Introduction to Galaxy

National Institute of Environmental Health Sciences Research Triangle Park, NC July 18, 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-Seg Example Part I 12:20 Lunch 1:35 Galaxy Project Overview 1:55 RNA-Seg Example Part II 2:45 Break Sharing, Publishing and Reproducibility 3:05 Setting up Galaxy on the Amazon Cloud Done 5:00

Introductions

In 46 seconds or less tell us

- your name
- your affiliation(s)
- something about your research
- something about your goals for today

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
 - Learn how to set up a 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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Basic Analysis: We have

an assembly of an archaeal organism gene annotation

TF binding sites

Which genes have most overlapping TFBs?

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

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

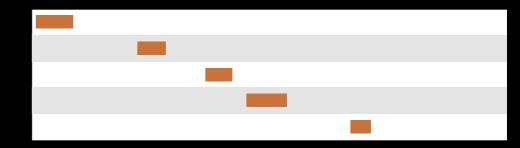
Genes & TFBs: A General Plan

- Get some data
 - Sequence, genes/exons, TFBs
- Mess with it
 - Identify which genes/exons have TFBs
 - Count TFBs per exon
 - Visualize, save, download, ... exons with most TFBs

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

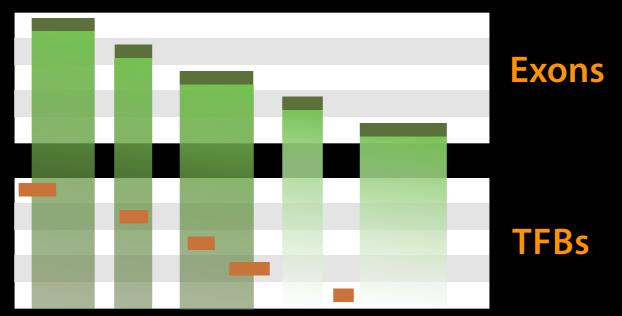
(~ http://usegalaxy.org/galaxy101)

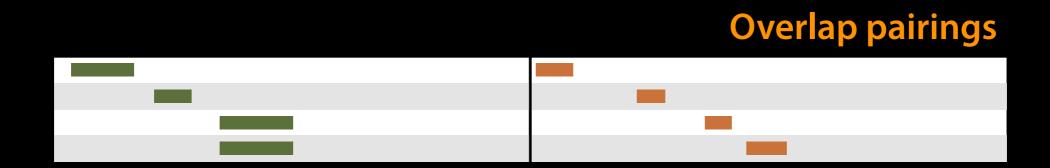


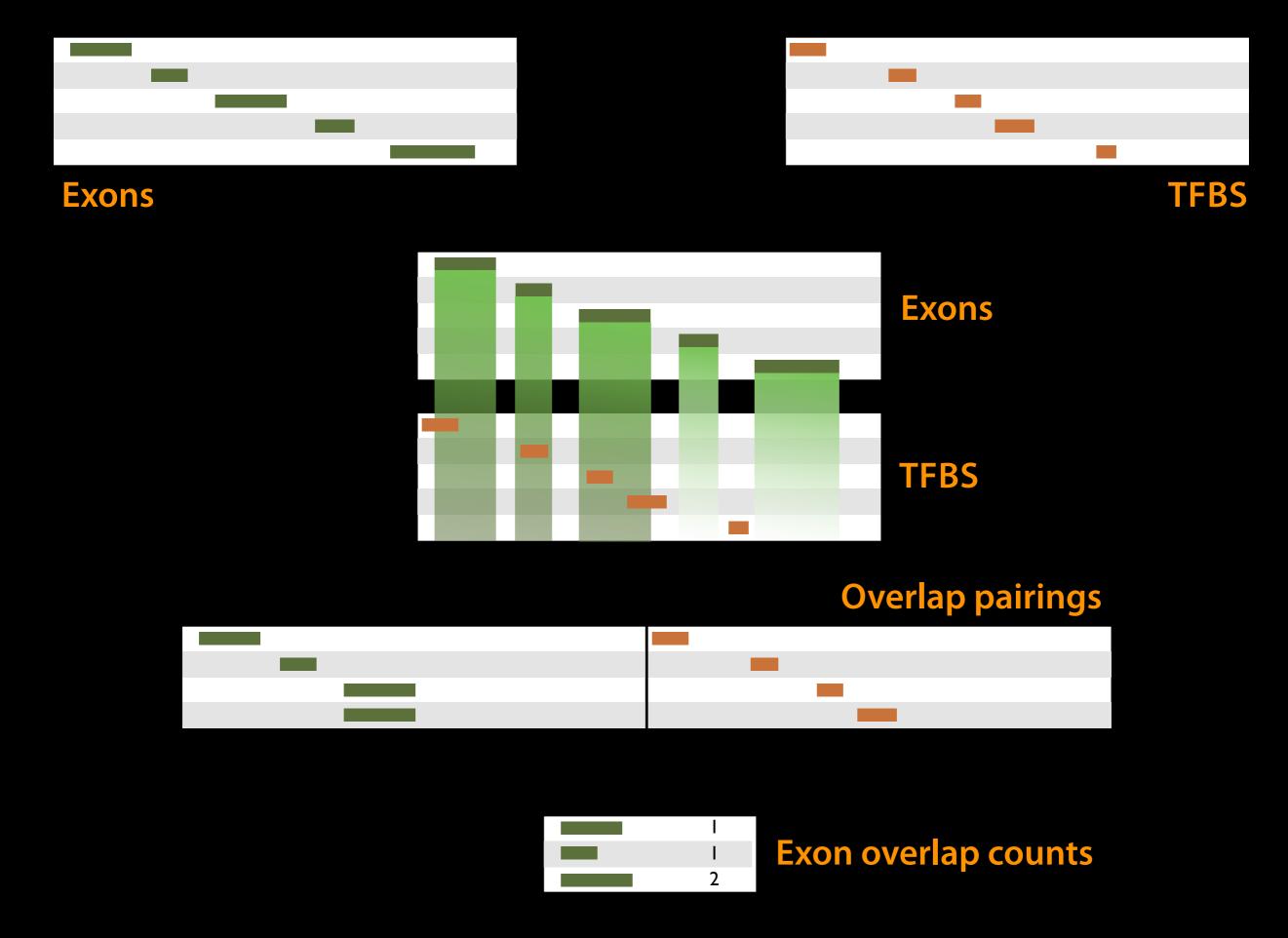


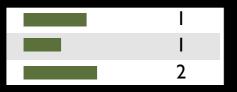
Exons TFBs











Exon overlap counts



Exons



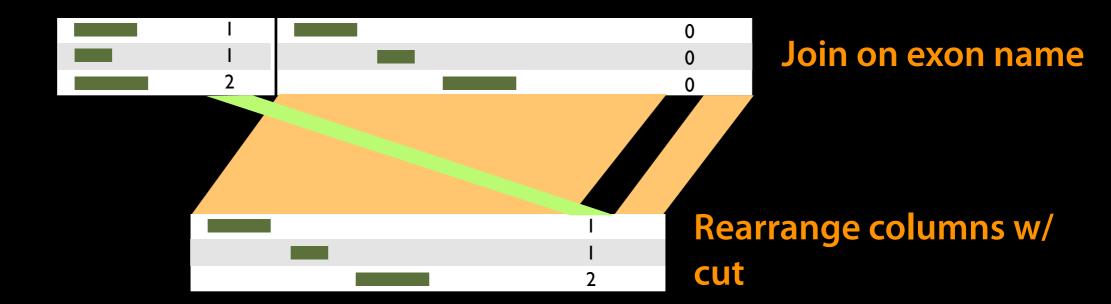


Exons

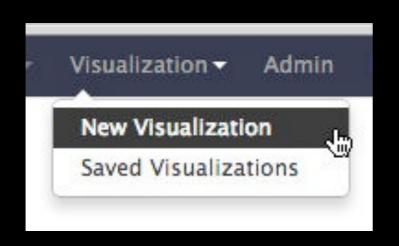








Visualize results







- 9:00 Welcome Basic Analysis with Galaxy 9:20 10:40 Break Basic Analysis into Reusable Workflows 11:00 RNA-Seq Example Part I 11:20 12:20 Lunch 1:35 Galaxy Project Overview 1:55 RNA-Seg Example Part II
 - 2:45 Break
 - 3:05 Sharing, Publishing and Reproducibility
 - 3:25 Setting up Galaxy on the Amazon Cloud
 - 5:00 Done

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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 TFBs *History* → Reusable *Workflow?*

- The analysis we just finished was about
 - An archaea
 - Overlap between exons and TFBs
- But, ...
 - there is nothing inherently in the analysis about archaea, exons or TFBs
 - 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

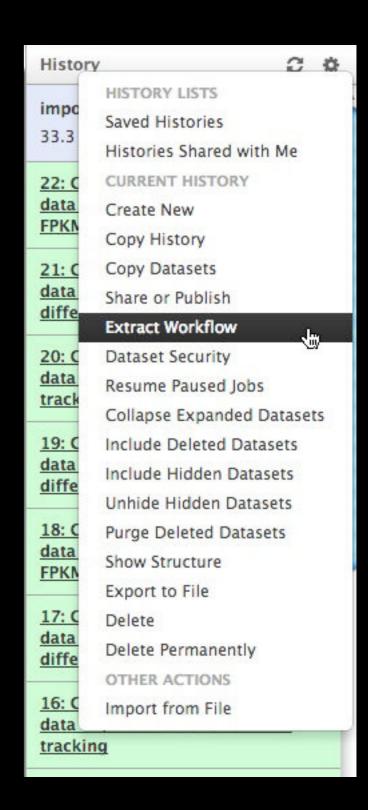
Create a workflow from this history. Edit it to make some things clearer.

Run / test it

Guided: rerun with same inputs Did that work?

On your own:

Count # of exons in each TFBS 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
- Visualize it

- Get input datasets; hg19, will mostly map to chr19
 - All datasets are FASTQ and from the Body Map
 2.0 project
 - Shared Data → Published Pages → RNA-Seq
 Analysis Exercise
 - or Shared Data → Data Libraries → RNA-Seq
 Example

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:

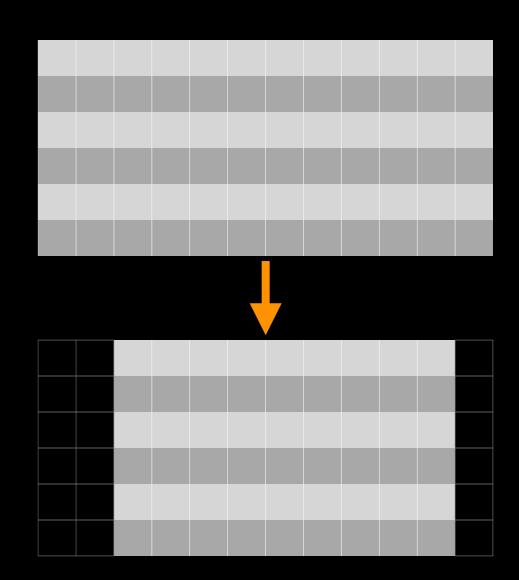
- 1. NGS QC and Manipulation → Compute Quality Statistics
 NGS QC and Manipulation → Draw quality score boxplot
 No control over how it is calculated or presented.
- 2. NGS QC and Manipulation → FastQ Summary Statistics,
 Graph / Display Data → Boxplot of quality statistics

Lots of control over what the box plot looks like, Statistics in text and graphic formats

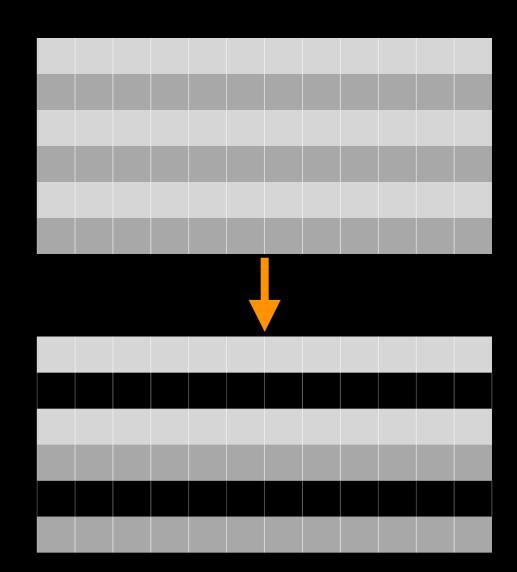
- Get input datasets; hg19, will mostly map to chr19
- Look at quality: Option 3
 - NGS QC and Manipulation → FastQC
 - Gives you a lot a lot more information but little control over how it is calculated or presented.

http://bit.ly/FastQCBoxPlot

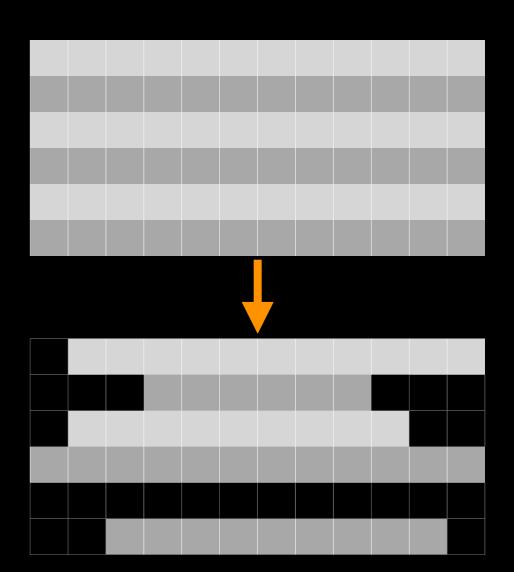
- Look at quality
- Trim as we see fit: Option 1
 - NGS QC and Manipulation →
 FASTQ Trimmer by column
 - Trim same number of columns from every record
 - Can specify different trim for 5' and 3'ends



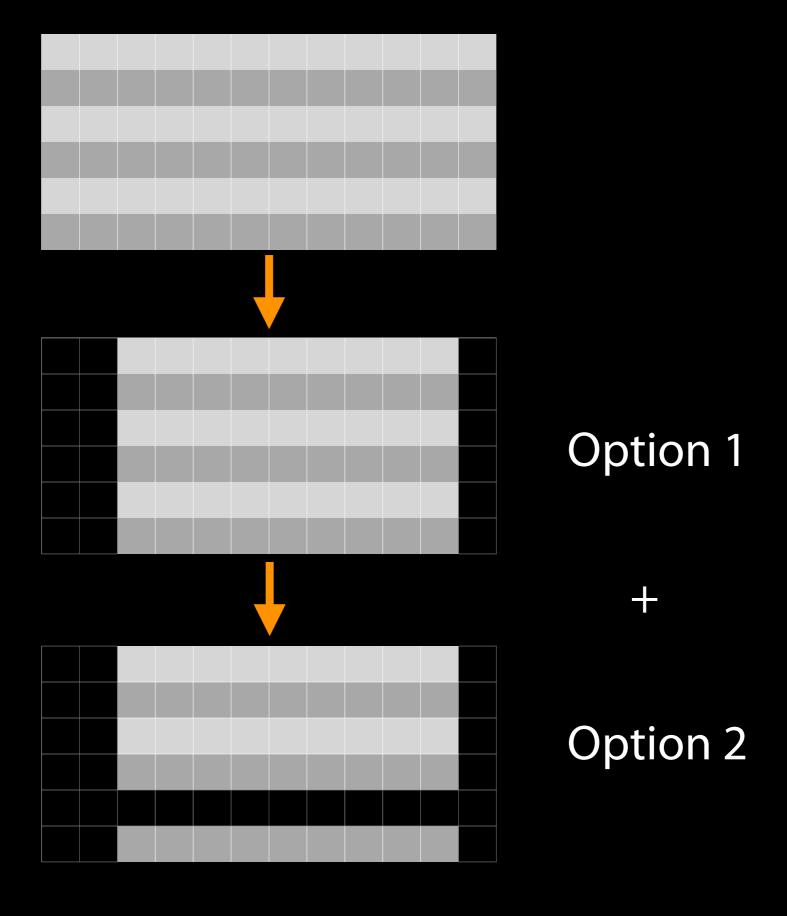
- Look at quality
- Trim Filter as we see fit: Option 2
 - NGS QC and Manipulation →
 Filter FASTQ reads by quality
 score and length
 - Keep or discard whole reads
 - Can have different thresholds for different regions of the reads.
 - Keeps original read length.



- 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 high-quality 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
 - Tophat looks for best place(s) to map reads, and best places to insert introns
 - Imagine pages and pages of discussion on the intricacies and pitfalls of RNA-seq mapping here.

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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

However, 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

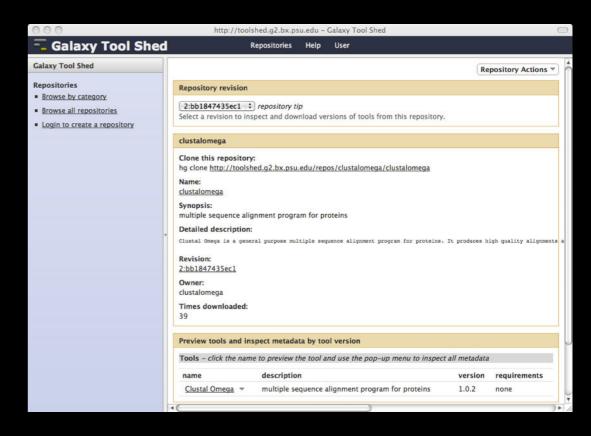
- Galaxy is designed for local installation and customization
 - Easily integrate new tools
 - Easy to deploy and manage on nearly any (unix) system
 - Run jobs on existing compute clusters
- Requires a computational resource on which to be deployed

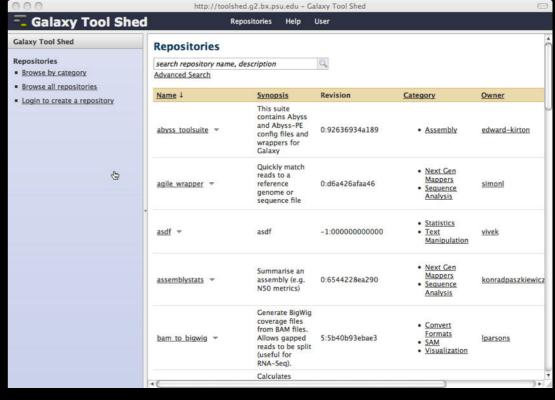
http://getgalaxy.org

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

http://getgalaxy.org

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 we will demonstrate how to do this later today

http://aws.amazon.com/education

Galaxy is available ...

- As a free (for everyone) web service
- As open source software
- On the Cloud
- With Commercial Support



Cloud-based solutions (Appistry, ABgenomica, AIS)

Consulting & Customization (Arctix, Deena Bioinformatics)



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 in 2012, 2100+ members)

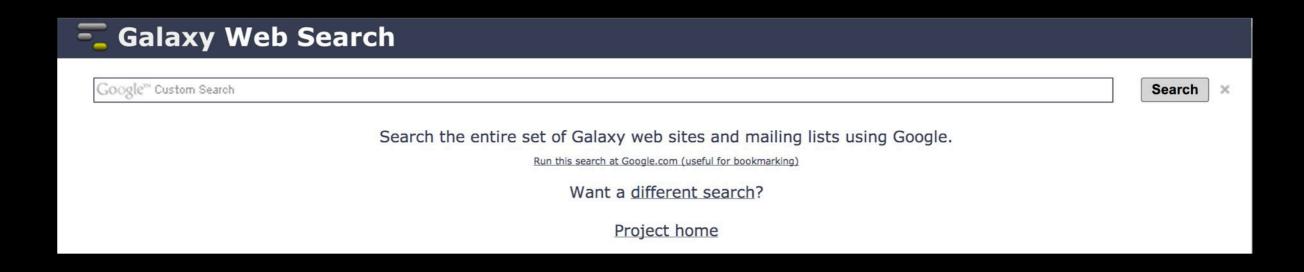
Galaxy-User

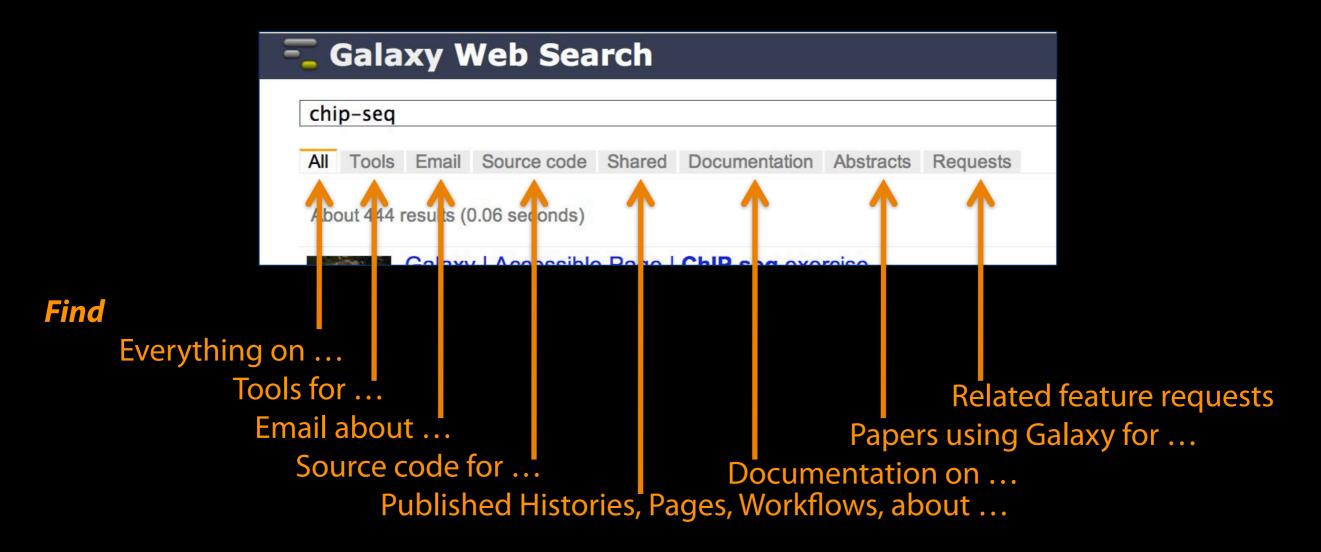
Questions about using Galaxy and usegalaxy.org High volume (2900 posts in 2012, 2700+ members)

Galaxy-Dev

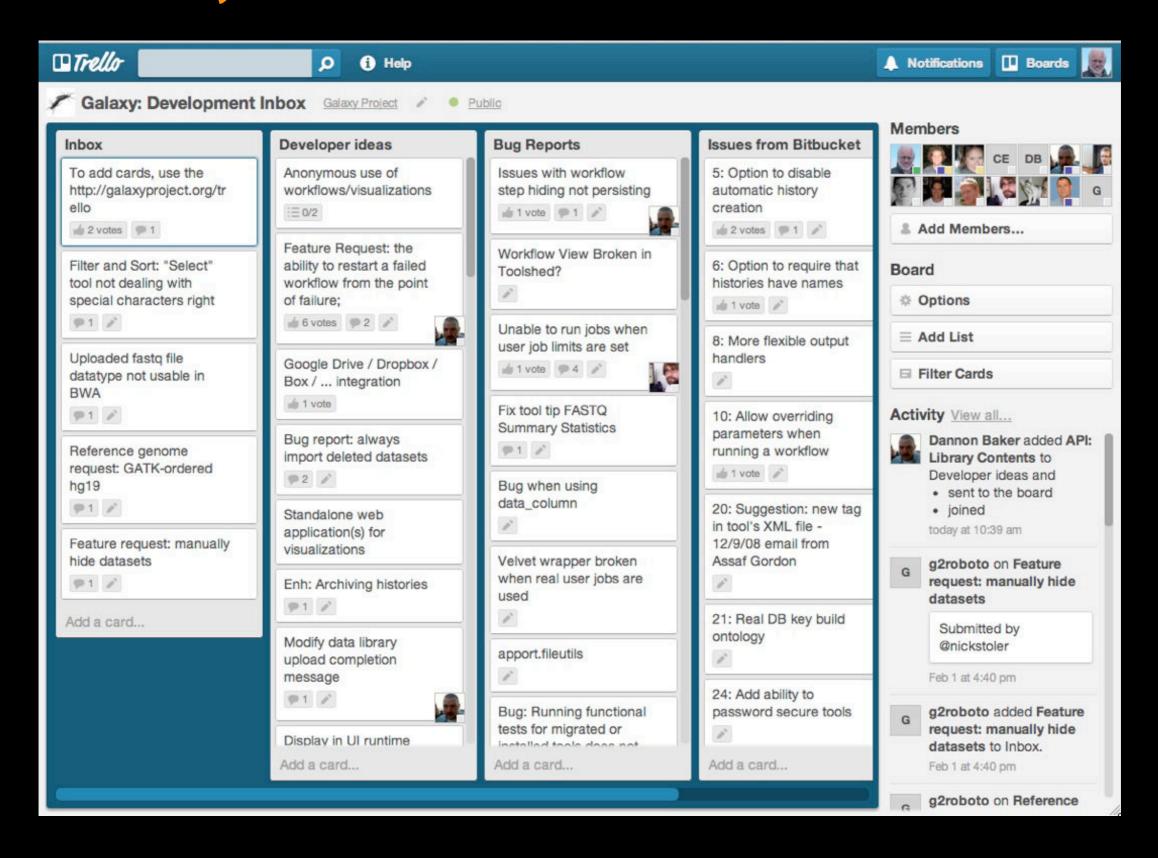
Questions about developing for and deploying Galaxy High volume (4500 posts in 2012, 900+ members)

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

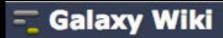




Community can create, vote and comment on issues



http://wiki.galaxyproject.org



DaveClements Settings Logout |

Search:

Titles Text



FrontPage

Edit 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.

=usegalaxy.org

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
- Galaxy Appliance

getgalaxy.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!



Use Galaxy

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

Communication

Support . News [3] 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

Galaxy Wiki

DaveClements Settings Logout

Galaxy Wiki

DaveClements Settings Logout | Search:

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 .

Upcoming Events







Date	Topic/Event	Venue/Location
July 18-23	Introduction to Galaxy Workshop National Institute of Environmental Health Sciences (NIEHS)	2013 Research Triangle W Tour, North Carolina, Unite
	Introduction to Galaxy Workshop University of North Carolina, Chapel Hill	
	Galaxy Installation Tutorial 2013 GMOD Summer School	
	Introduction to Galaxy Workshop North Carolina State University	
July 19-23	ISMB/ECCB, BOSC and MS SIG 2013 Talks, posters and workshops. Lots of them.	Berlin, Germany
July 21-25	Experiences in building a Next-Generation Sequencing Analysis Service using Galaxy, Globus Online, and Amazon Web Services	XSEDE13, San Diego, Ca United States
	A Sustainable National Gateway for Biological Computation	
	Supporting Genomics and other Biological Research	
September 28 - October 1	Galaxy Workshop	The Genomic Bioinformatics Workshop, Sydney, Australi
October 1-3	Galaxy	Beyond the Genome 2013 Francisco, California, United
October 7-8	TBD	NGS & Bioinformatics Su Europe
	Using Galaxy to Provide a NGS Analysis Platform	
October 9-11	Galaxy Training Days	GenoToul bioinformatics fac INRA, Toulouse Auzeville, F
October 22- 26	High Throughput Data Analysis and Visualization with Galaxy	ASHG 2013, Boston, Massac United States
November 6-	What are stated and an area of the state of	Cold Spring Harbor Laborate York, United States
**	Application Deadline: July 15, 2013	Tork, Officed States

News

News

Announcements of interest to the Galaxy Community. These can include items from the Galaxy Team or the Galaxy community and can address anything that is of wide interest to the community.

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

New CloudMan Release SlipStream Appliance: Galaxy Edition July 2013 Galaxy Update 1000th Galaxy CiteULike Paper GCC2013 Registration Ends 14 June June 3, 2013 Galaxy Distribution June 2013 Galaxy Update Software Carpentry Boot Camp: Oslo GCC2013 Early Registration Ends 24 May Duplicate Accounts on Main

News Archive

News Items

New CloudMan Release

We just released an update to Galaxy CloudMan. CloudMan offers an easy way to get a personal and completely functional instance of Galaxy in the cloud in just a few minutes, without any manual configuration.

IMPORTANT - please read

Any new cluster will automatically start using this version of CloudMan. Existing clusters will be given an option to do an automatic update once the main interface page is refreshed. Note that this upgrade is a major version upgrade and thus the migration is rather complicated. The migration process has been automated but will take a little while to complete. If you have made customizations to your cluster in terms of adding file systems, upgrading the database, or similar, we do not recommend you perform the upgrade. Note that this upgrade comes with (and requires) a new AMI (ami-118bfc78), which will automatically be used when starting an instance via CloudLaunch.

This update brings a large number of updates and new features, the most prominent ones being:

- . Unification of galaxyTools and galaxyData file systems into a single galaxy filesystem. This change makes it possible to utilize the Galaxy Tool Shed when installing tools into Galaxy.
- · Added initial support for Hadoop-type workloads
- · Added initial support for cluster federation via HTCondor
- · Added a new file system service for an instance's transient storage, allowing it to be used across the cluster over NFS
- · Added a service for the Galaxy Reports webapp
- · Added optional Loggly based off-site logging support
- · Added tags to all resources utilized by CloudMan

For more details on the new features, see the the CHANGELOG and for even more details see, all 291 commit messages from 7 contributors.

Enjoy and please let us know what you think,

Enis Afgan

Posted to the Galaxy News on 2013-07-08

SlipStream Appliance: Galaxy Edition





http://bit.ly/gcc2014







The Galaxy Team



http://wiki.galaxyproject.org/GalaxyTeam

Galaxy is hiring post-docs and software engineers



Please help.

http://wiki.galaxyproject.org/GalaxylsHiring

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RNA-seq Exercise: A Plan

- ...
- Map the reads to the human reference using Tophat
- Run Cufflinks on Tophat output to assemble reads into transcripts
 - Tophat does not make any predictions about how the reads it mapped, assemble together into transcripts.
 - Imagine pages and pages of discussion on the intricacies and pitfalls of RNA-seq transcript prediction here.

RNA-seq Exercise: A Plan

- ...
- Map the reads to the human reference using Tophat
- Run Cufflinks on Tophat output to assemble reads into transcripts
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 - Visualize it

Visualizing Genomics

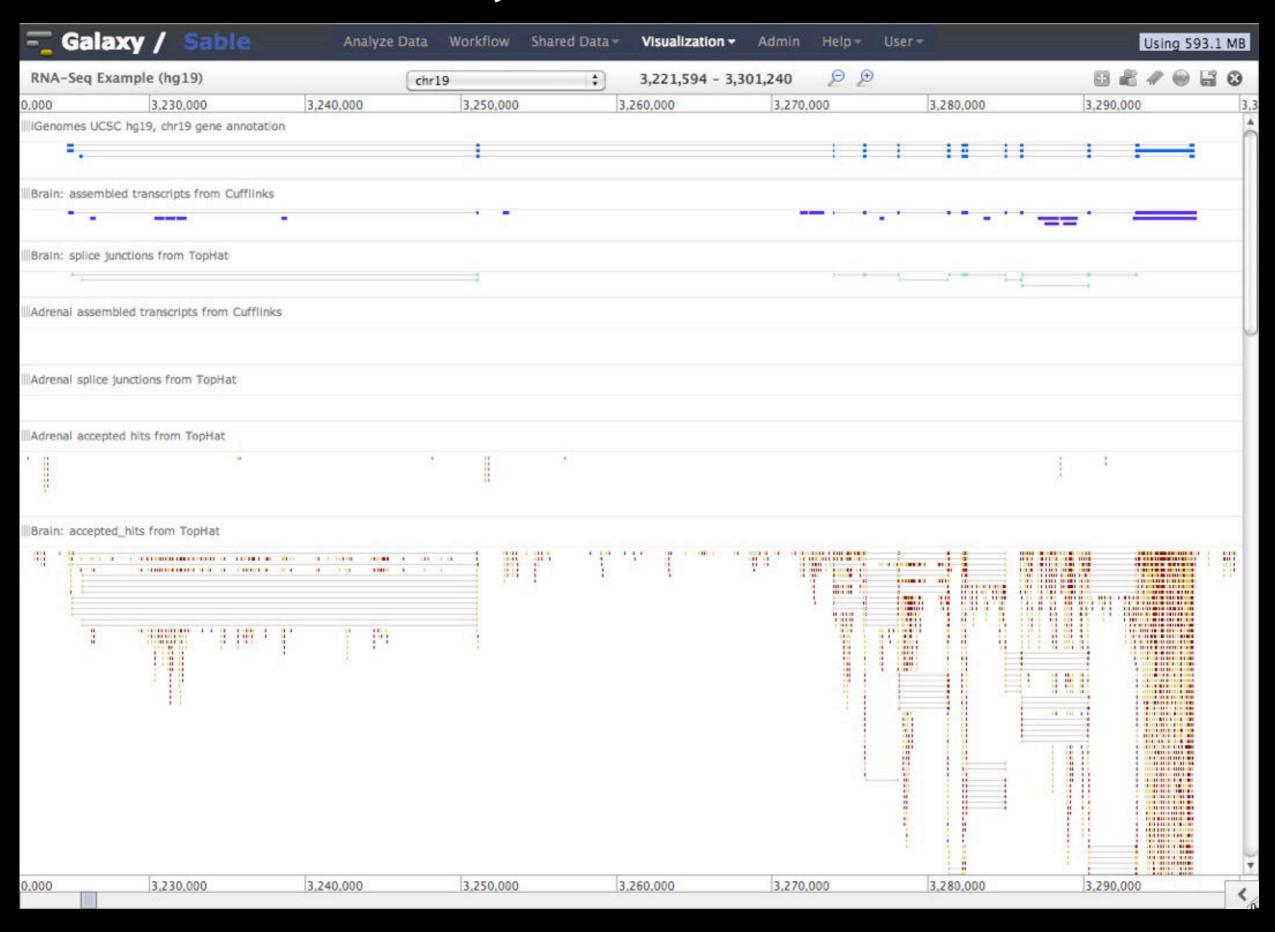
Supported external browsers

- UCSC
- Ensembl
- GBrowse
- IGB
- IGV

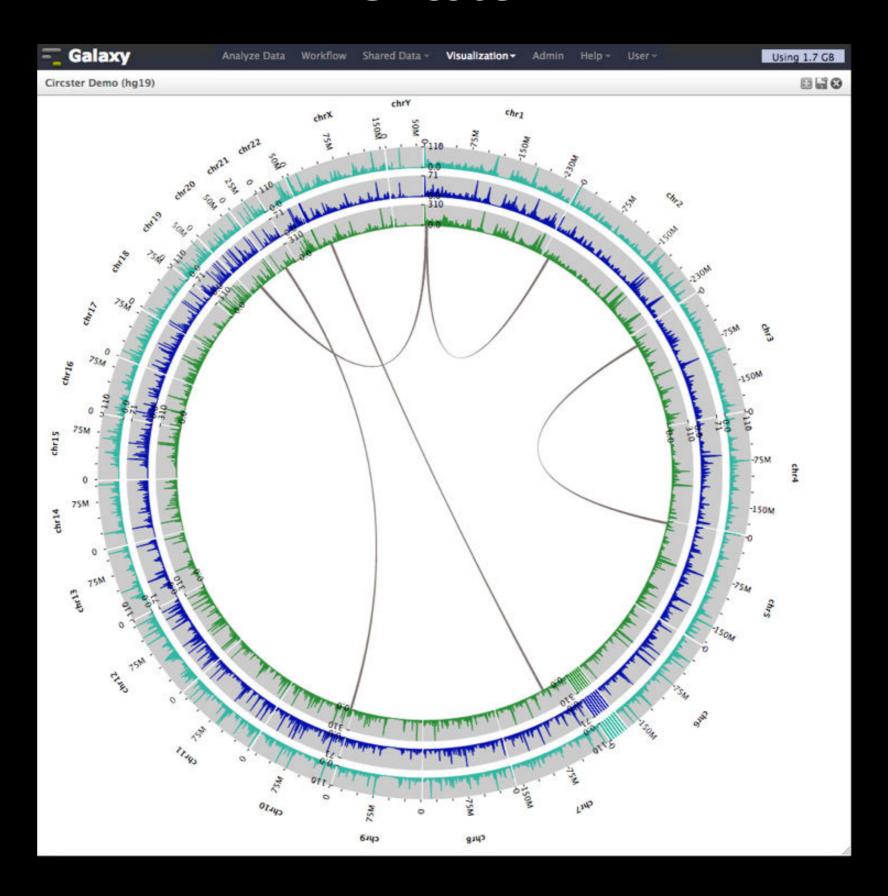
Traditional browser strengths:

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

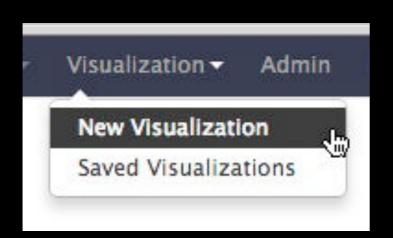
Trackster: Galaxy's embedded track browser



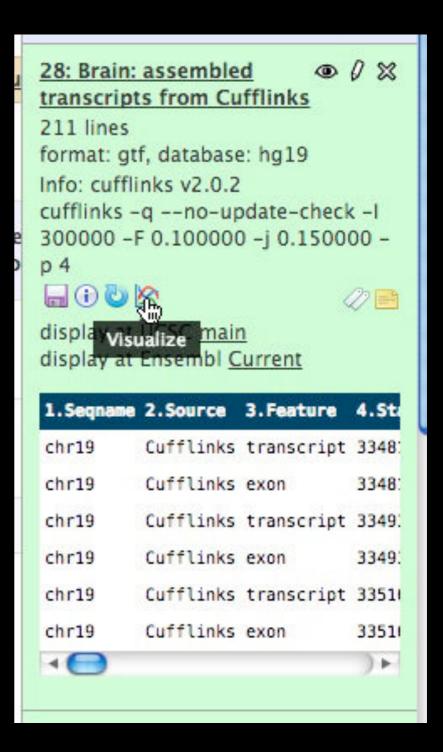
Circster



Create a visualization in Galaxy







Vizualization inside Galaxy

- Levarge visualization to evaluate and refine analyses
- Expose basic analyses in visualization to make it more informative
- Make the analyze-visualize-refine loop seamless and fast
- Enable experimenting with tools and their parameter space
- Support custom genome browsers

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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





HOME ABOUT ARCHIVE SUBMIT SUBSCRIBE ADVERTISE AUTHORINFO CONTACT HELP

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

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Abstract Free
 Full Tayt (PDE) Free

Current Issue

October 2010, 20 (10)



Sharing & Publishing enables Reproducibility





ABOUT ARCHIVE SUBMIT SUBSCRIBE ADVERTISE AUTHOR INFO CONTACT HELP

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,

Francesca Chiaromonte⁴, 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

OPEN ACCESS ARTICLE

This Article

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» Abstract Free

Current Issue October 2010, 20 (10)



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

SERGEI KOSAKOVSKY POND^{1,2,*}, SAMIR WADHAWAN^{3,6*}, FRANCESCA CHIAROMONTE⁴, GURUPRASAD ANANDA^{1,3}, WEN-YU CHUNG^{1,3,7}, JAMES TAYLOR^{1,5}, ANTON NEKRUTENKO^{1,3} and THE GALAXY TEAM^{1*}

Correspondence should addressed to SKP, JT, or AN.

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.



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



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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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 1:35 Galaxy Project Overview 1:55 RNA-Seq Example Part II 2:45 Break 3:05 Sharing, Publishing and Reproducibility Setting up Galaxy on the Amazon Cloud 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

ogin | Search:

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

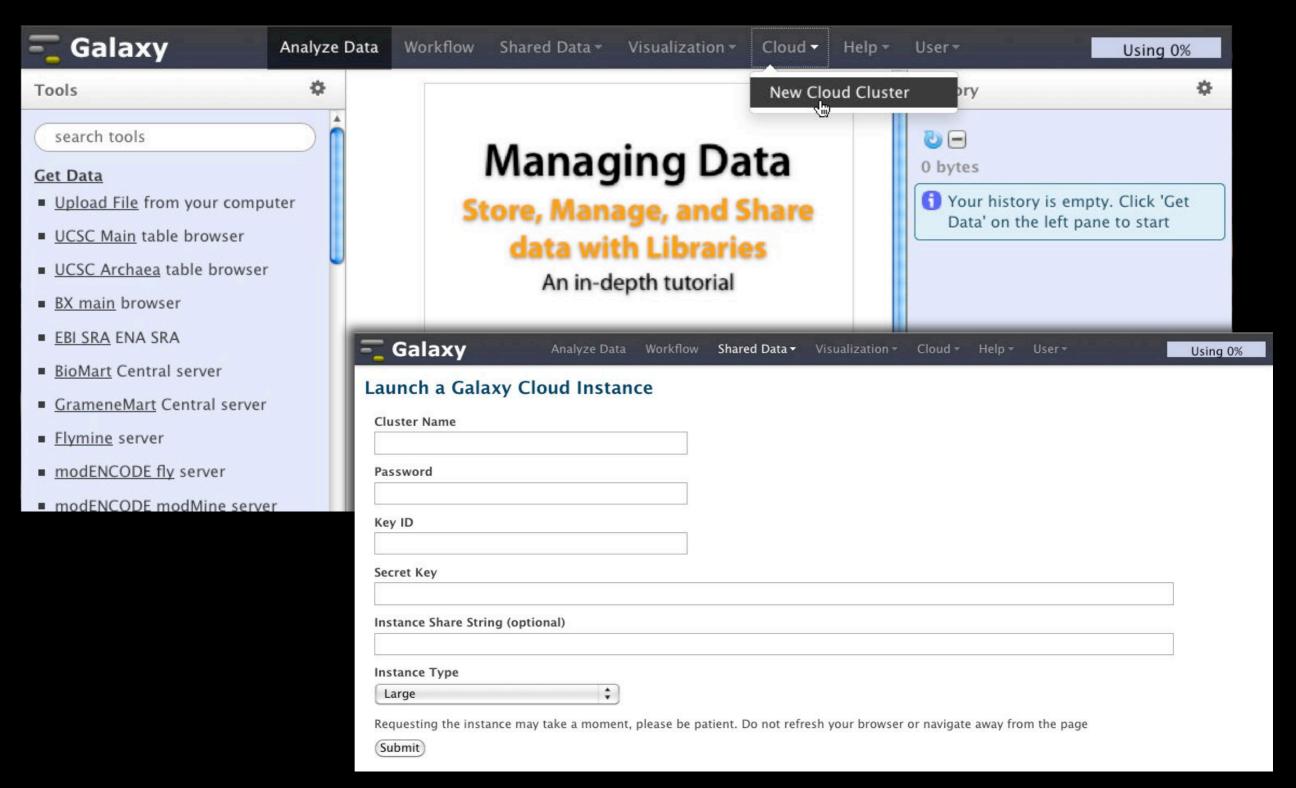
- Because AWS services implement pay-as-you-go access model for compute resources, it is necessary for every user of the service to register with Amazon. You will need a credit card to register. (You can apply for a AWS Education Grant after you register).
- Once your account has been approved by Amazon (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



AWS Credentials

http://bit.ly/niehsAWS

Instant CloudMan http://usegalaxy.org/cloudlaunch



http://bit.ly/niehsAWS

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Instant Feedback

http://bit.ly/20130718Gxy

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