

Galaxy Community Conference

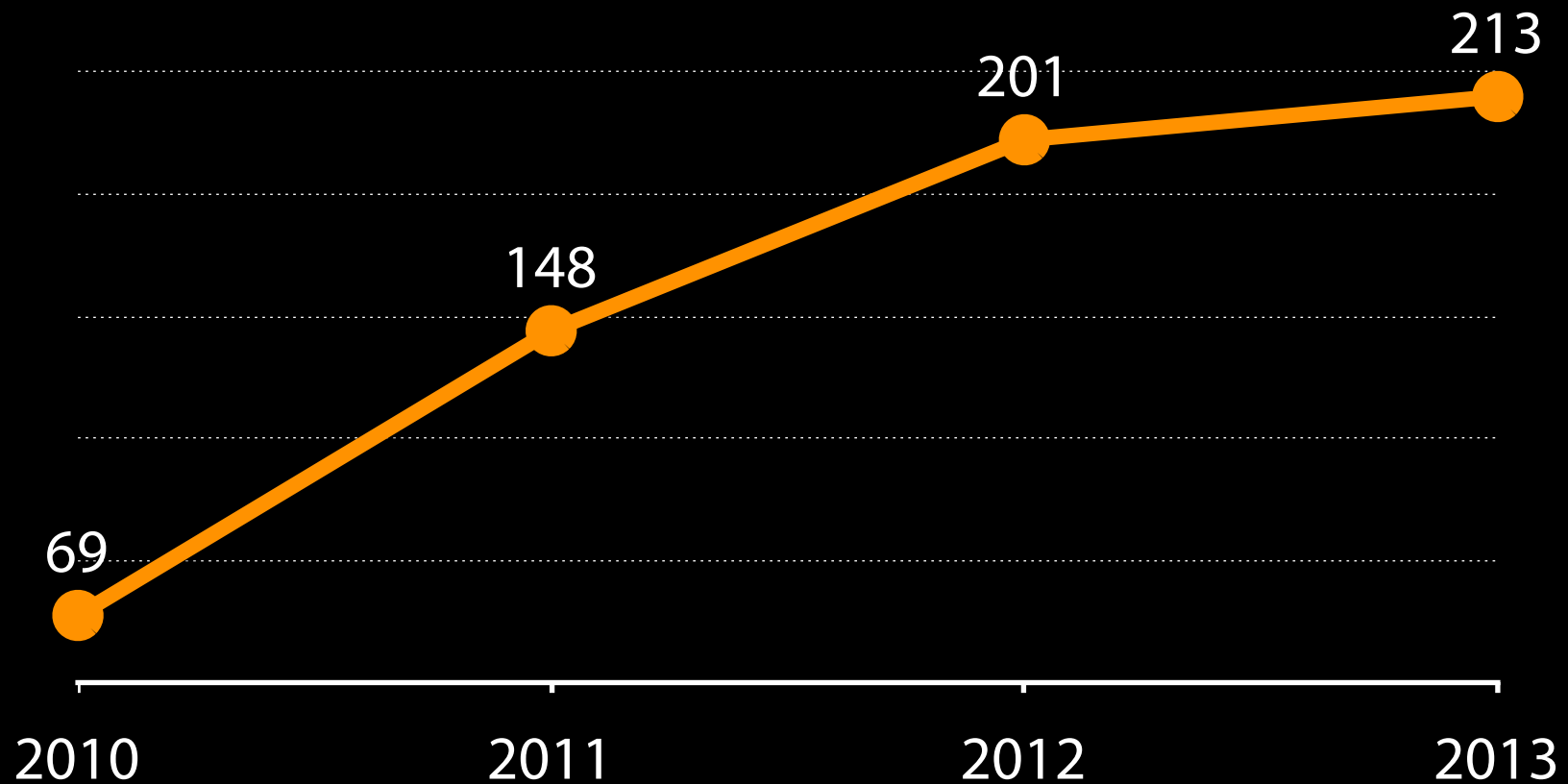
30 June
- 2 July

2013



UiO : University of Oslo

GCC attendance through the years

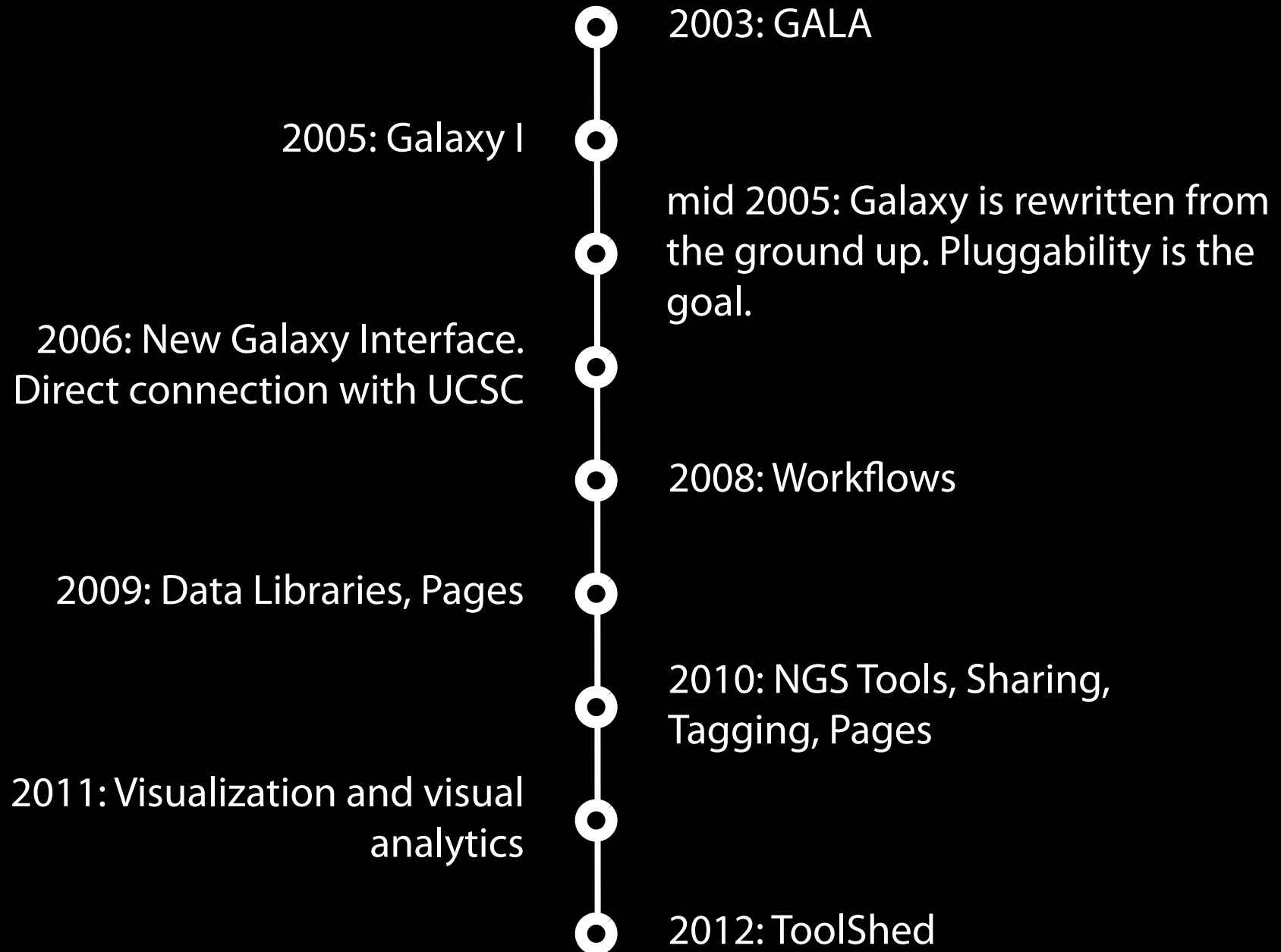




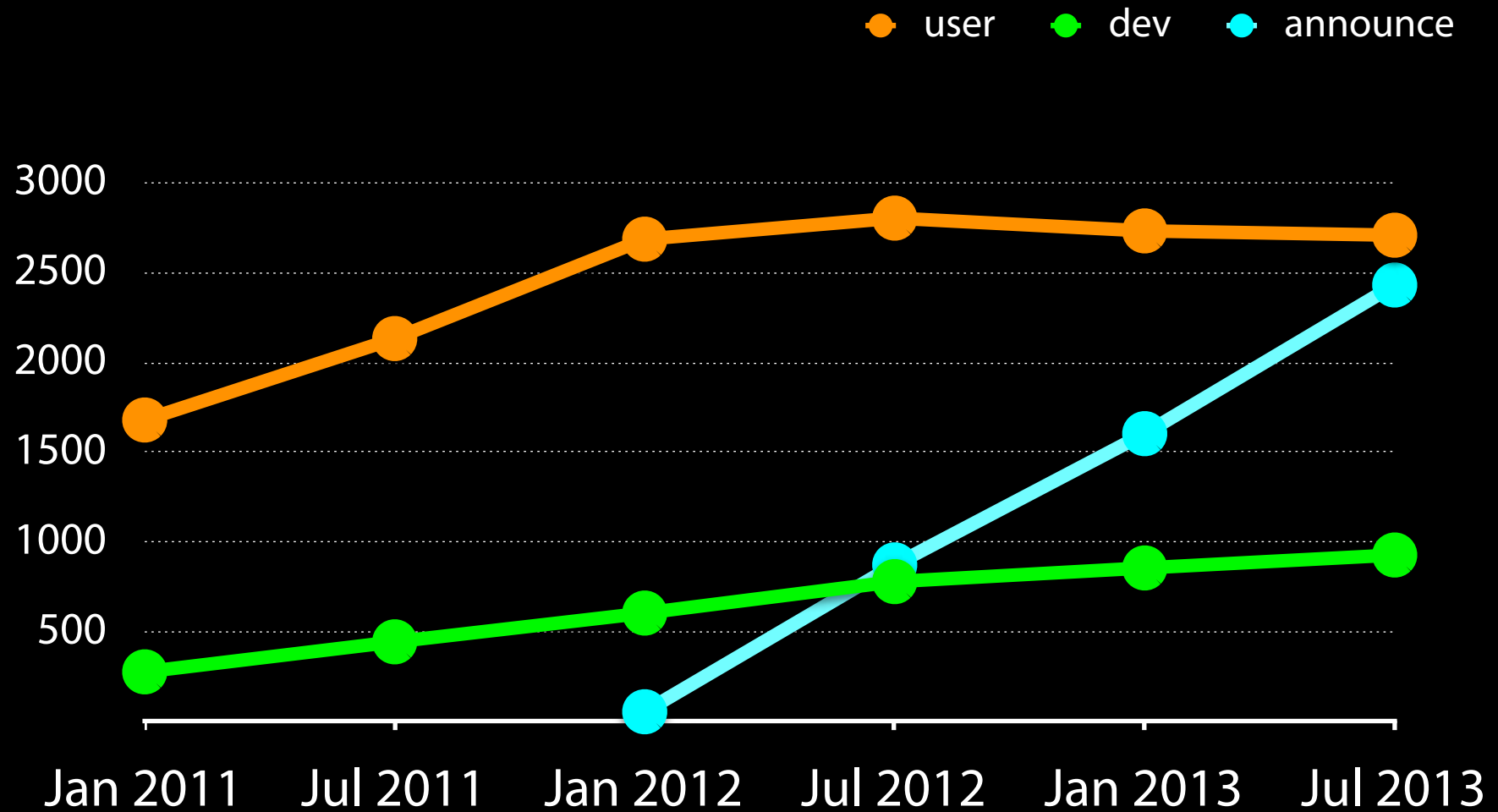
Wednesday, July 17, 13

The State of Galaxy

Galaxy timeline



Mailing List Membership



New Users per Month



Publications from others on Galaxy: ~1000 @ CiteULike



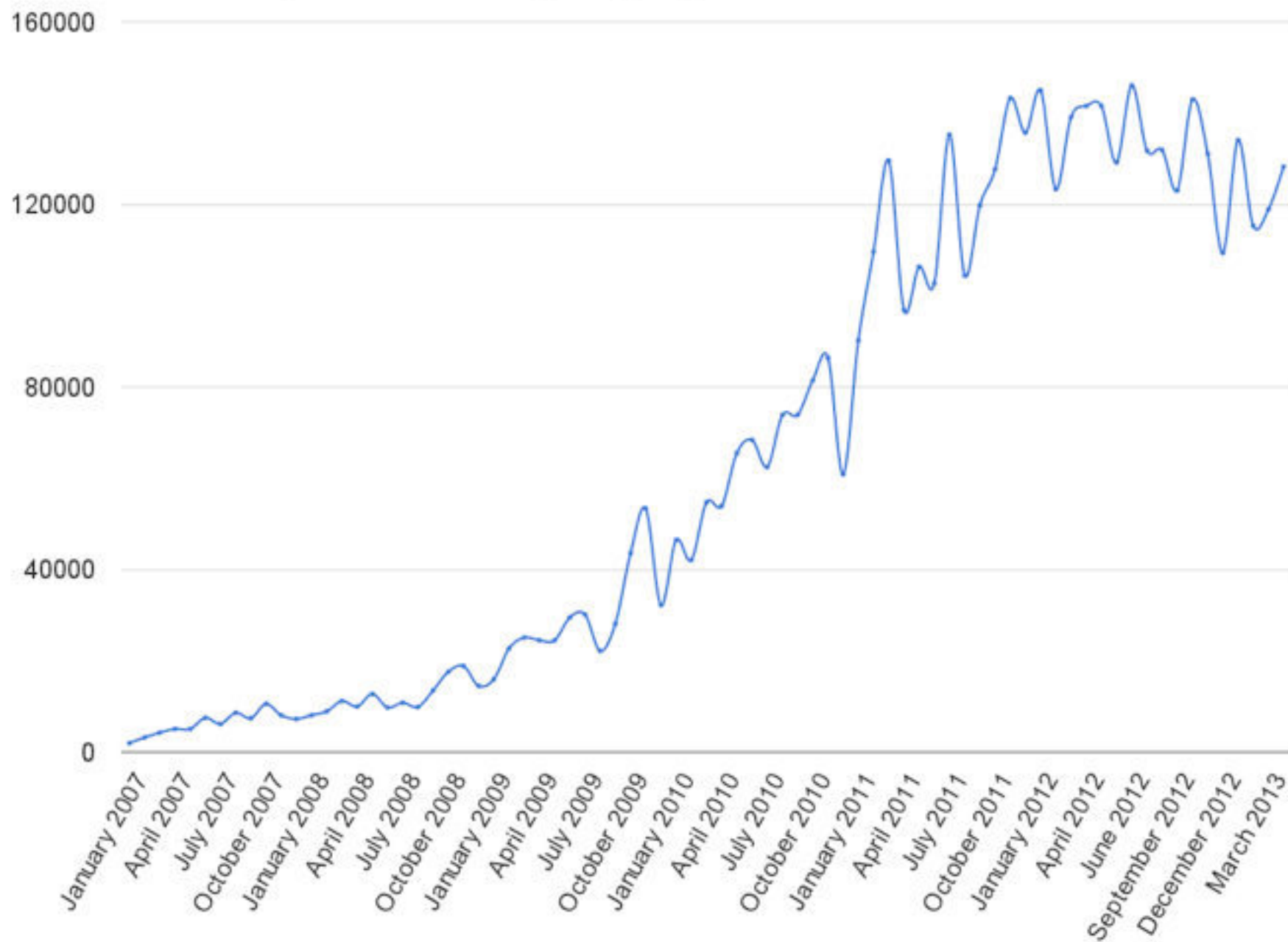
36,228

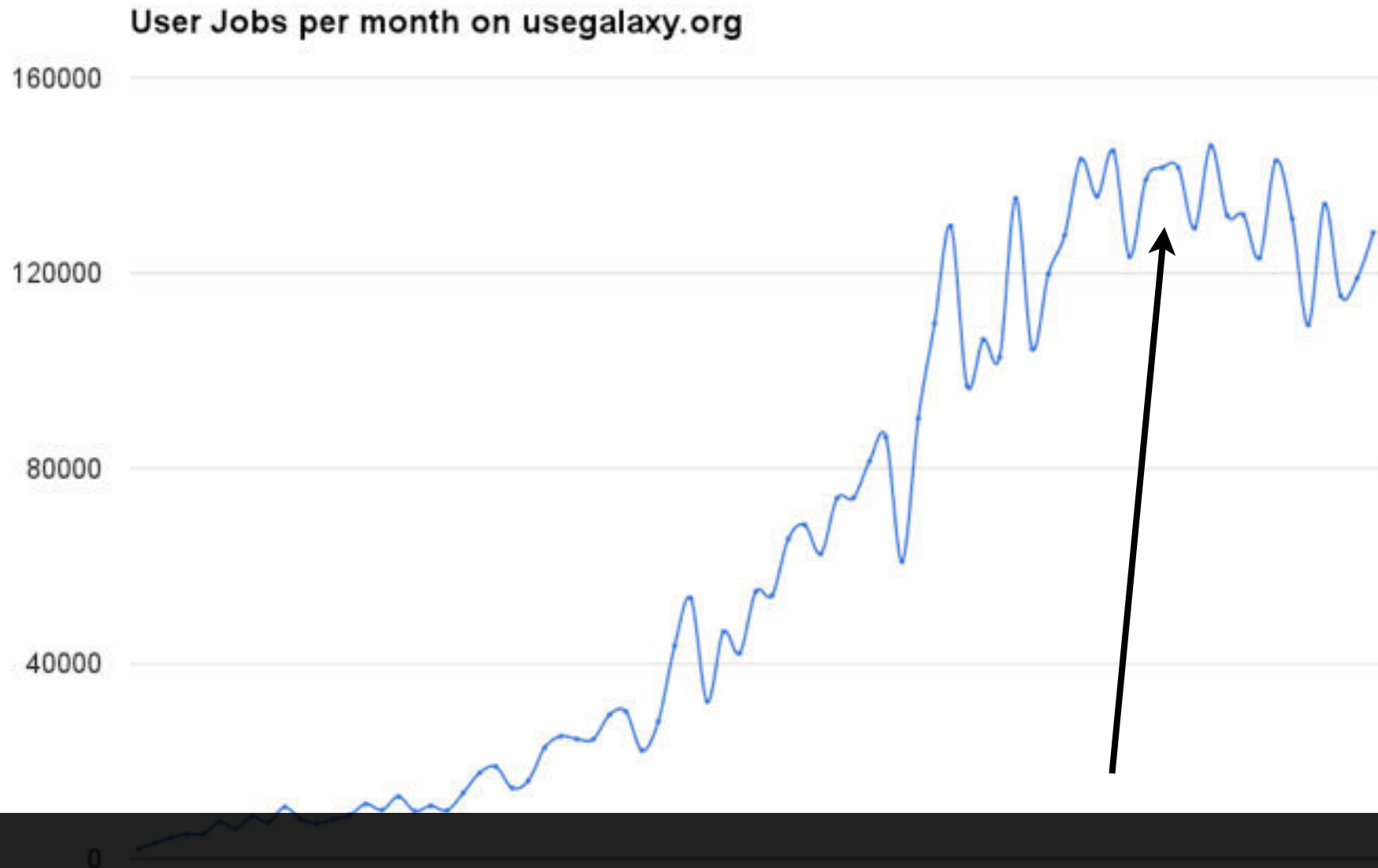
0.8 Pb

Most popular NGS tools (jobs in 2012)

- bowtie (50,693)
- cufflinks (31,085)
- tophat (31,085)
- fastQC (26,217)
- MACS (26,553)
- BWA (17,465)

User Jobs per month on usegalaxy.org





Plateau is due to resource constraints not reduced demand, runtime of individual jobs getting longer

More than 30 known public Galaxy servers

Ballaxy for structure based computational biology,
Cistrome for regulatory sequence analysis,
Genomic Hyperbrowser: statistical integration of genomic data,
GigaGalaxy: integrating workflows published in GigaScience,
Pathogen Portal: comparative analysis of host response to pathogens,
...

Dozens of large scale private Galaxy instances

NIH projects involving Galaxy

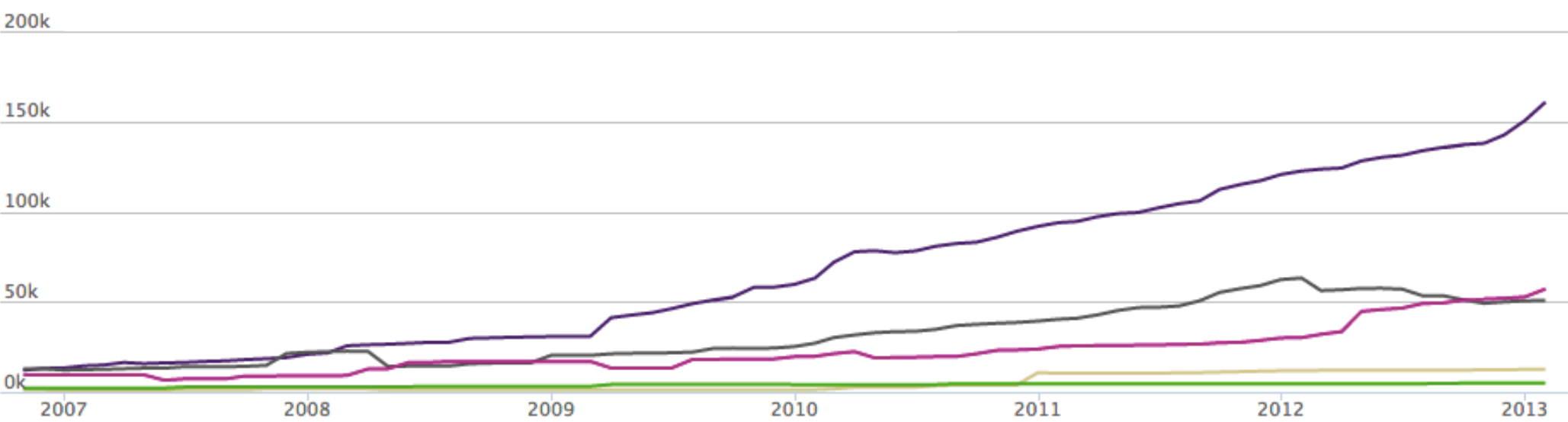
Project Title	Institute	Project Number	PI	Institution
GENE ONTOLOGY CONSORTIUM	NHGRI	2U41HG002273-12	BLAKE, JUDITH A	JAX
A DATA COORDINATING CENTER FOR ENCODE	NHGRI	1U41HG006992-01	CHERRY, JOE MICHAEL	STANFORD
ADVANCING THE SCIENTIFIC POTENTIAL OF TRANSCRIPTOMICS IN AQUATIC MODELS	OD	8R24OD011199-02	CRESKO, WILLIAM A	U Oregon
ENHANCING THE GMOD SUITE OF GENOME ANNOTATION AND VISUALIZATION TOOLS	NHGRI	5R01HG004483-05	HOLMES, IAN H	UC Berkeley
STATISTICAL ANALYSIS METHODS AND SOFTWARE FOR CHIP-SEQ DATA	NHGRI	2R01HG003747-05A1	KELES, SUNDUZ	U Wisconsin
STATISTICAL POWER CALCULATIONS FOR CHIP-SEQ EXPERIMENTS	NHGRI	1R21HG006716-01	KELES, SUNDUZ	U Wisconsin
A DATA ANALYSIS CENTER FOR INTEGRATION OF FLY AND WORM MODENCODE DATASETS	NHGRI	3RC2HG005639-02S1	KELLIS, MANOLIS	MIT
COMPUTATIONAL MODELS FOR MECHANISMS OF GLOBAL TRANSCRIPTION	NHGRI	5R01HG004069-07	LIU, XIAOLE SHIRLEY	DANA-FARBER
ROBUST SOFTWARE TOOLS FOR VARIANT IDENTIFICATION AND FUNCTIONAL ASSESSMENT	NHGRI	3U01HG006513-02S1	MARTH, GABOR T	Boston College
GENOMESPACE: A COMMUNITY WEB ENVIRONMENT FOR INTEGRATIVE GENOMIC ANALYSIS	NHGRI	5P01HG005062-04	MESIROV, JILL P.	Broad
UNLOCKING TRANSCRIPT DIVERSITY VIA DIFFERENTIAL ANALYSES OF SPLICE GRAPHS	NHGRI	1R01HG006272-01A1	PRINS, JAN F	UNC CH
NEW ALGORITHMS AND TOOLS FOR LARGE-SCALE GENOMIC ANALYSES	NHGRI	1R01HG006693-01	QUINLAN, AARON R	UVa
INTEGRATIVE TOOLS FOR PROTOZOAN PARASITE RESEARCH	NIGMS	5R01GM093132-03	STOECKERT, CHRISTIAN J.	UPenn
PROJECT III - COMPUTATIONAL ANALYSIS OF PHENOTYPES AND	NICHD	2P01HD039691-11	SUCGANG, RICHARD	Baylor
ECOLI HUB2.0: A NEXT-GENERATION E. COLI MODEL ORGANISM RESOURCE (SRI PROPOSAL ECU	NIGMS	5U24GM088849-04	THOMAS, PAUL D.	USC
MEGA2: MANIPULATION ENVIRONMENT FOR GENETIC ANALYSES	NIGMS	5R01GM076667-07	WEEKS, DANIEL E	Pitt
INIA: BIOINFORMATICS CORE	NIAAA	5U01AA016662-07	WILLIAMS, ROBERT W.	U Tennessee
NEW BAYESIAN ALGORITHMS FOR GENOME-WIDE ASSOCIATION MAPPING	NHGRI	2R01HG004718-04A1	ZHANG, YU	Penn State

NSF projects involving Galaxy

Project Title	Award Number	PI	Institution
GALAXY-P: A NEW COMMUNITY-BASED INFORMATICS PARADIGM FOR MS-BASED PROTEIOMICS	1147079	GRIFFIN, TIMOTHY	UMN
SOFTWARE AND SERVER FOR TAXONOMIC BINNING OF METAGENOMIC SEQUENCES	850103	TOVCHIGRENKO, ANDREY	JC Venter Inst.
GENERATION AND ANALYSIS OF A REFERENCE SEQUENCE FOR THE WEST AFRICAN CULTIVATED RICE - ORYZA	822284	WING, ROD	U Arizona
COMPUTATIONAL TOOLS AND STATISTICAL ANALYSIS OF CO-VARYING RATES OF DIFFERENT MUTATION TYPES	965596	MAKOVA, KATERYNA	Penn State

Developer involvement

Language	Code Lines	Comment Lines	Comment Ratio	Blank Lines	Total Lines	Total Percentage
Python	160,951	35,478	18.1%	18,060	214,489	55.3%
JavaScript	57,177	15,482	21.3%	10,569	83,228	21.5%
XML	50,805	1,810	3.4%	8,340	60,955	15.7%
Perl	12,473	3,004	19.4%	2,485	17,962	4.6%
HTML	4,960	142	2.8%	182	5,284	1.4%
CSS	2,604	113	4.2%	151	2,868	0.7%
shell script	2,117	420	16.6%	362	2,899	0.7%
Make	165	34	17.1%	46	245	0.1%
Totals	291,252	56,483		40,195	387,930	



Contributors outside the core team customize Galaxy through **forks**

The screenshot shows the Bitbucket web interface for the 'galaxy-central' repository. The 'Pull requests' tab is selected and circled in orange. An orange arrow points from the 'Forks' icon in the repository statistics (147 forks) to the 'Pull requests' tab. Another orange arrow points from the 'Pull requests' tab to the main content area of the repository page.

Bitbucket Pricing & signup What's new owner/repository ? Sign up Log in

galaxy-central galaxy Follow

Clone Fork Compare Pull request

Overview Source Commits **Pull requests 16** Wiki Downloads

GALAXY
=====

<http://galaxyproject.org/>

The latest information about Galaxy is always available via the Galaxy website above.

HOW TO START
=====

Galaxy requires Python 2.5, 2.6 or 2.7. To check your python version, run:

```
% python -V
Python 2.7.3
```

Start Galaxy:

```
% sh run.sh
```

Once Galaxy completes startup, you should be able to view Galaxy in your browser at:

<http://localhost:8080>

You may wish to make changes from the default configuration. This can be done in the universe_wsgi.ini file. Tools are configured in tool_conf.xml. Details

HTTPS - <https://bitbucket.org/galaxy/>

2 Branches 3 Tags **147 Forks** 151 Followers

Owner galaxy
Website <http://galaxyproject.org/>
Access level Public
Type Mercurial
Last updated 5 hours ago
Created 2009-02-23
Size 227.4 MB (download)

...and contribute changes back through **pull requests**

galaxy / galaxy-central / x

Atlassian, Inc. [US] <https://bitbucket.org/galaxy/galaxy-central/pull-requests/merged>

main Audio-Сказки Homemade "Bus Sh Read mapping and SRA-cancer RNA-seq The Fraenkel Lab Other Bookmarks

Atlassian Bitbucket Pricing Latest features owner/repository ? Sign up Log in

galaxy-central galaxy

Clone Fork Compare Pull request

Overview Source Commits **Pull requests 21** Wiki Downloads

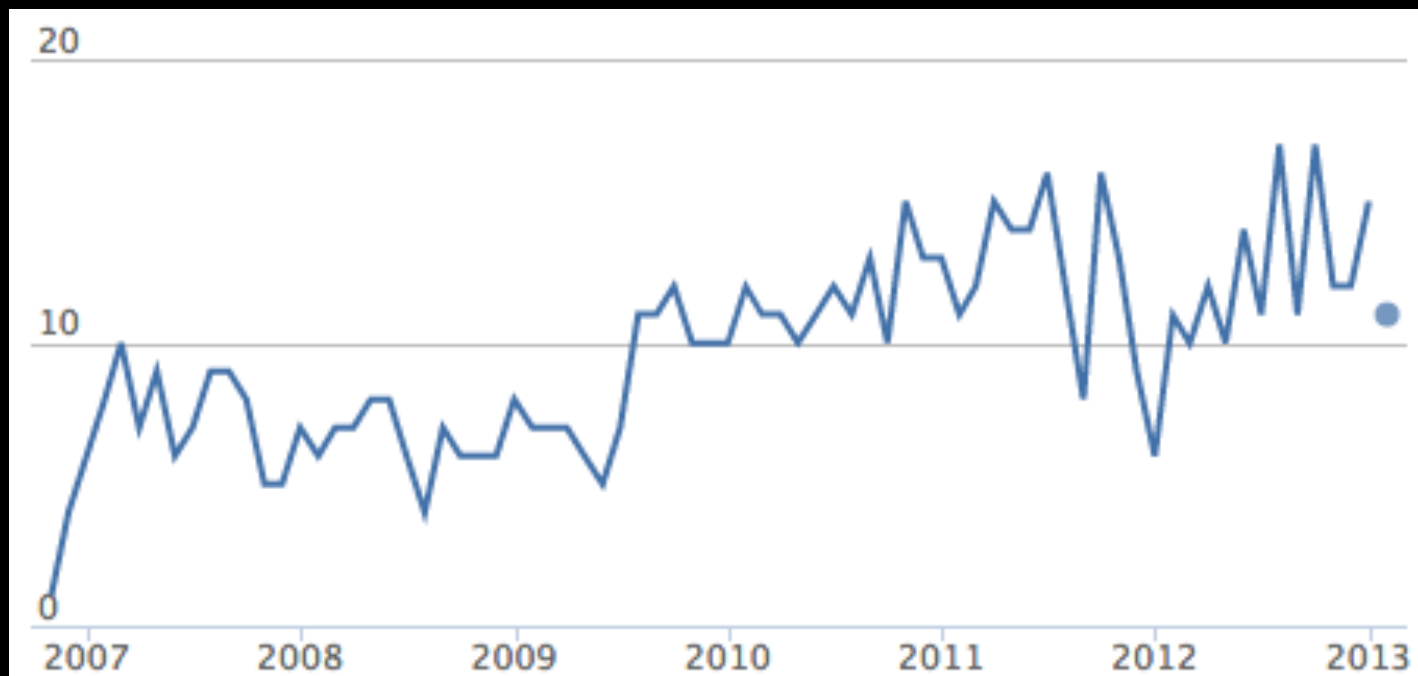
Filters: Open Merged Declined

Author	Title	Updated
John Chilton	#189: Small Unit Testing Improvements	19 hours ago
Adam Brenner	#192: eXpress tool requirements tag updated - replaced binary with package	4 days ago
Nicola Soranzo	#188: New loc file for SAMtools indexes to support genome variants (backward compatible)	2 2013-06-24
Saket Choudh...	#183: UI Add Support for directly exporting pulished workflows from the main 'list_public'	4 1 2013-06-21
Kyle Ellrott	#186: BugFix: Casting UUIDs to strings for JSON serialization in provenance report.	2013-06-20
Kyle Ellrott	#185: Provenance Bug Fix	3 2013-06-20
Kyle Ellrott	#182: Add ability to search Job data via the search api	2013-06-18
Kyle Ellrott	#174: Adding provenance output to the API	1 1 2013-06-17
John Chilton	#173: Improved exception and error handling conditions for the LWR job runner. PEP-8 fixes.	2013-06-16
Gert Hulselmans	#170: Fix detection of 2bit files when uploading them.	1 2013-06-15
John Chilton	#180: Introduce config option welcome_url	2013-06-14

21 open pull requests (as of 2/23), ~150 pull requests already merged

At least 66 distinct contributors to
the main code base

Number of distinct contributors per month,
gradually increasing:



	Name	Kudos	12 Month Commits	All Time Commits	5 Year Trend	Primary Language	First Commit	Last Commit
	Jeremy Goecks		521	1368		Python	over 3 years ago	4 days ago
	Greg Von Kuster		379	1730		Python	about 6 years ago	4 days ago
	Dan Blankenberg		288	1132		Python	about 6 years ago	5 days ago
	Dannon Baker		157	349		Python	almost 3 years ago	8 days ago
	Nate Coraor		143	999		Python	about 6 years ago	4 days ago
	InitHello		133	133		Python	10 months ago	4 days ago
	Carl Eberhard		128	128		JavaScript	7 months ago	4 days ago
	jctx (Manager)		123	746		Python	over 6 years ago	15 days ago
	John Chilton		78	97		Python	almost 2 years ago	8 days ago
	Scott McManus		45	45		Python	9 months ago	4 months ago
	Ross Lazarus		24	223		Python	over 5 years ago	4 months ago
	cléments		18	20		Python	about 1 year ago	about 1 month ago
	Richard Burhans		12	56		XML	over 2 years ago	3 months ago
	Finn Bacall		11	11		Python	11 months ago	8 months ago
	Kyle Ellrott		11	11		Python	4 months ago	16 days ago

	Kyle Elliott		11	11		Python	4 months ago	16 days ago
	Enis Afgan		9	82		Python	over 3 years ago	5 months ago
	Remi Marenco		8	8		XML	8 months ago	6 months ago
	Brad Chapman		6	8		Python	over 2 years ago	5 months ago
	peterjc		6	88		XML	over 2 years ago	4 months ago
	Richard Park		5	9		Python	about 1 year ago	24 days ago
	Joachim Jacob		4	4		Python	about 1 month ago	11 days ago
	Hiral Vora		3	3		XML	10 months ago	10 months ago
	mgehring		2	2		Python	4 months ago	4 months ago
	nuwan_ag		2	2		Python	6 months ago	6 months ago
	Anton Nekrutenko		2	178		XML	about 6 years ago	10 months ago
	Brad Langhorst		1	1		Python	7 months ago	7 months ago
	Guru Ananda		1	204		XML	about 6 years ago	9 months ago
	Nicola Soranzo		1	1		XML	about 1 month ago	about 1 month ago
	Lance Parsons		1	4		Python	over 1 year ago	3 months ago
	James		1	1		Python	6 days ago	6 days ago

greg@bx.psu.edu	439975	*****
james@jamestaylor.org	433227	*****
jeremy.goecks@emory.edu	236491	*****
nate@bx.psu.edu	118044	*****
dan@bx.psu.edu	106226	*****
kanwei@gmail.com	61444	*****
rc	56488	*****
ian@localhost.localdomain	46319	*****
carlfeherhard@gmail.com	32294	*****
inithello@gmail.com	30999	*****
afgane@gmail.com	29337	*****
kpvincent@bx.psu.edu	24798	*****
guru	19287	*****
rubar: ross Lazarus at gmail period com	19232	*****
burchans@bx.psu.edu	18878	*****
anton@bx.psu.edu	18707	*****
dannonbaker@me.com	16373	*****
ross.lazarus@gmail.com	13650	****
wychung@bx.psu.edu	10210	***
guaillo@bx.psu.edu	9548	**
chinmay@bx.psu.edu	7415	**
ian@bx.psu.edu	6491	**
jmchilton@gmail.com	5333	**
guaillo	5122	*
scottmcmanus@gatech.edu	4490	*
p.j.a.cock@googlemail.com	3943	*
jbhe@bx.psu.edu	3885	*
ianschenck@bhruskee.local	2444	*
clements	2118	*
jduddy@illumina.com	2112	*
tomithy.too@gmail.com	2061	*
jeremy.goecks at emory.edu	2039	*
remimarengo@gmail.com	2027	*
wychung	1892	*
clements@galaxyproject.org	1710	*
dan@scofield.bx.psu.edu	1395	*
dannon.baker@emory.edu	1047	*
yizhang@bx.psu.edu	1025	*
rpark37	800	*
ichorny	792	*
ianschenck@Thugunit.local	660	*
rubar/ross period lazarus at gmail d0t com	611	*
jduddy@Bruno-Proto6-illumina.com	601	*
anton@grusha.bx.psu.edu	598	*
scottmcmanus@emory.edu	491	*
afgane@enis-afgans-macbook-pro.local	473	*
florient.angly@gmail.com	437	*
anton@nekruit-mbp.bx.psu.edu	416	*
jfrey@cs.wisc.edu	387	*
dckind@bx.psu.edu	385	*
finn.bacall@cs.man.ac.uk	345	*
rossl@bx.psu.edu	336	*
m.vermaat.hg@lumc.nl	332	*
rob.hooff@nbic.nl	331	*
hiralv	328	*
kellrott@gmail.com	260	*
arjun@bx.psu.edu	229	*
greg	207	*
ad9075@gmail.com	194	*
vdtoorn@hotmail.com	146	*
lparsons@princeton.edu	130	*
trevor@well.com	114	*
roryk	101	*
rc@bx.psu.edu	89	*
Guru Ananda	81	*
rerla@localhost	80	*
jj@umn.edu	77	*
semenko@alum.mit.edu	76	*
dan	56	*
anton@client-75-102-65-120.mobility-up.psu.edu	56	*
chapmanb@50mail.com	53	*
smcmanus	49	*
mgehrin@emory.edu	40	*
langhorst@neb.com	40	*
Rory Kirchner (roryk@mit.edu)	37	*
chapmanb	35	*
pvh@sanbi.ac.za	32	*
nuwan_ag	31	*
kellrott@soe.uscs.edu	21	*
sloc@unimelb.edu.au	10	*
radhesh@bx.psu.edu	9	*
guaillo@scofield.bx.psu.edu	8	*
jen	8	*
jen@bx.psu.edu	8	*
takadonet	6	*
h-morita@esm.co.jp	5	*
hvorai@uncc.edu	5	*
freek.de.bruijn@nbic.nl	3	*
paniagua.cshl@gmail.com	2	*
jj@msi.umn.edu	2	*
afgane@dhcp243061.rollins.emory.edu	2	*
soranzo@crs4.it	1	*
carlos.borroto@gmail.com	1	*

We have also recently redesigned our release process

All development happens in “galaxy-central”, we previously released monthly to “galaxy-dist”

However, as the number of production instances has grown, their maintainers were finding it difficult to keep up with this release cycle

We are now releasing on a cycle of approximately three months with a longer testing period before releases

However, we are also maintaining a dist release branch for releasing bug fixes or security fixes on the current distribution

The path to sustainability

Leverage existing compute infrastructure

Currently engaged in several efforts to leverage national cyberinfrastructure in Galaxy

10 Gig dedicated link from Galaxy server room to XSEDE network via PSC

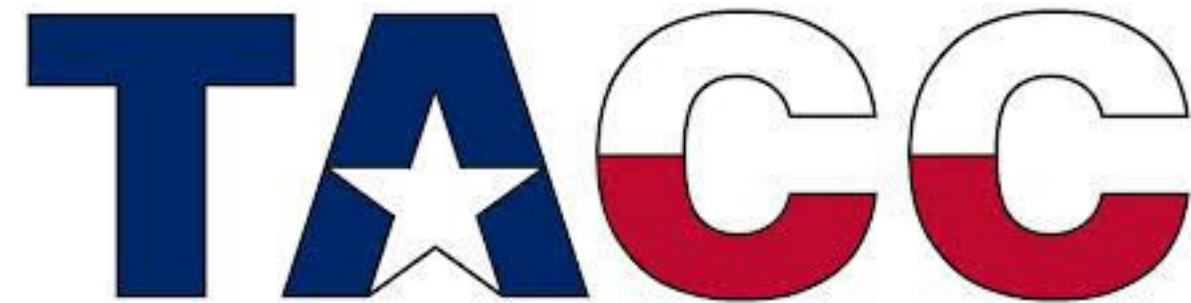
Mirror of all Galaxy data on PSC's SLASH2 store

Ongoing work with XSEDE Extended Support group enabling job submission to XSEDE

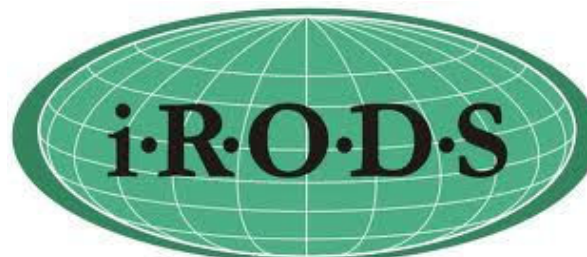
Integration with Globus Online from Ian Foster's group

Goal is to allow users to link XSEDE allocations to Galaxy accounts, submit directly from Galaxy main

Using robust infrastructure



Extreme Science and Engineering
Discovery Environment



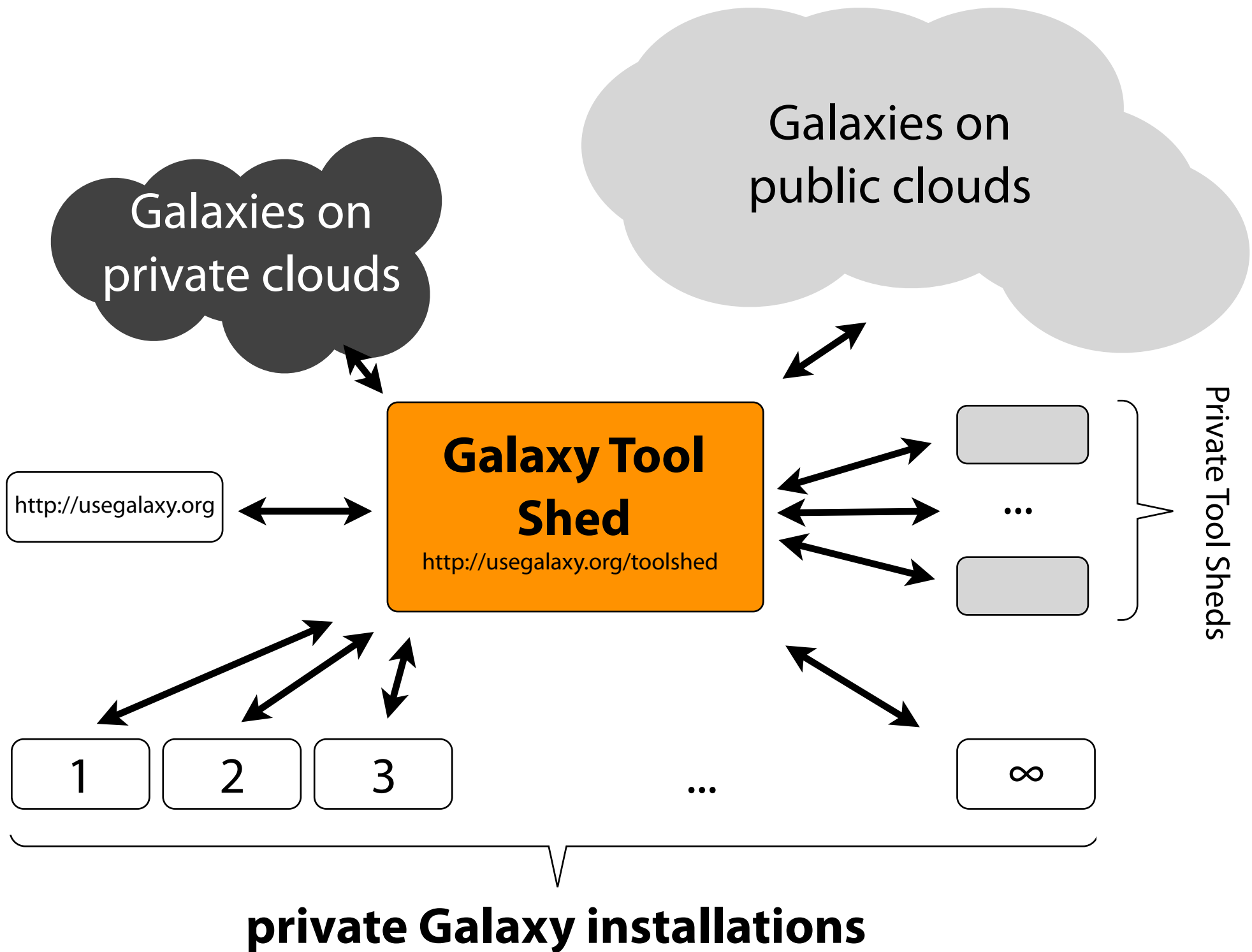
Integrated Rule-Oriented Data System



The Galaxy Toolshed

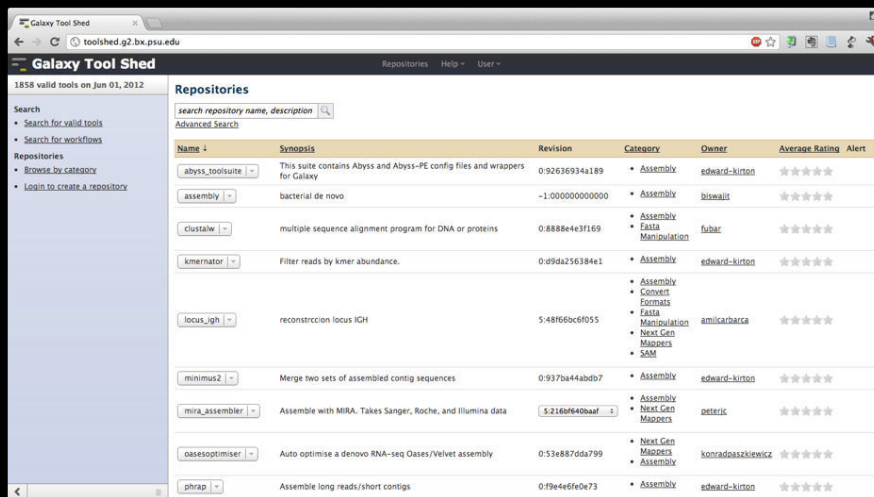
Scaling Galaxy: two distinct problems

- So much data, not enough infrastructure.
 - Solution, encourage local Galaxy instances, cloud Galaxy, support increasingly decentralized model, *improve access to exiting resources*
- So many tools and workflows, not enough manpower
 - Focus on building infrastructure to allow community to integrate and share tools, workflows, and best practices

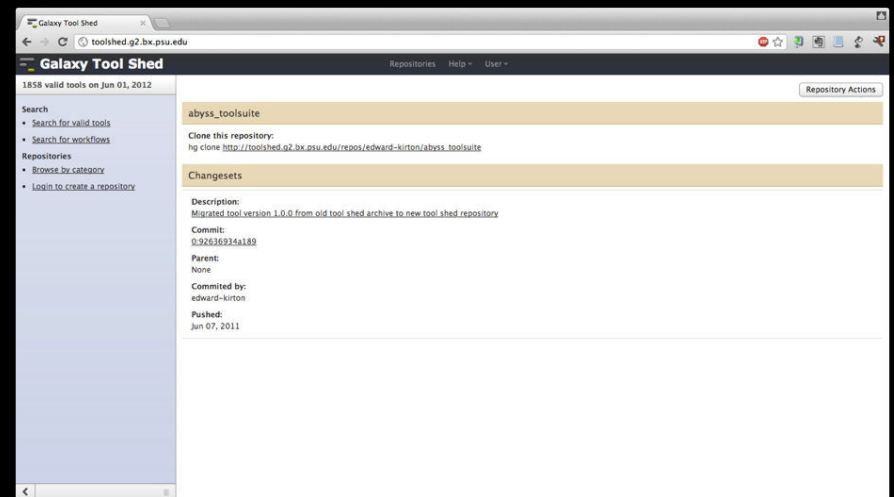


Galaxy toolshed vision

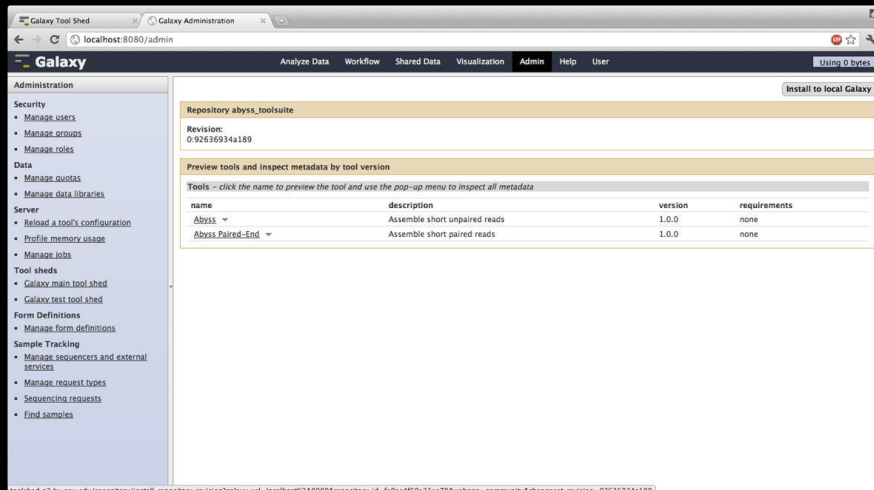
- Allow users to share “suites” containing tools, datatypes, workflows, sample data, and automated installation scripts for tool dependencies
- Version controlled
- Community annotation, rating, comments, review
- Dependency resolution
- Integration with Galaxy instances to automate tool installation and updates



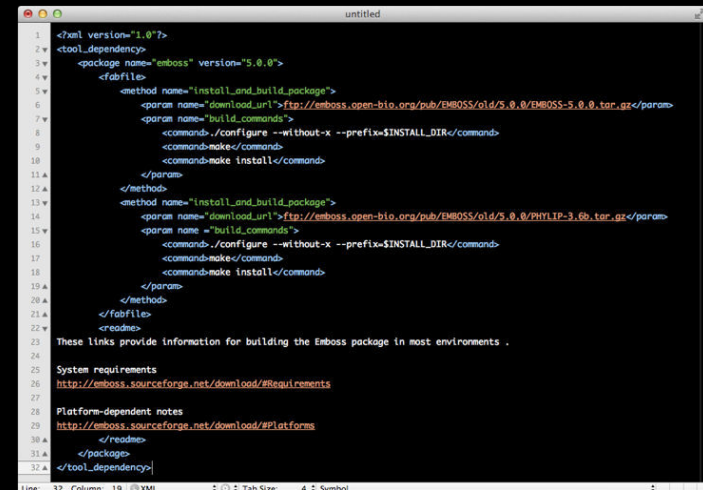
Repositories are owned by the contributor, can contain tools, workflows, etc.



Backed by version control, a complete version history is retained for everything that passes through the toolshed



Galaxy instance admins can install tools directly from the toolshed using only a web UI



Support for recipes for installing the underlying software that tools depend on (also versioned)

Toolshed oversight committee

- Ira Cooke | La Trobe
- JJ Johnson | UMN
- Ed Kirton | DOE JGI
- Peter Cock | Hutton Institute
- Brad Chapman | HSPH
- Björn Grüning | Freiburg
- Ross Lazarus | Baker IDI

Improving robustness and performance of the Galaxy UI

Although the core of the Galaxy framework is robust and scalable, there are some areas we need to invest engineering effort in revisiting

Some features currently perform poorly due to inefficient use of the database

Many components communicate through synchronization on the database, need to refactor the framework with a proper message bus

Supporting analysis at massive scale

One of the most common requests from users is to
run tools or workflows on many samples

For example, a user might have a few dozen (paired)
samples, want to run each through a workflow of
several dozen steps, and aggregate the results in
some way

A simple analysis quickly results in dozens of
workflow invocations and hundred of individual tool
runs

Limitations of the Galaxy Workflow System

It isn't a workflow system

Launching large workflows is relatively slow

Scheduling is completely naive
(just scheduled as individual jobs)

Not robust to individual job failures, no way to
detect types of failures or rerun individual jobs or
parts of workflows

Plans

Schedule workflows in the background

Histories will be able to contain not just datasets, but pending workflows, dataset groups, other entities

Make workflow scheduling engine pluggable

Once it is a background process, can afford the time to delegate

Rewrite default workflow scheduling approach

Rather than scheduling all at once, monitor workflow progress, allow pausing in response to failure or user intervention, decision nodes, streaming data and intermediate datasets

Better integration of workflow planning with job level parallelism

Limitations of the Galaxy user interface

Very good at what is was designed for,
running one tool, or one workflow, on a few datasets
interactively

Very limited facilities for running on multiple
datasets

Galaxy

https://main.g2.bx.psu.edu/root?workflow_id=443736f7fc7e50cd

Galaxy

Analyze DataWorkflowShared DataLabVisualizationCloudAdminHelpUser

Using 30.9 GB

Tools

search tools

Get Data

Send Data

ENCODE Tools

Lift-Over

Text Manipulation

Convert Formats

FASTA manipulation

Filter and Sort

Join, Subtract and Group

Extract Features

Fetch Sequences

Fetch Alignments

Get Genomic Scores

Operate on Genomic Intervals

Statistics

Graph/Display Data

Regional Variation

Multiple regression

Multivariate Analysis

Evolution

Motif Tools

Multiple Alignments

Metagenomic analyses

Genome Diversity

Running workflow "Groom FASTQ"

Expand AllCollapse

Step 1: Input dataset

Input Dataset

2: Imported: GM12878...ple Dataset

type to filter

Step 2: FASTQ Groomer (version 1.0.4)

☐ Send results to a new history

Run workflow

History

RNA-seq exercise (full)

96.8 MB

28: UCSC Main on Human: all est (chr19:1-59128983)

27: Cuffdiff on data 8, data 10, and data 4: CDS diff

26: Cuffdiff on data 8, data 10, and data 4: promoters diff

25: Cuffdiff on data 8, data 10, and data 4: splicing diff

24: Cuffdiff on data 8, data 10, and data 4: CDS FPKM tracking

23: Cuffdiff on data 8, data 10, and data 4: TSS groups FPKM tracking

22: Cuffdiff on data 8, data 10, and data 4: gene FPKM tracking

21: Cuffdiff on data 8, data 10, and data 4: isoform FPKM tracking

20: Cuffdiff on data 8, data 10, and data 4: CDS Expression FPKM Tracking

Galaxy

https://main.g2.bx.psu.edu/root?workflow_id=443736f7fc7e50cd

Galaxy

Analyze DataWorkflowShared DataLabVisualizationCloudAdminHelpUser

Using 30.9 GB

Tools

search tools

Get Data

Send Data

ENCODE Tools

Lift-Over

Text Manipulation

Convert Formats

FASTA manipulation

Filter and Sort

Join, Subtract and Group

Extract Features

Fetch Sequences

Fetch Alignments

Get Genomic Scores

Operate on Genomic Intervals

Statistics

Graph/Display Data

Regional Variation

Multiple regression

Multivariate Analysis

Evolution

Motif Tools

Multiple Alignments

Metagenomic analyses

Genome Diversity

Running workflow "Groom FASTQ"

Expand AllCollapse

Step 1: Input dataset

Input Dataset

1: Imported: h1-hESC..ple Dataset

2: Imported: GM12878..ple Dataset

type to filter, [enter] to select all

Step 2: FASTQ Groomer (version 1.0.4)

☐ Send results to a new history

Run workflow

History

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21: Cuffdiff on data 8, data 10, and data 4: isoform FPKM tracking

20: Cuffdiff on data 8, data 10, and data 4: CDS Expression FPKM Tracking

Need to support much more complex combinations of multiple inputs

Parallel execution on some datasets, cross products on others, match up paired datasets, annotations, ...

Need to provide better feedback to users running large-scale analysis on shared resources

Plans

Completely new view in Galaxy for multiple dataset execution

Given a workflow to run, use rules to select sets of datasets that it will be run on

Define tools or workflows for aggregating results

Completely new interfaces for monitoring progress of running workflows and jobs, not limited to single history

Better feedback on queue position and resource utilization

***Galaxy Team* Roadmap for 2014**

- ToolShed
- Cloud
- Improving data integration & management
- User Interface refactoring/redesign
- Visualization framework and API
- Robust federated infrastructure for main site
- Working more closely with journals

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SCIENCE



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This will not be possible without

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- Dave Clements
- Ingeborg Engh
- Mohammad Heydarian
- Geir Kjetil Sandve

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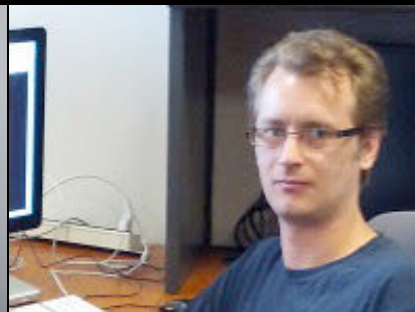
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<http://wiki.galaxyproject.org/GalaxyTeam>