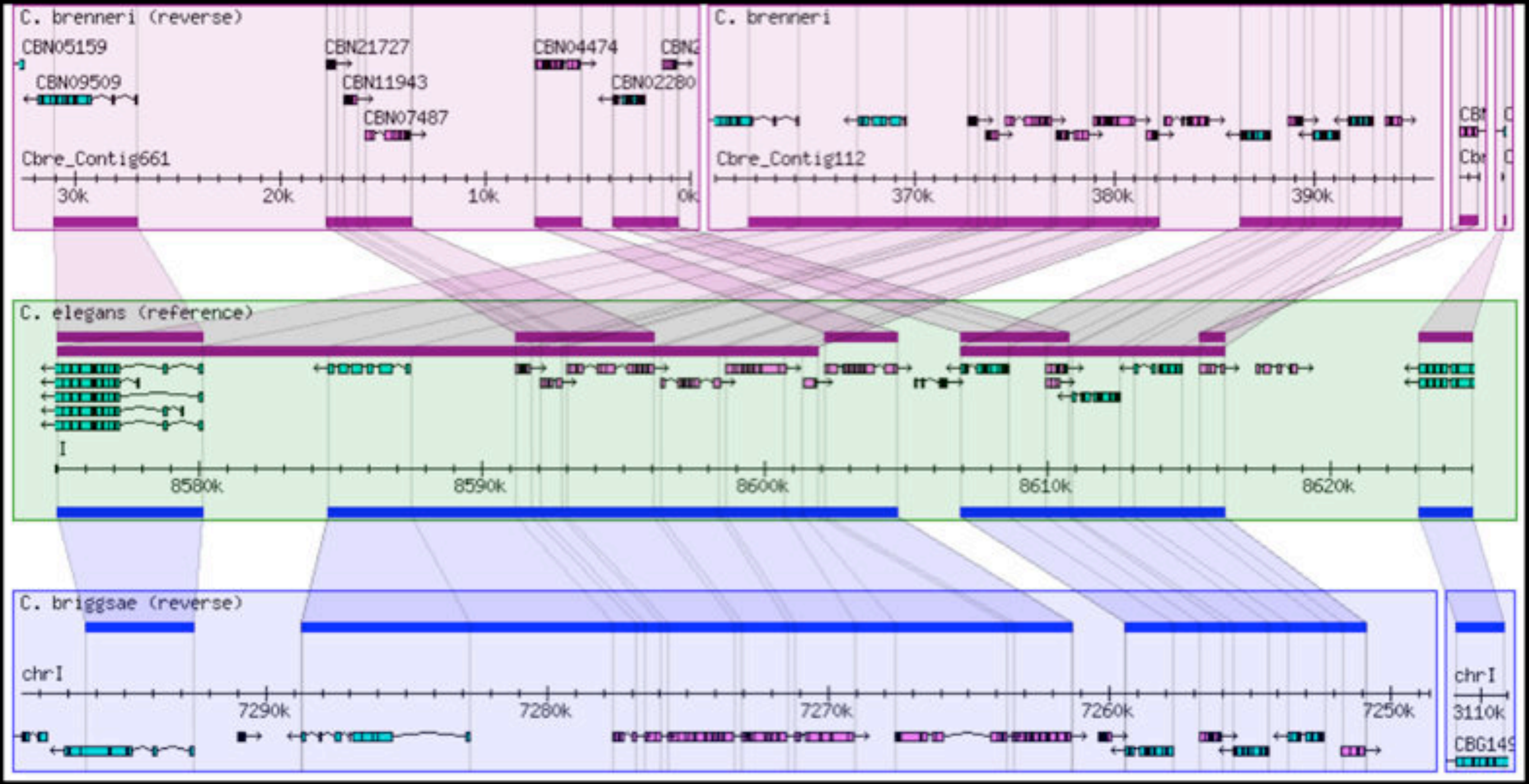
Nucleotide-level alignment
(PECAN, MAVID, *etc.*)

GBrowse_syn

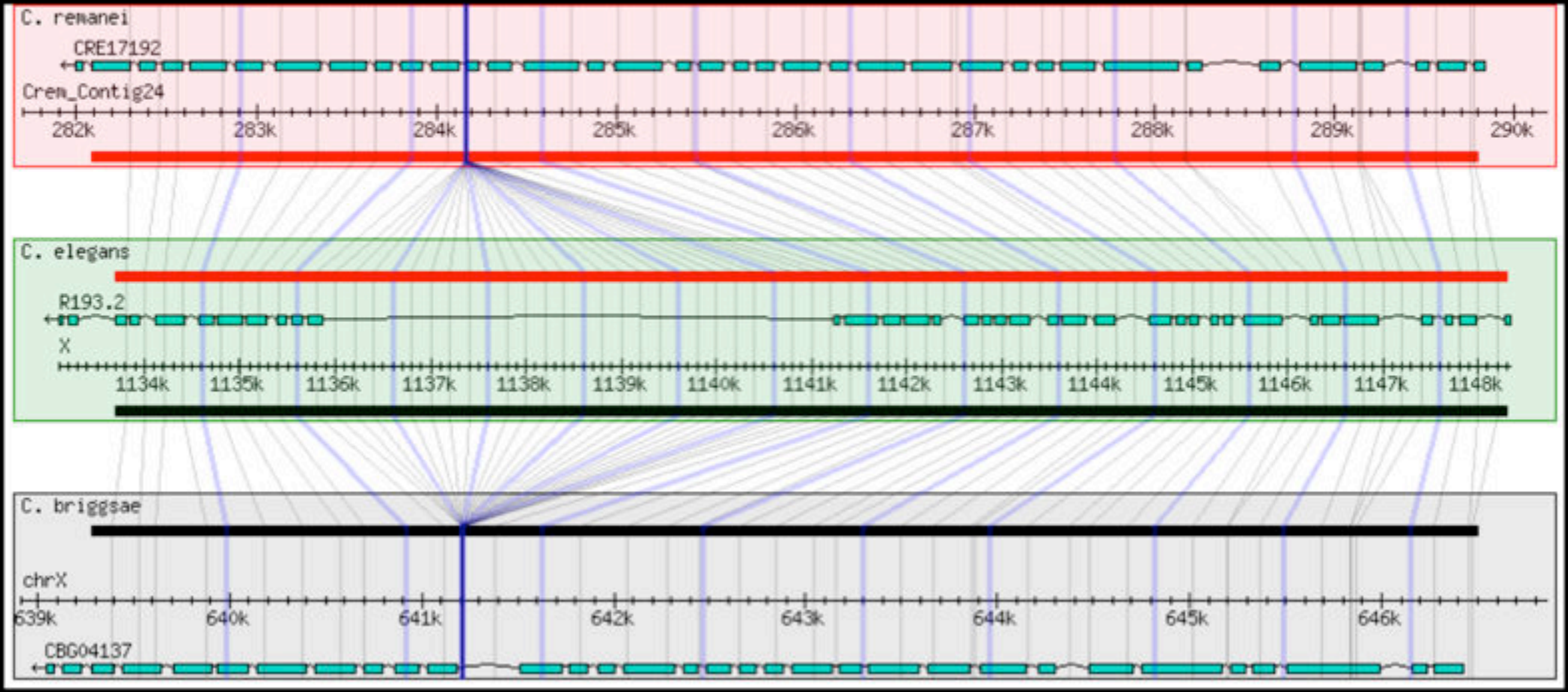
Further processing (GERT)

GBrowse

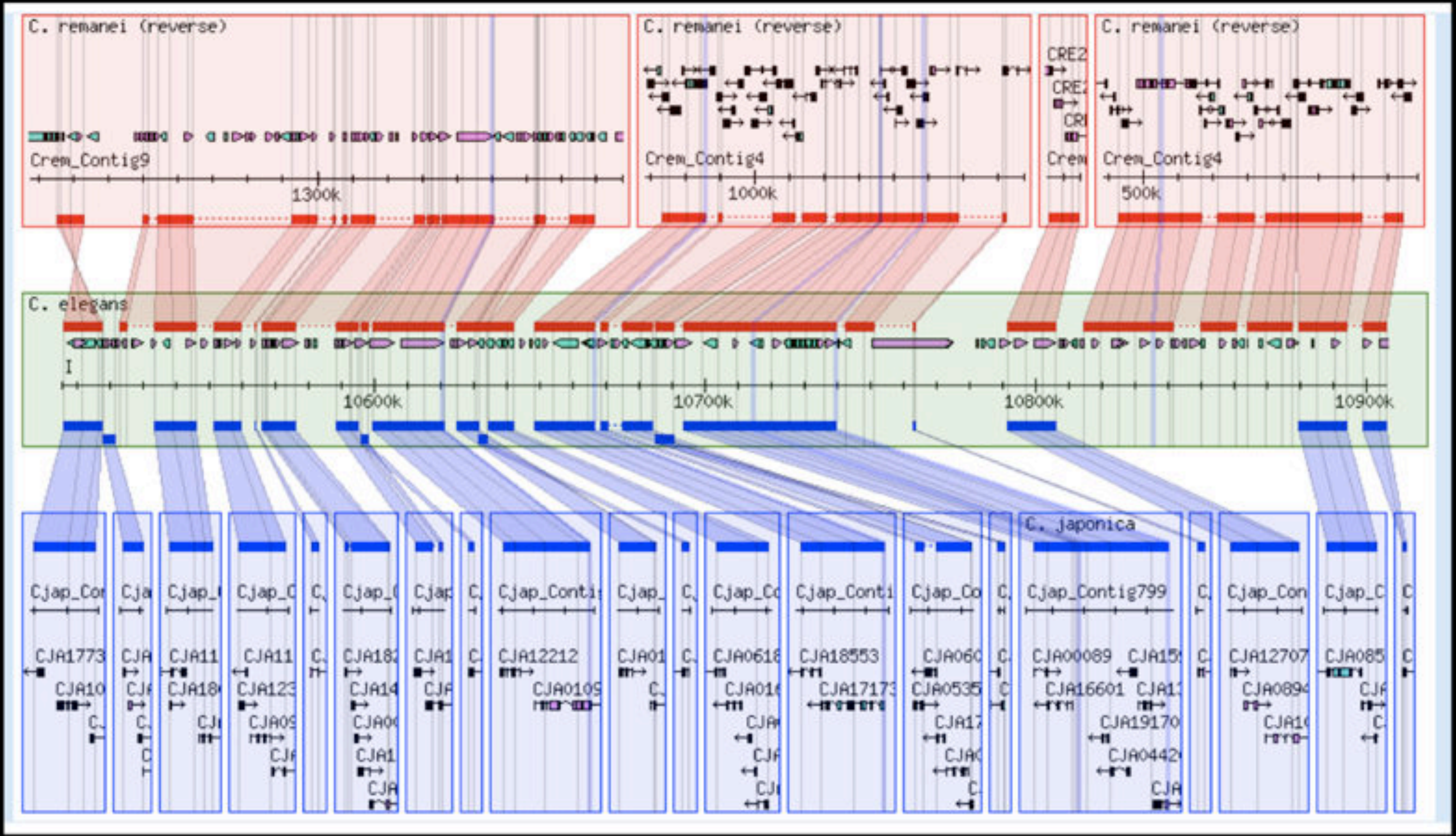
GBrowse_syn: Duplications



GBrowse_syn: Base level alignments



GBrowse_syn: Visual feedback on assembly



Q: CMap or GBrowse_syn?
A: Not an either/or choice

CMap

- Typically used when you have non-sequence based markers
- Popular in the plant community

GBrowse_syn

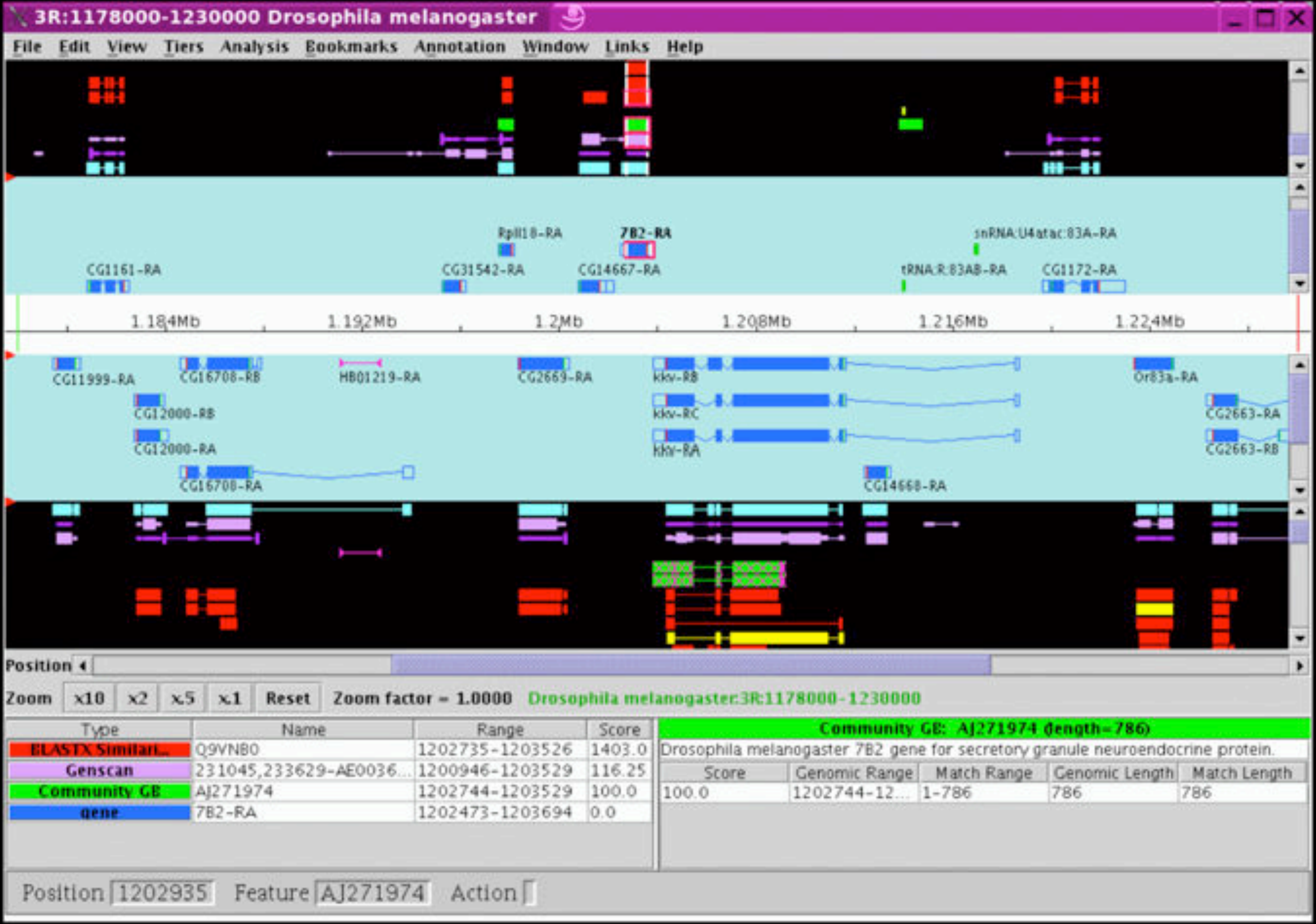
- Used when to show multiple alignment data
- Can be orthology, region, or sequence based alignments
- Exploits GBrowse data sources and infrastructure

Annotation: MAKER

- Genome annotation pipeline for creating gene models
- Produces GFF3 and FASTA which can be loaded into GBrowse, JBrowse, Apollo, Chado, Galaxy, BioMart, InterMine, ...
- Incorporates SNAP, RepeatMasker, exonerate, BLAST, Augsustus, FGENESH, GeneMark, MPI
- Can also map existing annotation on to new assemblies and update existing annotations with new evidence
- Also available as a hosted service.

Cantarel, *et al.,* MAKER: An Easy-to-use Annotation Pipeline Designed for Emerging Model Organism Genomes,. *Genome Research* 2008 18(1) 188-96.

Apollo: Manual genome annotation editor



Zoom factor = 1.0000 Drosophila melanogaster:3R:1178000-1230000

Type	Name	Range	Score
BLASTX Similari...	Q9VNB0	1202735-1203526	1403.0
Genscan	231045,233629-AE0036...	1200946-1203529	116.25
Community GB	AJ271974	1202744-1203529	100.0
gene	7B2-RA	1202473-1203694	0.0

Community GB: AJ271974 (length=786)

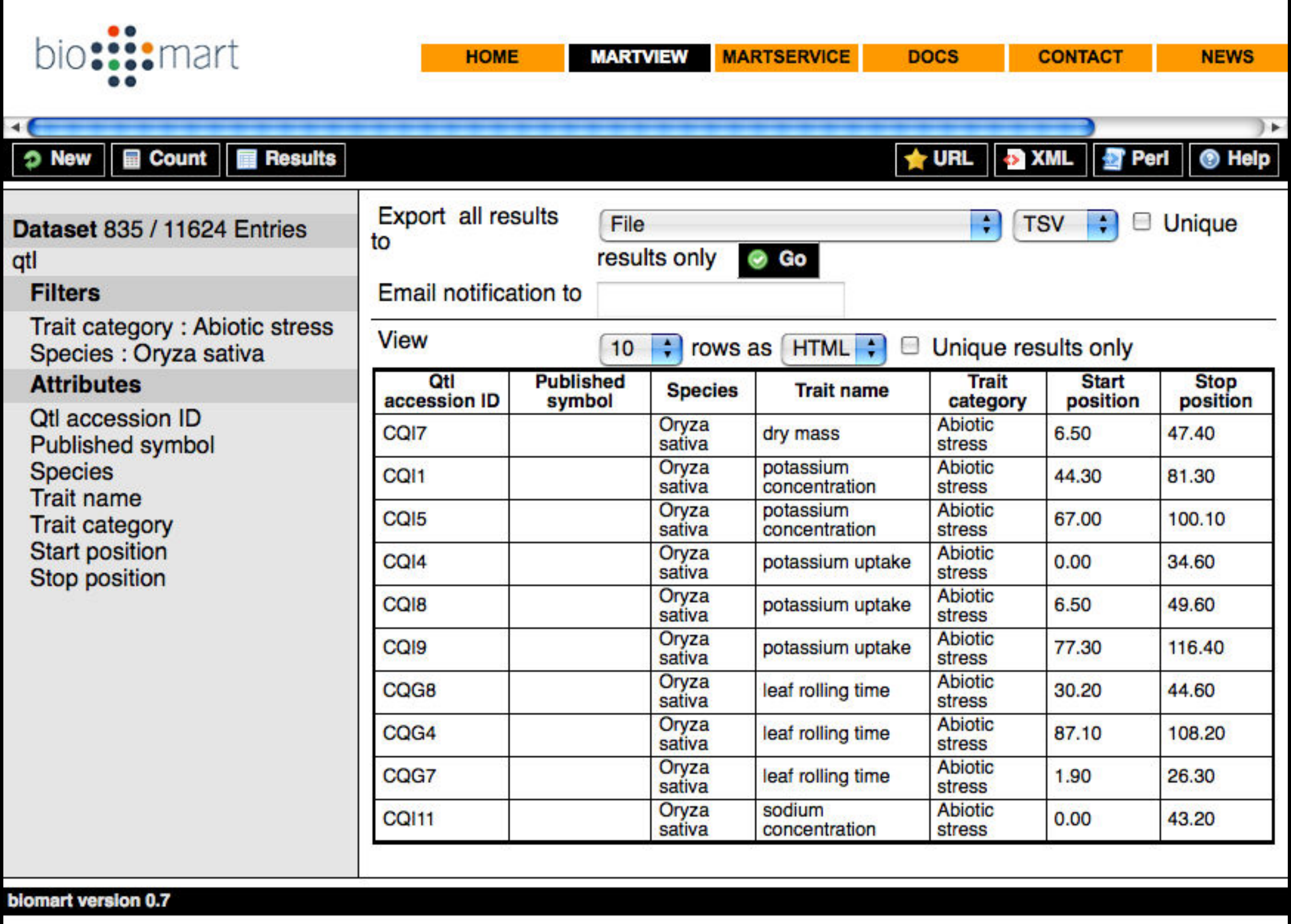
Drosophila melanogaster 7B2 gene for secretory granule neuroendocrine protein.

Score	Genomic Range	Match Range	Genomic Length	Match Length
100.0	1202744-12...	1-786	786	786

Position 1202935 Feature AJ271974 Action

Lewis *et al.*, Apollo: a sequence annotation editor., *Genome Biology* 2002, 3(12)

Data Integration & Querying: BioMart



Dataset 835 / 11624 Entries
qtl

Filters
Trait category : Abiotic stress
Species : Oryza sativa

Attributes
Qtl accession ID
Published symbol
Species
Trait name
Trait category
Start position
Stop position

Export all results to File TSV ☐ Unique results only

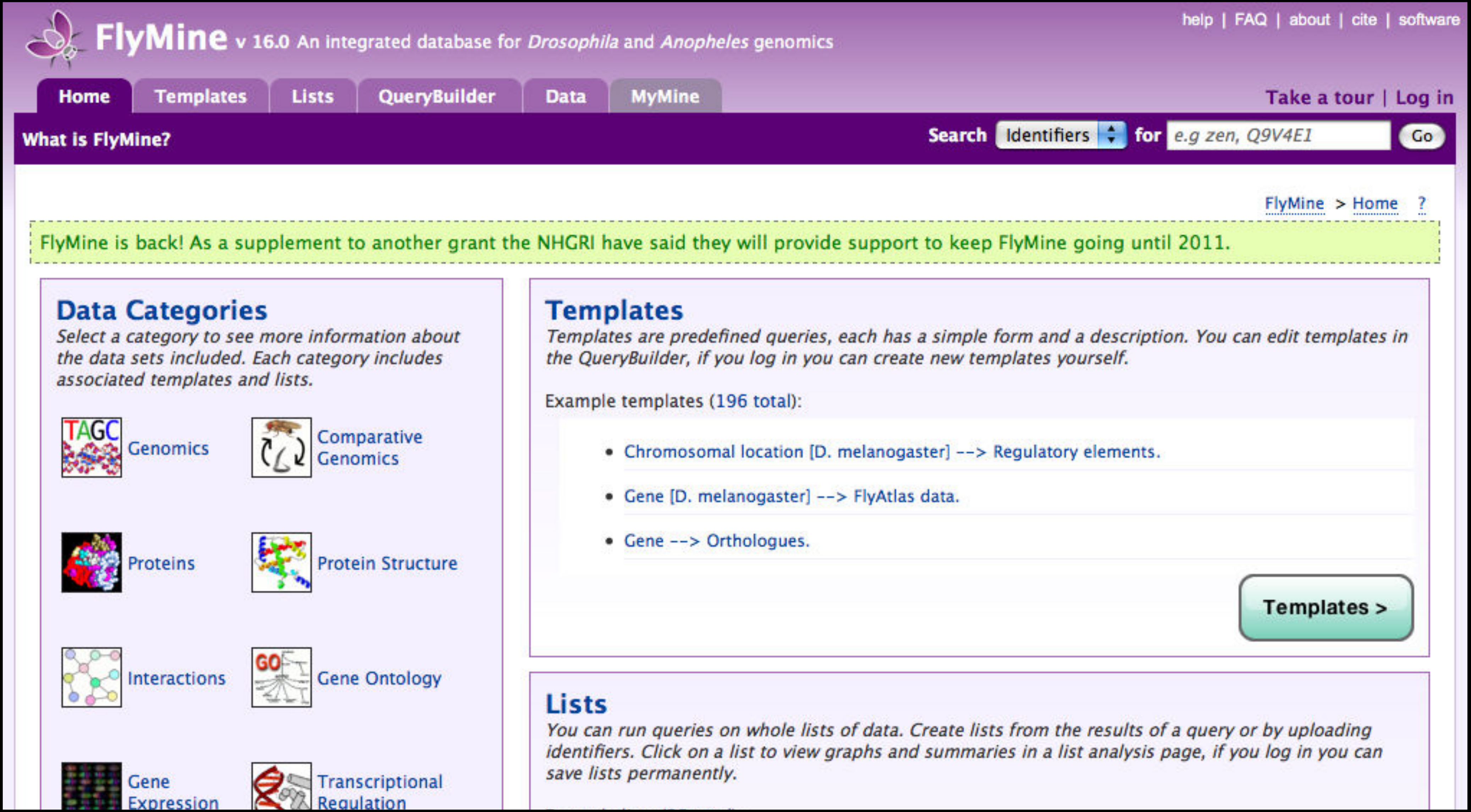
Email notification to

View 10 rows as HTML ☐ Unique results only

Qtl accession ID	Published symbol	Species	Trait name	Trait category	Start position	Stop position
CQI7		Oryza sativa	dry mass	Abiotic stress	6.50	47.40
CQI1		Oryza sativa	potassium concentration	Abiotic stress	44.30	81.30
CQI5		Oryza sativa	potassium concentration	Abiotic stress	67.00	100.10
CQI4		Oryza sativa	potassium uptake	Abiotic stress	0.00	34.60
CQI8		Oryza sativa	potassium uptake	Abiotic stress	6.50	49.60
CQI9		Oryza sativa	potassium uptake	Abiotic stress	77.30	116.40
CQG8		Oryza sativa	leaf rolling time	Abiotic stress	30.20	44.60
CQG4		Oryza sativa	leaf rolling time	Abiotic stress	87.10	108.20
CQG7		Oryza sativa	leaf rolling time	Abiotic stress	1.90	26.30
CQI11		Oryza sativa	sodium concentration	Abiotic stress	0.00	43.20

Smedley, *et al.*, BioMart – biological queries made easy, *BMC Genomics* 2009, 10:22

Data Integration & Querying: InterMine



FlyMine is back! As a supplement to another grant the NHGRI have said they will provide support to keep FlyMine going until 2011.

Data Categories

Select a category to see more information about the data sets included. Each category includes associated templates and lists.

Templates

Templates are predefined queries, each has a simple form and a description. You can edit templates in the QueryBuilder, if you log in you can create new templates yourself.

Example templates (196 total):

- Chromosomal location [D. melanogaster] --> Regulatory elements.
- Gene [D. melanogaster] --> FlyAtlas data.
- Gene --> Orthologues.

Lists

You can run queries on whole lists of data. Create lists from the results of a query or by uploading identifiers. Click on a list to view graphs and summaries in a list analysis page, if you log in you can save lists permanently.

Data Integration & Querying: Chado

- Chado is GMOD’s core database *schema*
- A blueprint for organizing biological data
- Modular and extensible.
- Modules for IDs, sequence features, ontologies, attribution, ...
- Database backing many web sites from FlyBase to ParameciumDB

Agenda

Introduction

Galaxy

Worked example
Deployment Options
Community

GMOD

Software
Community

GMOD Community

- Mailing lists (very active)
- Annual week long course
- Tutorials
- Events Calendar, News Feed
- Community Wiki
- Semi-Annual Community Meetings
    - Tomorrow! Toronto
    - April 2012, Washington, DC

http://gmod.org/

GMOD Contributors

Scott Cain
Carson Holt
Brian Osborne
Ed Lee
Stephen Ficklin
Mitch Skinner
Ian Holmes
Gos Micklem
Barry Moore
Dave Emmert
Alex Kalderimis
Steve Taylor
Dorie Main
Brian O’Connor
Sook Jung
…

Sheldon McKay
Lincoln Stein
Jim Hu
Daniel Renfro
Todd Vision
Nathan Liles
Chris Hemmerich
James Taylor
LBCC Adv. Design
Seth Redmond
Chris Fields
Ben Faga
Joshua Orvis
Junjun Zhang
Naama Menda
…

Hilmar Lapp
Dan Blankenberg
John Aikman
Robert Buels
Richard Smith
Ken Youens-Clark
Nicole Washington
Alexie Papanicolaou
Josh Goodman
Yuri Bendana
Jason Stajich
Suzi Lewis
Mark Yandell
Don Gilbert
Meg Staton
…

Plus hundreds, if not thousands, of others

Thanks

CSIRO

AMATA
conference canberra 2011

CSIRO

Dr Jen Taylor

Dr Annette McGrath

Dr Alexie Papanicolaou

AMATA 2011 Organizing Committee