Introduction to Galaxy

Washington University St. Louis, Missouri May 1, 2013

Dave Clements, Emory University http://galaxyproject.org/











9:00 Welcome Basic Analysis with Galaxy 9:20 10:40 Break 11:00 Basic Analysis into Reusable Workflows 11:20 RNA-Seq Example Part I 12:20 Lunch (on your own) 1:35 Galaxy Project Overview 1:55 RNA-Seq Example Part II 2:45 Break 3:05 Sharing, Publishing and Reproducibility Setting up your own Galaxy Cluster on AWS 5:00 Done

Introductions

In 60 seconds or less tell us

- your name
- your affiliation(s)
- something about your research
- something about what you want to learn

Goals

- 1. Introduce Galaxy
- 2. Introduce bioinformatics concepts and formats
- 3. Hands-on experience
 - Load and integrate data
 - Perform bioinformatic analysis with Galaxy
 - Save, share describe and publish your analyses
 - Visualize your results
 - Set up your own Galaxy server in the cloud

This workshop will not cover details of how tools are implemented, or new algorithm designs, or which assembler or mapper or ... is best for you.

```
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 5:00
      Done
```

Basic Analysis

On human chromosome 22, which coding exons have the most repeats in them?

```
http://cloud1.galaxyproject.org/
http://cloud2.galaxyproject.org/
http://cloud3.galaxyproject.org/
```

(~ http://usegalaxy.org/galaxy101)

Exons & Repeats: A General Plan

- Get some data
 - Coding exons on chromosome 22
 - Repeats on chromosome 22
- Mess with it
 - Identify which exons have repeats
 - Count repeats per exon
 - Save, download, ... exons with most repeats

```
http://cloud1.galaxyproject.org/
http://cloud2.galaxyproject.org/
http://cloud3.galaxyproject.org/
```

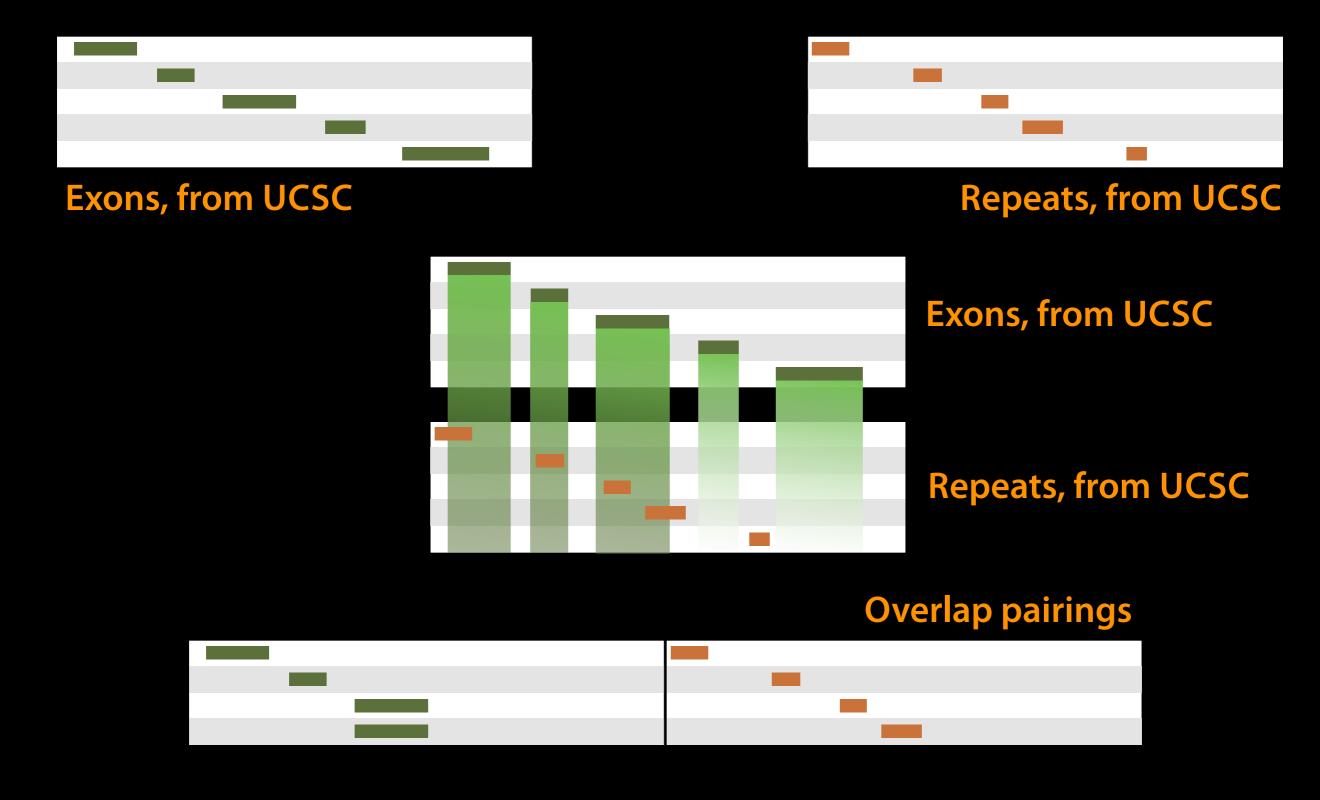
(~ http://usegalaxy.org/galaxy101)

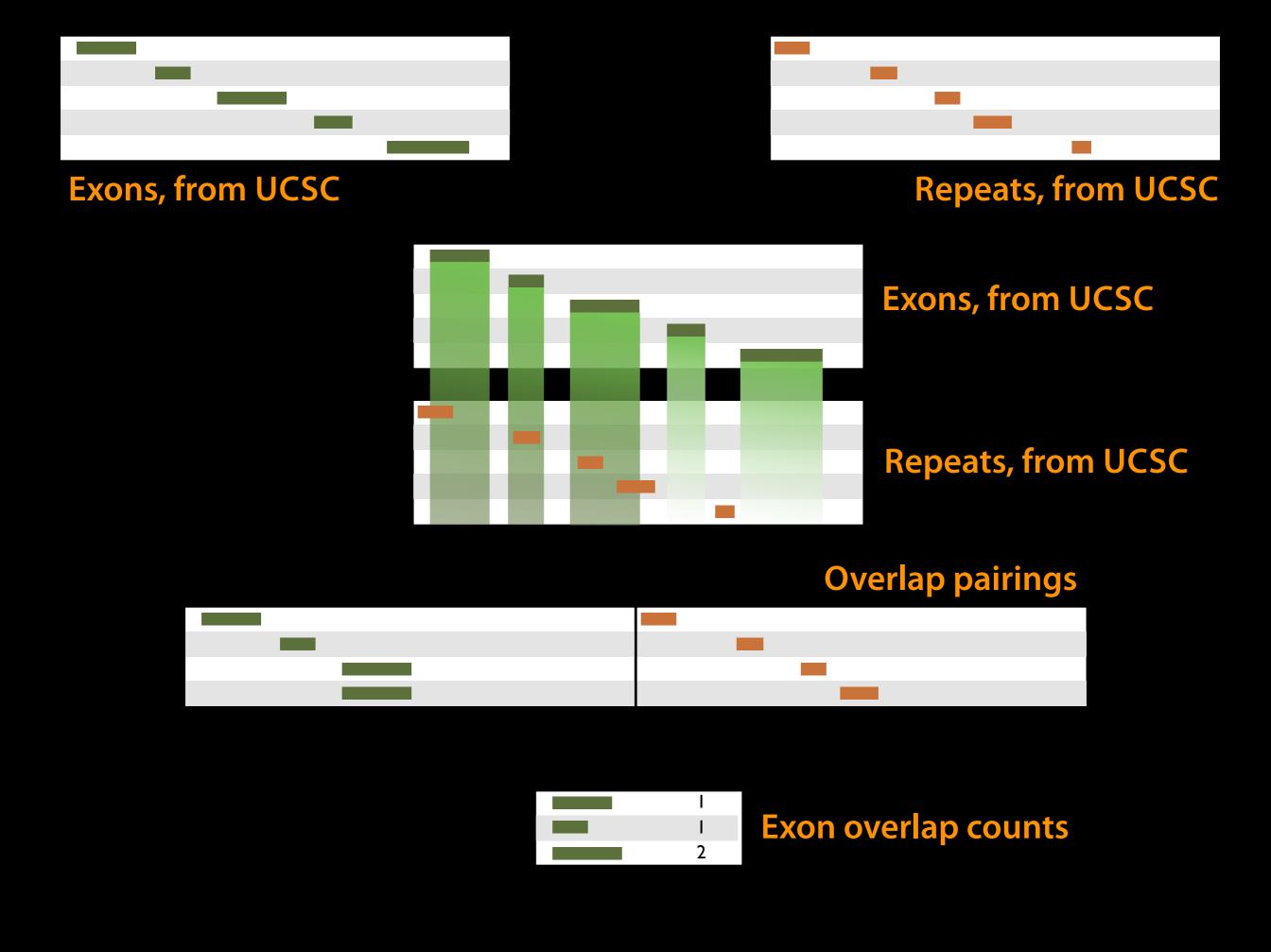


Exons, from UCSC



Repeats, from UCSC







Exon overlap counts



Exons, from UCSC



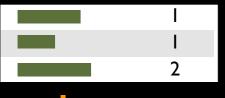
Exon overlap counts



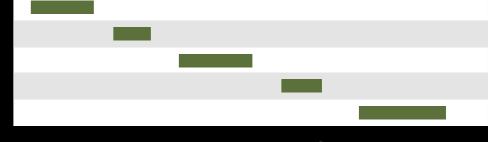
Exons, from UCSC

0	o Join	0
0	0	0
I	I	2

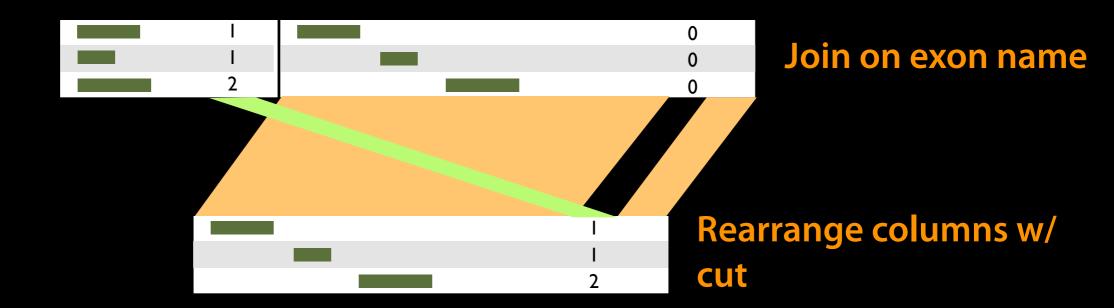
Join on exon name



Exon overlap counts



Exons, from UCSC



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Some Galaxy Terminology

Dataset:

Any input, output or intermediate set of data + metadata

History:

A series of inputs, analysis steps, intermediate datasets, and outputs

Workflow:

A series of analysis steps

Can be repeated with different data

Exons and Repeats *History* → Reusable *Workflow?*

- The analysis we just finished was about
 - Human chromosome 22
 - Overlap between exons and repeats
- But, ...
 - there is nothing inherently in the analysis about humans, chromosomes, exons or repeats
 - It is a series of steps that sets the score of one set of features to the number of overlaps from another set of features.

Create a generic Overlap Workflow

Extract Workflow from history

Create a workflow from this history. Edit it to make some things clearer.

Run / test it

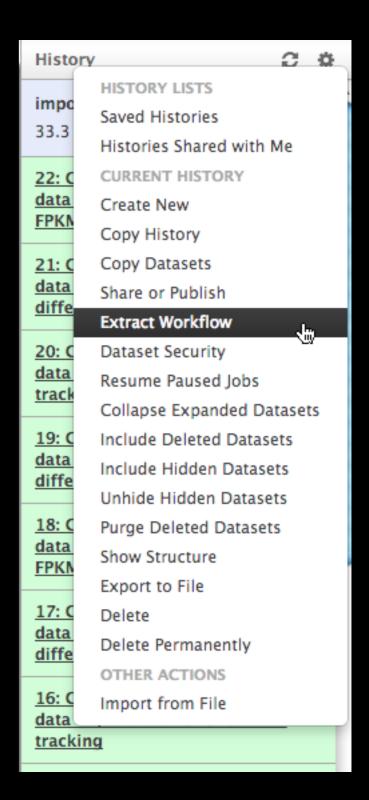
Guided: rerun with same inputs

On your own:

Count # CpG islands in each exon Did that work?

On your own:

Count # of exons in each repeat Did that work? *Why not?* Edit workflow: doc assumptions



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RNA-seq Exercise

Shared Data → Published Pages

→ RNA-Seq Analysis Exercise

- Get input datasets; hg19, will mostly map to chr19
- Look at quality
- Trim as we see fit.
- Map the reads to the human reference using Tophat
- Run Cufflinks on Tophat output to assemble reads into transcripts
- Run Cuffdiff on Tophat output to find significant differences

RNA-seq Exercise: A Plan, Except ...

- At WashU, these steps have likely already been done:
 - Trim as we see fit.
 - Map the reads to the human reference using Tophat
- So, we won't run them today, but we will explain them.

GTAC: http://bit.ly/WashURNA

- Get input datasets; hg19, will mostly map to chr19
 - All datasets are FASTQ and from the Body Map
 2.0 project

 Shared Data → Published Histories → RNA-Seq with QC through Tophat

What is FASTQ?

- Specifies sequence (FASTA) and quality scores (PHRED)
- Text format, 4 lines per entry

```
@SEQ_ID
GATTTGGGGTTCAAAGCAGTATCGATCAAATAGTAAATCCATTTGTTCAACTCACAGTTT
+
!''*((((***+))%%%++)(%%%%).1***-+*''))**55CCF>>>>>CCCCCCC65
```

FASTQ is such a cool standard, there are 3 (or 5) of them!

Look at quality Options 1 & 2:

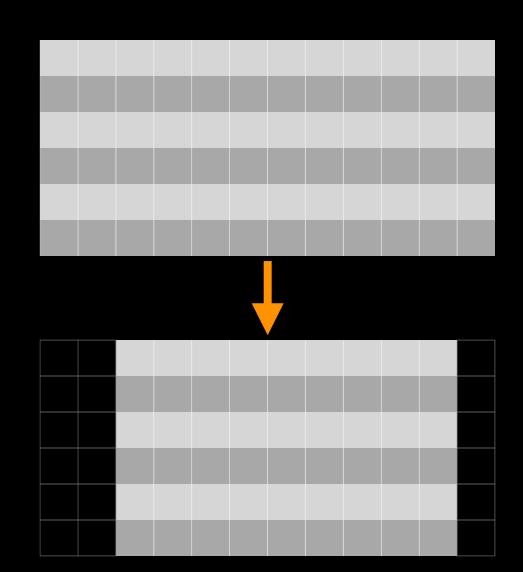
- NGS QC and Manipulation → Compute Quality
 Statistics and then Draw quality score boxplot
 No control over how it is calculated or presented.
- 2. NGS QC and Manipulation → FastQ Summary Statistics,
 Graph / Display Data → Boxplot of quality statistics
 Lots of control over what the box plot looks like, info

available in both graphical and text formats

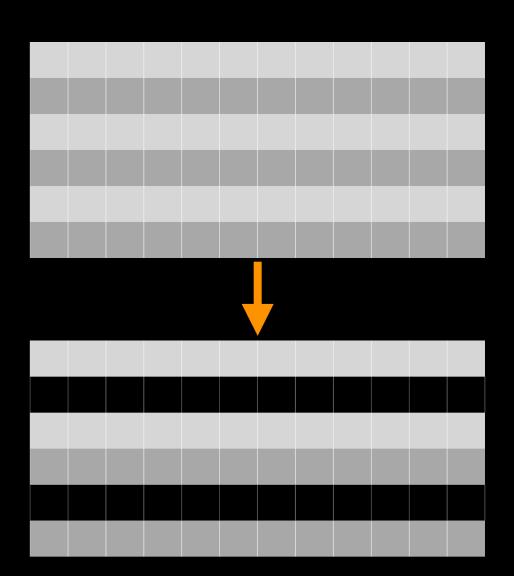
- Look at quality: Option 3
 - NGS QC and Manipulation → FastQC
 - Gives you a lot a lot more information but little control over how it is calculated or presented.
- This is what we have done

"For the love of all that is holy, please trim your reads!" Chris Mason, ABRF NGS Study Report, March 4, 2013

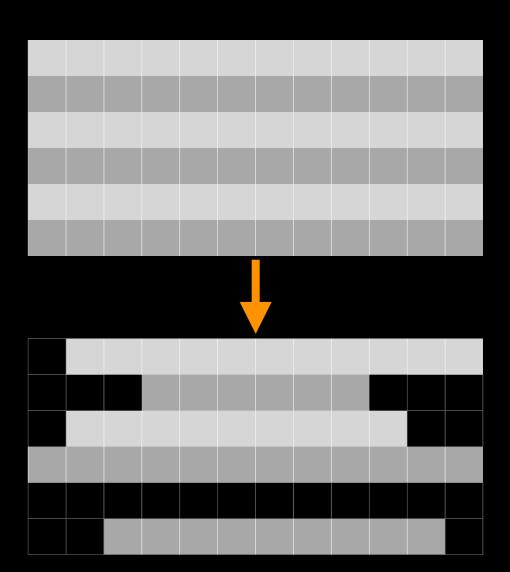
- Look at quality
- Trim as we see fit: Option 1
 - NGS QC and Manipulation →
 FASTQ Trimmer by column
 - Trim same number of columns from every record
 - Can specify different trim for 5' and 3'ends



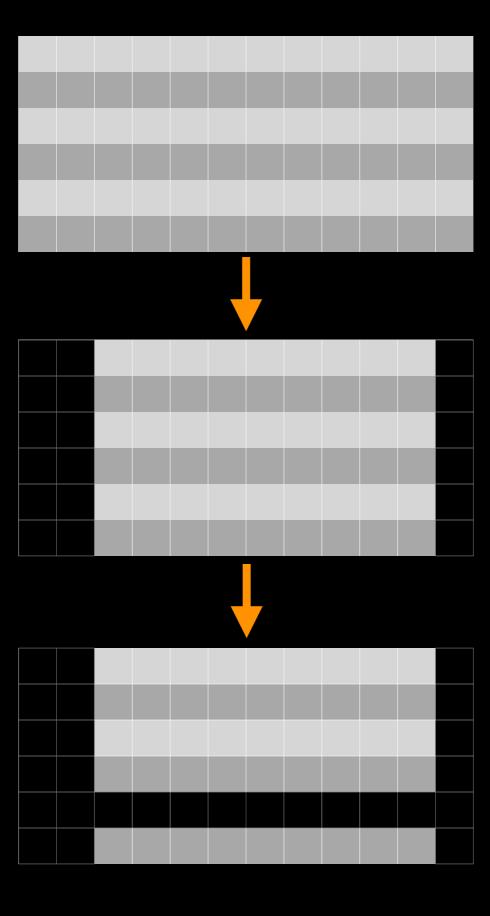
- Look at quality
- Trim Filter as we see fit: Option 2
 - NGS QC and Manipulation → Filter FASTQ reads by quality score and length
 - Keep or discard whole reads at a time
 - Can have different thresholds for different regions of the reads.
 - Keeps original read length.



- Look at quality
- Trim as we see fit: Option 3
 - NGS QC and Manipulation →
 FASTQ Quality Trimmer by
 sliding window
 - Trim from both ends, using sliding windows, until you hit a highquality section.
 - Produces variable length reads



Options are not mutually exclusive



Trim? As we see fit?

- Introduced 3 options
 - One preserves original read length, two don't
 - One preserves number of reads, two don't
 - Two keep/make every read the same length, one does not
 - One preserves pairings, two don't

Trim? As we see fit?

- Choice depends on downstream tools
- Find out assumptions & requirements for downstream tools and make appropriate choice(s) now.
- How to do that?
 - http://biostars.org/
 - http://seqanswers.com/
 - http://galaxyproject.org/search





- Get input datasets; hg19, will mostly map to chr19
- Look at quality
- Trim as we see fit.
- Map the reads to the human reference using Tophat
 - Imagine pages and pages of discussion on the intricacies and pitfalls of RNA-seq mapping here.
 - And thanks to GTAC, we won't run it today.

- Map the reads to the human reference using Tophat
- Run Cufflinks on Tophat output to assemble reads into transcripts
 - Imagine pages and pages of discussion on the intricacies and pitfalls of RNA-seq transcript prediction here.

http://bit.ly/11Qvnwh: Lance Parsons' RNA-Seq Tutorial

http://bit.ly/Y7yKzv: UC Davis (Nik Joshi?) RNA-Seq Tutorial

http://bit.ly/Yfl0E0: UAB RNA-Seq Tutorial @ GCC2012

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What is Galaxy?

- A free (for everyone) web service integrating a wealth of tools, compute resources, terabytes of reference data and permanent storage
- Open source software that makes integrating your own tools and data and customizing for your own site simple
- These options result in several ways to use Galaxy

http://galaxyproject.org

Galaxy is available ...

As a free (for everyone) web service

http://usegalaxy.org

A centralized solution cannot scale to meet the analysis needs of the entire world.

Galaxy is available ...

- As a free (for everyone) web service http://usegalaxy.org
- As open source software

http://getgalaxy.org

As Open Source Software: Local Galaxy Instances

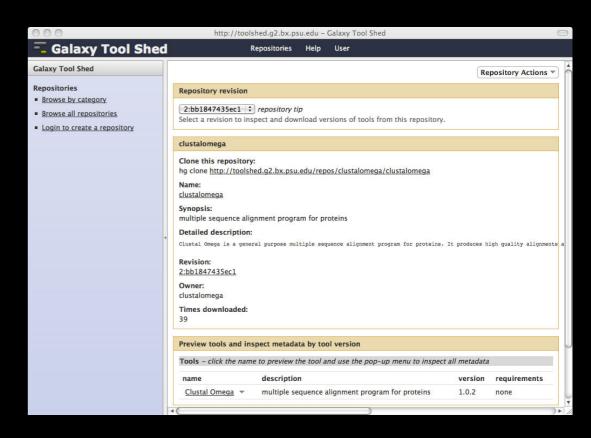
- Galaxy is designed for local installation and customization
 - Easily integrate new tools
 - Easy to deploy and manage on nearly any (unix) system
 - Run jobs on existing compute clusters
- Requires a computational resource on which to be deployed

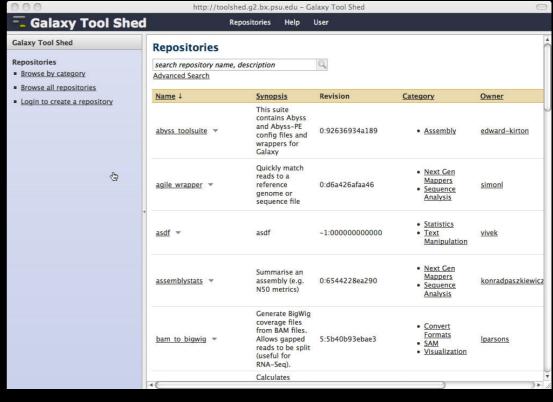
http://getgalaxy.org

Encourage Local Galaxy Instances

- Encourage and support Local Galaxy Instances
 - Support increasingly decentralized model and improve access to existing resources
 - Focus on building infrastructure to enable the community to integrate and share tools, workflows, and best practices

Galaxy Tool Shed http://toolshed.g2.bx.psu.edu





Encourage Public Galaxy Instances

http://bit.ly/gxyServers

Interested in:

ChIP-chip and ChIP-seq?

✓ Cistrome

Statistical Analysis?

✓ Genomic Hyperbrowser

Protein synthesis?

✓ GWIPS-viz

de novo assembly?

✓ CBIIT Galaxy

Reasoning with ontologies?

✓ OPPL Galaxy

Repeats!

✓ RepeatExplorer

Everything?

✓ Andromeda

Plus many more

As Open Source Software: Local Galaxy Instances

- Galaxy is designed for local installation and customization
 - Easily integrate new tools
 - Easy to deploy and manage on nearly any (unix) system
 - Run jobs on existing compute clusters
- Requires a computational resource on which to be deployed

Got your own cluster?

- Galaxy works with any DRMAA compliant cluster job scheduler (which is most of them).
- Galaxy is just another client to your scheduler.









Galaxy is available ...

As a free (for everyone) web service

http://usegalaxy.org

As open source software

http://getgalaxy.org



On the Cloud

http://usegalaxy.org/cloud

We are using this right now, and you will set up your own instance today

http://aws.amazon.com/education

Galaxy Resources and Community

Mailing Lists (very active)

Unified Search

Issues Board

Events Calendar, News Feed

Community Wiki

GalaxyAdmins

Screencasts

Tool Shed

Public Installs

CiteULike group, Mendeley mirror

Annual Community Meting

http://wiki.galaxyproject.org

Galaxy Resources and Community: Mailing Lists http://wiki.galaxyproject.org/MailingLists

Galaxy-Announce

Project announcements, low volume, moderated Low volume (42 posts, 1600 members in 2012)

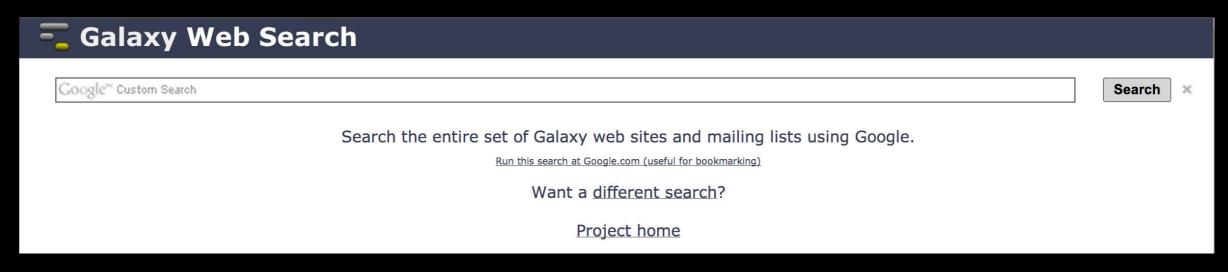
Galaxy-User

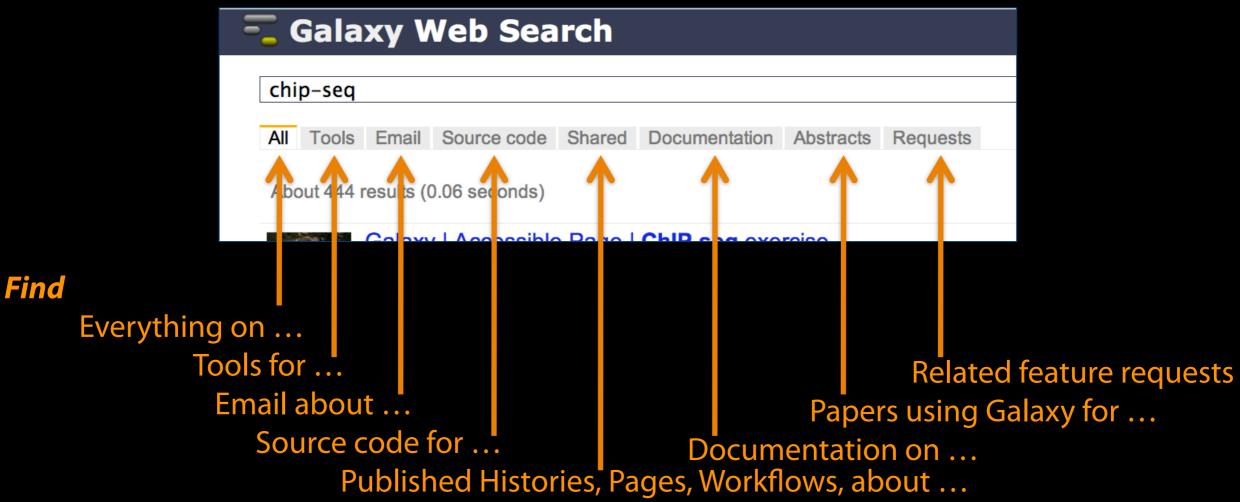
Questions about using Galaxy and usegalaxy.org High volume (2900 posts, 2700 members in 2012)

Galaxy-Dev

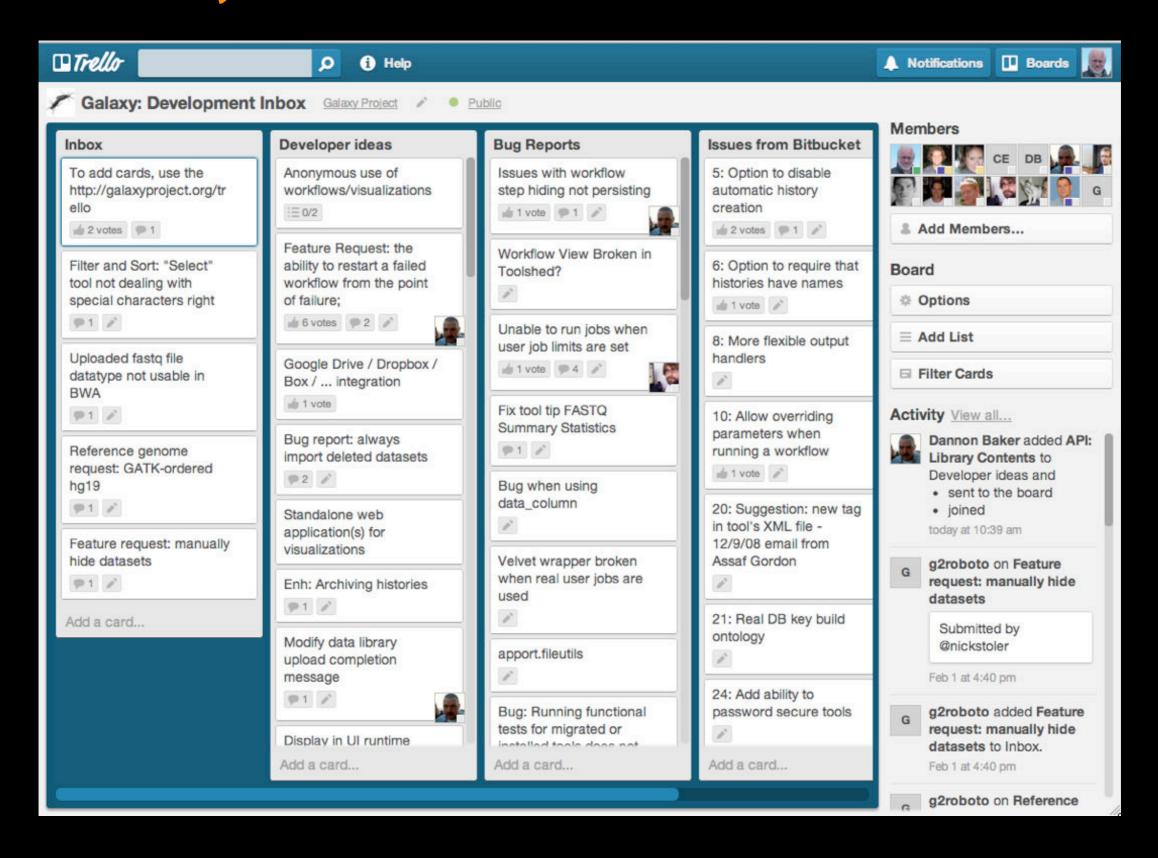
Questions about developing for and deploying Galaxy High volume (4500 posts, 850 members in 2012)

Unified Search: http://galaxyproject.org/search

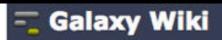




Community can create, vote and comment on issues



http://wiki.galaxyproject.org



Login | Search:

Titles Text

FrontPage

Locked History Actions



Galaxy is an open, web-based platform for accessible, reproducible, and transparent computational biomedical research.

- Accessible: Users without programming experience can easily specify parameters and run tools and workflows.
- · Reproducible: Galaxy captures information so that any user can repeat and understand a complete computational analysis.
- . Transparent: Users share and publish analyses via the web and create Pages, interactive, web-based documents that describe a complete analysis.

This is the Galaxy Community Wiki. It describes all things Galaxy.

Use Galaxy

Galaxy's public service web site makes analysis tools, genomic data, tutorial demonstrations, persistent workspaces, and publication services available to any scientist. Extensive user documentation (applicable to any public or local Galaxy instance) is available on this wiki and elsewhere.

Deploy Galaxy

Galaxy is open source for all organizations. Local Galaxy servers can be set up by downloading and customizing the Galaxy application.

- Admin
- Cloud

=getgalaxy.org

=usegalaxy.org

Community & Project

Galaxy has a large and active user community and many ways to Get Involved.

- Community
- News
- Events
- Support
- Galaxy Project

Contribute

- · Users: Share your histories, workflows, visualizations, data libraries, and Galaxy Pages, enabling others to use and learn from them.
- . Deployers and Developers: Contribute tool definitions to the Galaxy Tool Shed (making it easy for others to use those tools on their installations), and code to the core release.
- Everyone: Get Involved!



Poster abstracts due 3 May

Use Galaxy

Use Main (about) Use Others! . Learn Share . Search

Communication

Support . News M Events • Twitter Mailing Lists (search)

Deploy Galaxy

Get Galaxy . Cloud Admin . Tool Config Tool Shed . Search

Contribute

Tool Shed . Share Issues & Requests Support

Galaxy Project

Home . About Community Big Picture

Wiki

Help . All Pages

Events

News

Galaxy Wiki Titles = Galaxy Wiki Login | Search: Login | Search: Titles Text News Locked History Actions Locked History

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Gala web sea

Community

Big Picture

Wiki

Support

Galaxy Event Horizon

Events with Galaxy-related content are listed here.



Also see the Galaxy Events Google Calendar for a listing of events and deadlines that are relevant to the Galaxy Community. This is also available as an RSS feed ...

If you know of any event that should be added to this page and/or to the Galaxy Event Calendar, please add it here or send it to outreach@glaxyproject.org .

Contents

- 1. Upcoming Events
- 2. Other Calendars
- 3. Past Events
 - 1. 2013
 - 2. Archive

Upcoming Events









Date	Topic/Event	Venue/Location	Contact
April 29 - May 2	Introduction to Galaxy Workshops 2013 Galaxy Workshop Tour	Washington University in St. Louis	Dave Clements
		Saint Louis University	
		University of Missouri Columbia	
May 14- 16	Tutorial: Exploring and Enabling Biomedical Data Analysis with Galaxy	Great Lakes Bioinformatics Conference (GLBIO) 2013, Pittsburgh, Pennsylvania, United States	Anton Nekrutenko
May 15	GalaxyAdmins May 2013 Meetup	GalaxyAdmins web meetup	Srinivas Maddhi, Dave Clements
May 16- 17	Galaxy Workflows for Bioinformatics Analysis, and Workshop 1A - Galaxy Workflows for Bioinformatics Analysis	Workshop in Next- Generation Sequence Analysis and Metabolomics (WiNGS), UNC-Charlotte, North Carolina, United States	James Taylor
May 21 May 29	Initiation à l'utilisation de Galaxy Les deux ateliers sont maintenant complets	Cycle "Bioinformatique par la pratique" 2013, INRA Jouy-en-Josas, France	Sandra Dèrozier, Valentin Loux, Véronique Martin <veronique.martin at="" dot="" fr="" inra="" jouy=""></veronique.martin>
May 22 May 30	Analyse de données issues de séquenceurs nouvelle génération sous Galaxy Les deux ateliers sont maintenant complets		Jean-François Gibrat, Valentin Loux, Véronique Martin <veronique.martin at="" dot="" fr="" inra="" jouy=""></veronique.martin>
May 24 June 19	Introduction to Galaxy	UC Davis Bioinformatics Core Davis, California, United States	Nikhil Joshi <najoshi at="" dot="" edu="" ucdavis=""></najoshi>
	A Genomics Virtual Lab for Cancer Research		Dominique Gorse

News



The Galaxy News is also available as an RSS feed .

See Add a News Item below for how to get an item on this page, and the RSS feed. Older news items are available in the Galaxy News Archive.

See also

- · Galaxy News Briefs
- Galaxy Updates
- · Galaxy on Twitter
- Events
- Learn
- Support
- · About the Galaxy Project

News Items

Environmental Metabolomics + Galaxy

A new UK-China collaboration in environmental metabolomics between the University of Birmingham, BGI and GigaScience has received funding from the UK's Natural Environment Research Council (NERC).

BIRMINGHAM

The first metabolomics project will send a developer from the University of Birmingham's School of Biosciences, to Hong Kong to work with GigaScience personnel on extending Galaxy for use in metabolomics data analyses.

"Metabolomics involves the detection and quantification of small molecules (metabolites) in living organisms and can provide an indication of their cellular condition and health. The toxicological responses of organisms to pollutants can be studied using environmental metabolomics, enabling researchers to discover diagnostic markers for monitoring and risk assessment of our environment. Research at Birmingham focuses extensively on the metabolic responses of the freshwater model organism, Daphnia, to both pollutants and engineered nanomaterials."

See the official announcement for more details.

Peter Li GigaScience

Posted to the Galaxy News on 2013-04-22

Galaxy @ ASMS 2013

Galaxy will have a significant presence at the 61st ASMS Conference on Mass Spectrometry and Allied Topics being held in Minneapolis, Minnesota, June 9-13. Galaxy related content includes the Galaxy Framework as a Solution for MSbased Informatics workshop and at least 9 posters either directly about or using



If you do research in proteomics than please consider attending.

Dave Clements

Posted to the Galaxy News on 2013-04-19

News Items Environmental Metabolomics + Galaxy

Galaxy @ ASMS 2013 April 8, 2013 Galaxy Security Release GCC2013 & Galaxy GigaScience Series April 2013 Galaxy Update April 1, 2013 Galaxy Distribution Galaxy LinkedIn Group March 2013 GalaxyAdmins Meetup Main & Test ServerDowntime: 3/14 March 2013 Galaxy Update GCC2013 Abstract Submission & Registration

News Archive



Poster abstracts due 3 May

Use Galaxy

Use Main (about) Use Others! . Learn Share • Search

Communication

Support • News 🔊 Events • Twitter Mailing Lists (search)

Deploy Galaxy

Get Galaxy . Cloud Admin . Tool Config Tool Shed . Search

Contribute

Tool Shed . Share Issues & Requests Support

Galaxy Project

Home . About Community Big Picture

Wiki

Help • All Pages Recent Changes 🔝 Search • Create Page





April 8, 2013 Galaxy Security Release

Galaxy Community 30 June - 2 July Conference 2013 UiO: University of Oslo





\$125



Poster abstracts due May 3





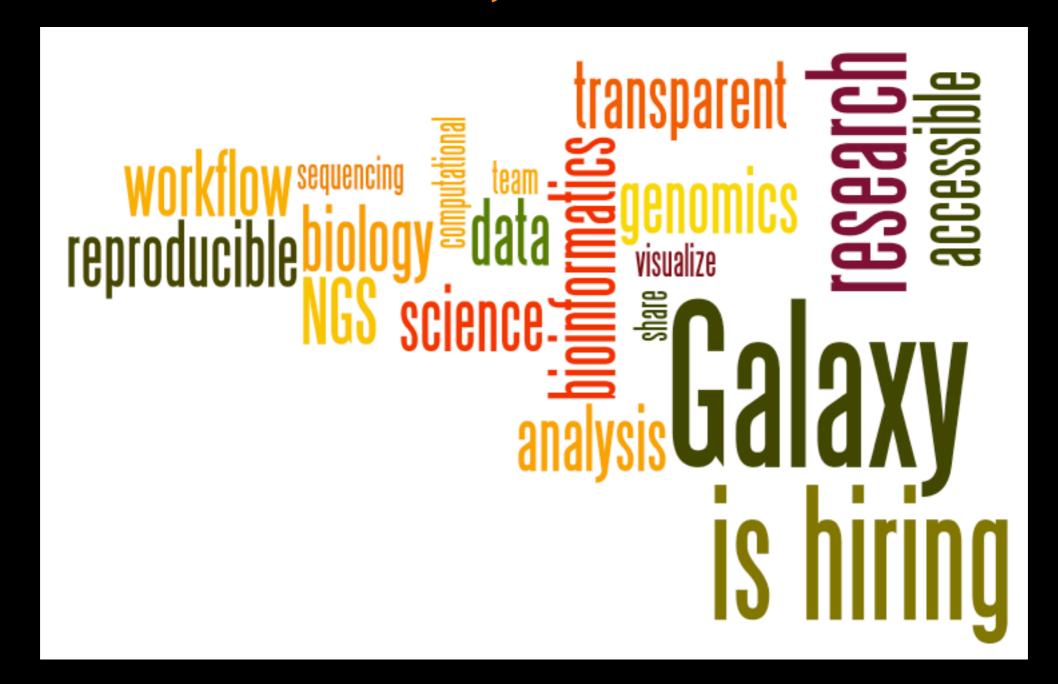
(a) 5125

The Galaxy Team



http://wiki.galaxyproject.org/GalaxyTeam

Galaxy is hiring post-docs and software engineers at both Emory and Penn State.



Please help.

http://wiki.galaxyproject.org/GalaxylsHiring

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RNA-seq Exercise: A Plan

- ...
- Run Cufflinks on Tophat output to assemble reads into transcripts
- Run Cuffdiff on Tophat output compare expression
 - Imagine pages and pages of discussion on the intricacies and pitfalls of RNA-seq differential expression analysis here.

RNA-seq Exercise: A Different (better?) Plan

- We've now walked through the analysis
- Suggests our level of iteration / experimentation is the whole workflow.
- Use Visualization as we go, to guide analysis as we go.

Visualizing Genomics

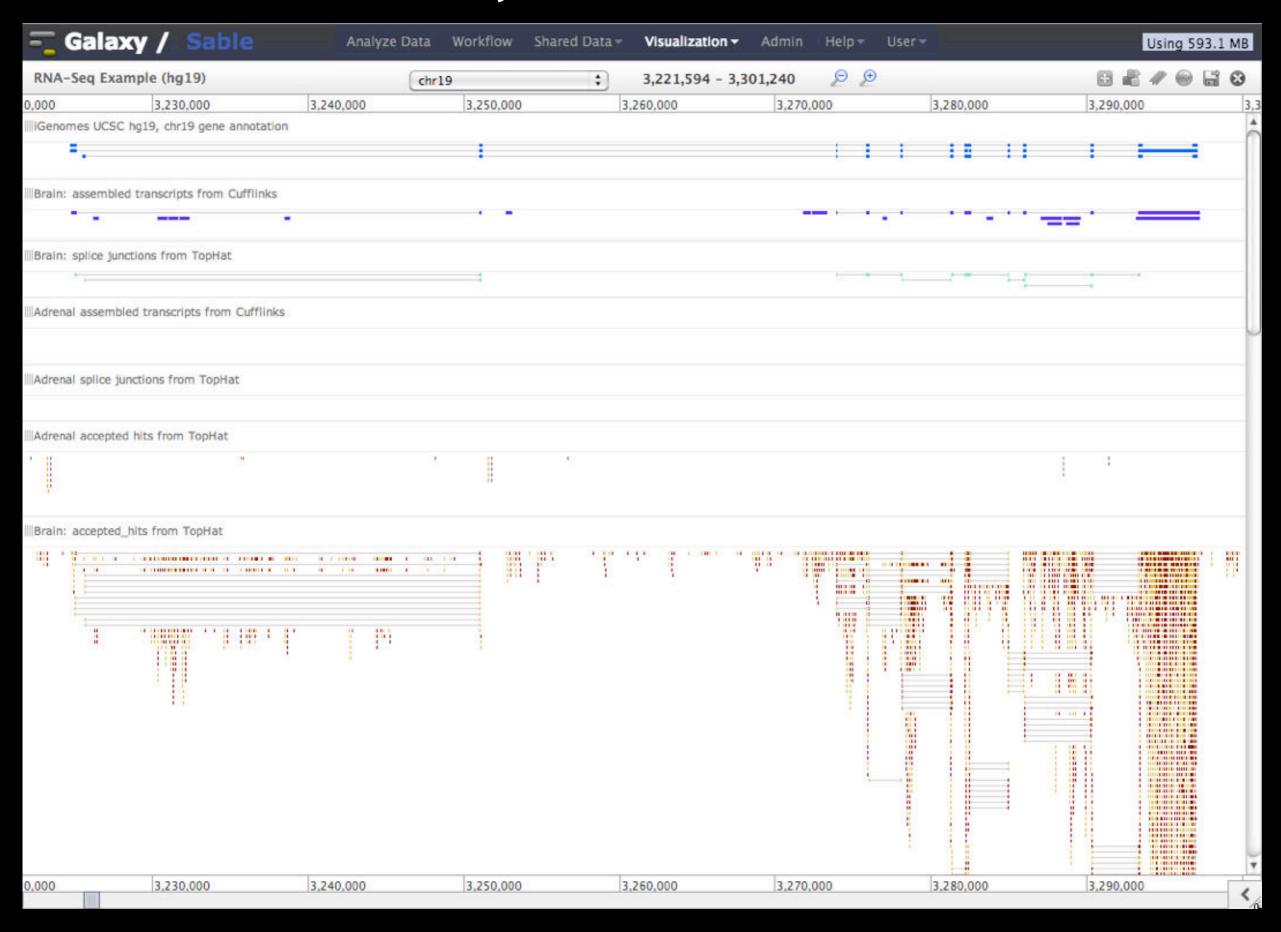
Supported external browsers

- UCSC
- Ensembl
- GBrowse
- IGB
- IGV

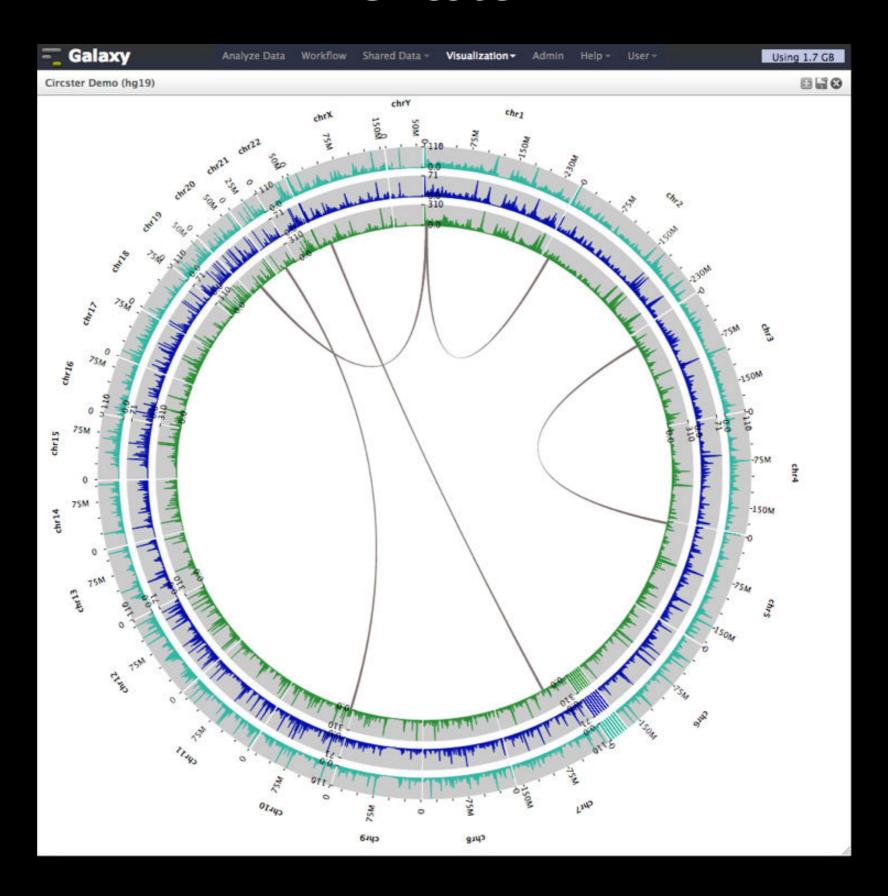
Traditional browser strengths:

- Showing what is nearby
- what else is happening here
- highlighting correlations
- integrating many datasets

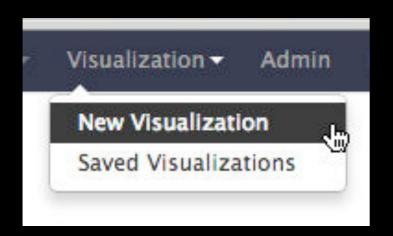
Trackster: Galaxy's embedded track browser



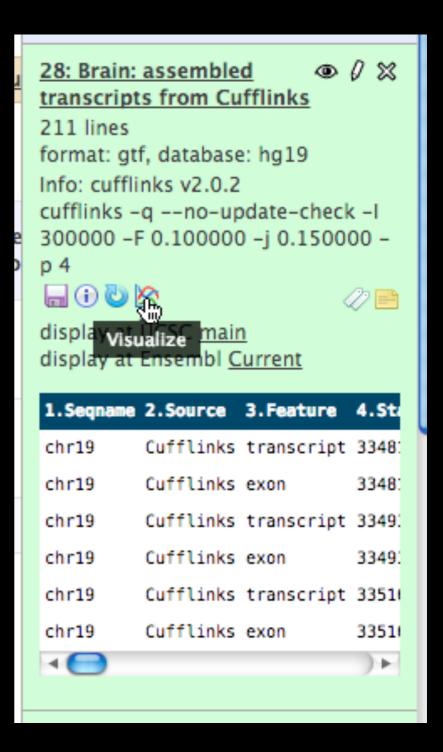
Circster



Create a visualization in Galaxy







Vizualization inside Galaxy

- Levarges visualization to evaluate and refine analyses
- Exposes basic analyses in visualization to make it more informative
- Makea that analyze-visualize-refine loop seamless and fast
- Enables learning tools and exploring their parameter space
- Supports custom genome browsers, without a predefined reference genome

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```

More Galaxy Terminology

Share:

Make something available to someone else

Publish:

Make something available to everyone

Galaxy Page:

Analysis documentation within Galaxy; easy to embed any Galaxy object

Sharing & Publishing enables Reproducibility

Reproducibility: Everybody talks about it, but ...

Galaxy aims to push the goal of reproducibility from the bench to the bioinformatics realm

All analysis in Galaxy is recorded without any extra effort from the user.

Histories, workflows, visualizations and *pages* can be shared with others or published to the world.

Sharing & Publishing enables Reproducibility





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Institution: PENN STATE UNIV Sign In via User Name/Password

Search for Keyword: Go
Advanced Search

Windshield splatter analysis with the Galaxy metagenomic pipeline

Sergei Kosakovsky Pond 1,2,6,9, Samir Wadhawan 3,6,7,

Francesca Chiaromonte⁴, Guruprasad Ananda^{1,3}, Wen-Yu Chung^{1,3,8},

James Taylor1,5,9, Anton Nekrutenko1,3,9 and The Galaxy Team1

OPEN ACCESS ARTICLE

This Article

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

Copyright © 2009 by Cold Spring Harbor Laboratory Press

Abstract Free
 Full Tayt (PDE) Free

Current Issue

October 2010, 20 (10)



Sharing & Publishing enables Reproducibility





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Institution: PENN STATE UNIV Sign In via User Name/Password

Search for Keyword: Advanced Search

Windshield splatter analysis with the Galaxy metagenomic pipeline

Sergei Kosakovsky Pond 1,2,6,9, Samir Wadhawan 3,6,7,

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» Abstract Free

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Footpotes

[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.]

Published Pages | aun1 | Windshield Splatter

Windshield splatter analysis with the Galaxy metagenomic pipeline: A live supplement

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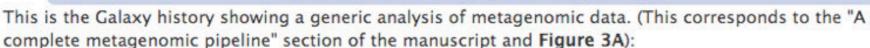
How to use this document

This document is a live copy of supplementary materials for the manuscript. It provides access to the exact analyses and workflows discussed in the paper, so you can play with them by re-running, changing parameters, or even applying them to your own data. Specifically, we provide the two histories and one workflow found below. You can view these items by clicking on their name to expand them. You can also import these items into your Galaxy workspace and start using them; click on the green plus to import an item. To import workflows you must create a Galaxy account (unless you already have one) – a hassle-free procedure where you are only asked for a username and password.

This is the Galaxy history detailing the comparison of our pipeline to MEGAN:



Galaxy History | Galaxy vs MEGAN Comparison of Galaxy vs. MEGAN pipeline.





Galaxy History | metagenomic analysis



This is the Galaxy workflow for generic analysis of metagenomic data. (This corresponds to the "A complete metagenomic pipeline" section of the manuscript and Figure 3B):



Galaxy Workflow | metagenomic analysis



Generic workflow for performing a metagenomic analysis on NGS data.

Accessing the Data

Windshield Splatter datasets analyzed in this manuscript can be accessed through this Galaxy Library. From

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Wrapping tools and datatypes

Agenda

```
9:00 Welcome
     Basic Analysis with Galaxy
 9:20
10:40 Break
11:00 Basic Analysis into Reusable Workflows
11:20 RNA-Seg Example Part I
12:20 Lunch (on your own)
 1:35 Galaxy Project Overview
 1:55 RNA-Seq Example Part II
 2:45 Break
 3:05 Sharing, Publishing and Reproducibility
     Setting up your own Galaxy Cluster on AWS
 5:00
      Done
```

Galaxy CloudMan http://usegalaxy.org/cloud

- Start with a fully configured and populated (tools and data) Galaxy instance.
- Allows you to scale up and down your compute assets as needed.
- Someone else manages the data center.
- We are using this today.



You will set up an instance now

http://aws.amazon.com/education

Could do this step by step, but ... http://bit.ly/GXYAWSGetStarted

🔁 Galaxy Wiki

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CloudMan/AWS/GettingStarted

Getting Started with Galaxy CloudMan

This page provides a step-by-step instructions on how to start your own instance of Galaxy on Amazon Web Services (AWS) Elastic Compute Cloud (EC2). More general information and instructions about Galaxy CloudMan (GC) can be found here.

AWS Get Started Capacity Planning AMIs † CloudMan

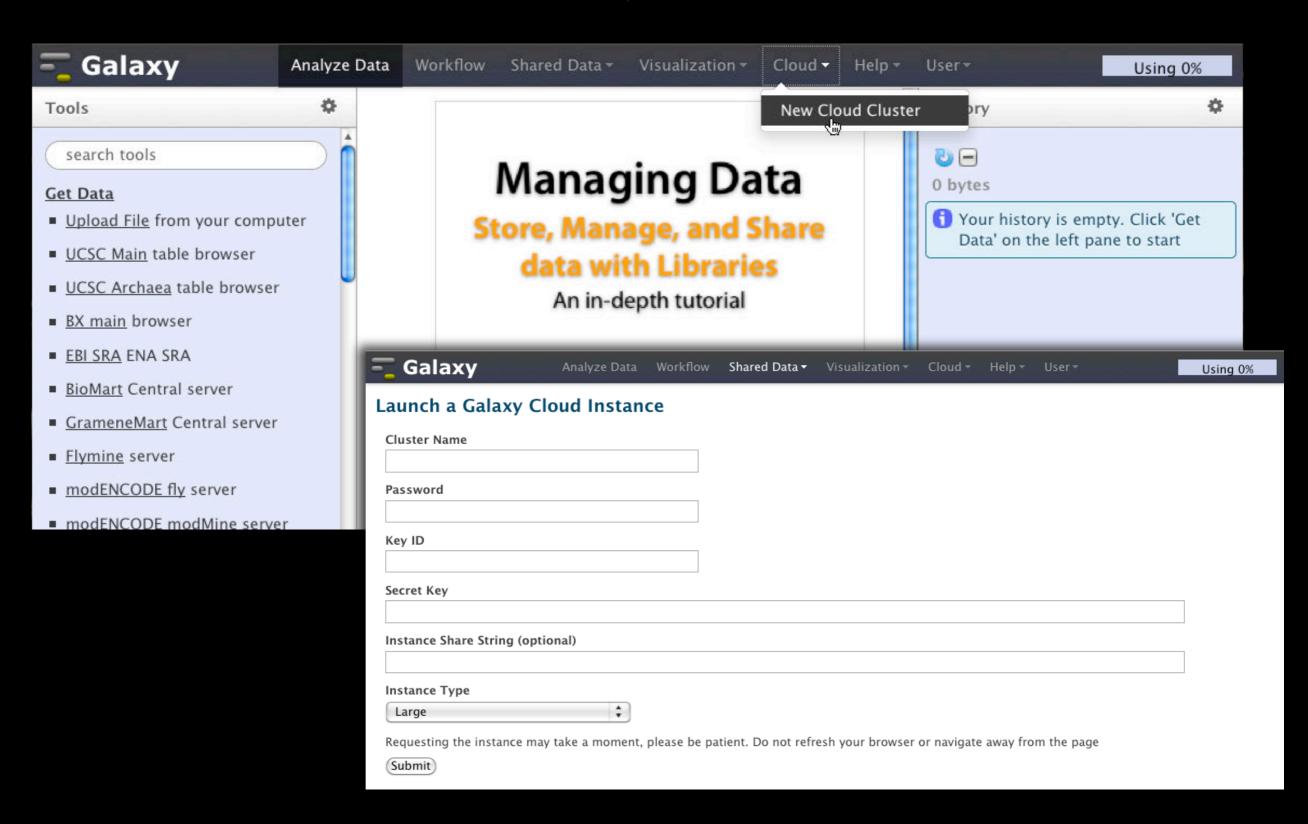
Contents

- 1. Step 1: One Time Amazon Setup
- 2. Step 2: Starting a Master Instance
- 3. Step 3: Galaxy CloudMan Web Interface
- 4. Step 4: Use Galaxy as you normally would
- 5. Step 5: Shutting Down

Step 1: One Time Amazon Setup

- Because AWS services implement pay-as-you-go access model for compute resources, it is necessary for every user of the service to register with Amazon. You will need a credit card to register. (You can apply for a AWS Education Grant after you register).
- Once your account has been approved by Amazon (note that this may take up to one business day), log into the EC2 AWS Management Console and set your AWS Region to US East (Virginia). This is the only region Galaxy CloudMan is fully supported in at this time (see screenshot 1.2).
- Click Network & Security → Key Pairs or My Resources → n Key Pairs (see screenshot 1.3 - if it does not look like this, then try using the Chrome browser) and then click Create Key Pair. Enter a memorable name for the key pair, e.g., GalaxyCloud and click Create.
- 4. Save your private key! The previous step creates the key pair and downloads a copy to your machine with the name MemorableName.pem. Save this file and protect it like you would your password. The key pair can be used to access started instances from

Instant CloudMan http://usegalaxy.org/cloudlaunch



Instant CloudMan

AWS Credentials

http://bit.ly/WashUWed

Instant Feedback

http://bit.ly/20130501Gxy

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Exploring Parameter Space with Trackster

