

# UF Research Computing

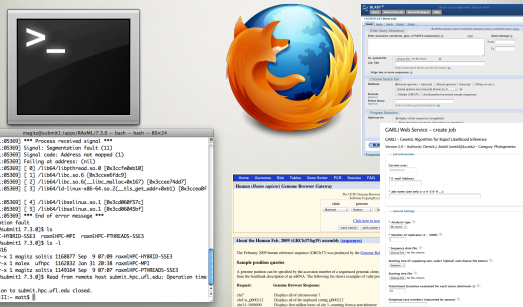
## Introduction to Galaxy at UF HPC

Matt Gitzendanner  
Oleksandr Moskalenko

## Today's research computing

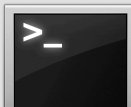



## Approaches




## Different approaches, same result

### Head node





### Scheduler




Interactive session or batch submission

### Computing resources





Your job runs on the cluster

## What is Galaxy?




### Galaxy Provides Life Support for NGS Exploration





powered by **Galaxy**

## What is Galaxy?



- ◆ Computational biology platform
  - Open and Web-based
  - Accessible
  - Reproducible
  - Transparent

## Galaxy Analysis Workspace

**Tools**

- Get Data
- Send Data
- ENCORE Tools
- LiCh-Over
- Text Manipulation
- Filter and Sort
- Join, Subtract and Group
- Convert Formats
- Extract Features
- Fetch Sequences
- Fetch Alignments
- Get Genomic Scores
- Operate on Genomic Intervals
- Statistics
- Graph/Display Data
- Regional Variation
- Multiple regression
- Multivariate Analysis
- Evolution
- Model Tools
- Metabolic Assessments
- Measurement analysis
- FASIS manipulation
- NCR BLAST
- NCR UC and manipulation
- NCR UC (beta)
- NCR Mapping
- NCR Index Analysis
- NCR RNA Analysis
- NCR SAM Tools

**MACS**

Treatment file: hg19.chr10.bam

Input file: Selection is Optional

Format: Auto

Effective Genome Size: (Human hg19) 5.3 Gb

Tag size (Optional): 25

P-Value: 1e-05

Keep duplicate tags at the exact same location?:  Keep ALL  Auto by Binomial  Keep Single

Use Model?:  True  False

small fold enrichment for model building: large fold: 10

Advanced Options:

**History**

- 0915 Macs Exercise 5.3 Gb
- 35: Summary Statistics on data.28
- 33: UCSC Main on Human: chr1:156690-165971
- 31: MACS job log on hg19.chr9.bam
- 30: MACS wiggle on hg19.chr9.bam
- 29: MACS xls on hg19.chr9.bam
- 28: MACS summits on hg19.chr9.bam
- 27: MACS peaks on hg19.chr9.bam
- 26: BAM to SAM on data
- 25: converted SAM
- 24: hg19.chr8.bam
- 23: hg19.chr7.bam

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**MACS**

chr9	179077	179078	MACS_peak_1	14.00
chr9	501305	501306	MACS_peak_2	27.00
chr9	764211	764212	MACS_peak_3	29.00
chr9	2241895	2241896	MACS_peak_4	25.00
chr9	3161896	3161897	MACS_peak_5	10.00
chr9	2487733	2487734	MACS_peak_6	14.00
chr9	3526275	3526276	MACS_peak_7	19.00
chr9	3809982	3809983	MACS_peak_8	17.00
chr9	3921930	3921931	MACS_peak_9	15.00
chr9	4315884	4315885	MACS_peak_10	17.00
chr9	4897865	4897866	MACS_peak_11	11.00
chr9	5186618	5186619	MACS_peak_12	13.00
chr9	5439021	5439022	MACS_peak_13	14.00
chr9	5510340	5510341	MACS_peak_14	13.00
chr9	5628255	5628256	MACS_peak_15	11.00
chr9	5699455	5699456	MACS_peak_16	9.00
chr9	5828255	5828256	MACS_peak_17	12.00
chr9	6015764	6015765	MACS_peak_18	17.00
chr9	6681231	6681232	MACS_peak_19	29.00
chr9	7028374	7028375	MACS_peak_20	11.00
chr9	7028374	7028375	MACS_peak_21	8.00
chr9	9442225	9442226	MACS_peak_22	5.00
chr9	9442225	9442226	MACS_peak_23	3.00
chr9	9524985	9524986	MACS_peak_24	5.00
chr9	9676511	9676512	MACS_peak_25	7.00
chr9	12776444	12776445	MACS_peak_26	14.00
chr9	13024578	13024579	MACS_peak_27	12.00
chr9	14021262	14021263	MACS_peak_28	12.00
chr9	15028466	15028467	MACS_peak_29	7.00
chr9	16371450	16371451	MACS_peak_30	12.00
chr9	16784786	16784787	MACS_peak_31	15.00
chr9	16968419	16968420	MACS_peak_32	11.00
chr9	17005970	17005971	MACS_peak_33	15.00
chr9	17663745	17663746	MACS_peak_34	16.00
chr9	18059354	18059355	MACS_peak_35	11.00
chr9	21805741	21805742	MACS_peak_36	41.00
chr9	21948229	21948230	MACS_peak_37	16.00
chr9	22016238	22016239	MACS_peak_38	7.00

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## Getting Data into Galaxy

- ◆ Upload a file from your computer
  - scp or copy files to HPC
  - Load from within Galaxy
    - [http://wiki.hpc.ufl.edu/index.php/Galaxy\\_Data\\_Import](http://wiki.hpc.ufl.edu/index.php/Galaxy_Data_Import)
- ◆ External data
  - UCSC table browser
  - Biomart
  - interMine / modMine
  - EuPathDB
  - EncodeDB
  - EpiGRAPH
  - FlyMine
  - GrameneMart...

## Data libraries

Name	Message	Uploaded By	Date	File Size
2010-11-17-12-hg19chr9.bam		omihpc@ufl.edu	2011-09-13	1.8 GB
2010-11-17-12-hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-13	1.4 GB
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	80.8 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	62.5 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	76.9 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	50.9 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	36.1 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	48.3 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	55.9 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	64.5 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	33.5 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	39.6 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	148.5 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	26.5 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	17.5 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	16.9 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	130.3 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	488.0 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	119.0 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	102.7 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	63.7 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	89.9 Mb
hg19chr9.bam		omihpc@ufl.edu	2011-09-14	65.9 Mb
hg19chr9.sorted.bam		omihpc@ufl.edu	2011-09-14	64.8 Mb

## Data Access Control

**Groups**

Name	Users	Roles
HPC	0	2
Taylor HPC Lab	2	1

**Roles**

Name	Description	Type	Groups
HPC	Role for group HPC	system	1
HPC-test-CHIP-seq-analyses	Test analyses of CHIP-seq data	admin	1

**Users**

Email	User Name	Groups	Roles	External	Last Login
adission@ufl.edu	adission	0	1	yes	Sep 15, 2011
bozwick@ufl.edu	bozwick	0	1	yes	Sep 15, 2011
cupress@ufl.edu	cupress13	0	1	yes	Sep 15, 2011
cliff@ufl.edu	cliffjerry	0	1	yes	Sep 15, 2011
coltr@ufl.edu	coltrd3	0	1	yes	Sep 15, 2011

## Galaxy Tool Suites

- ◆ Text Manipulation
- ◆ Format Converters
- ◆ Filtering and Sorting
- ◆ Join, Subtract, Group
- ◆ Sequence Tools
- ◆ Multi-species Alignment Tools
- ◆ Genomic Interval Operation
- ◆ Summary Statistics, graphing
- ◆ Regional Variation
- ◆ EMBOSS
- ◆ Evolution
- ◆ RNA-Seq
- ◆ ChIP-Seq
- ◆ GATK
- ◆ Phylogenetics ???

## A galaxy of tools

- QC and manipulation**
  - ILLUMINA DATA
  - FASTQ converter: convert between various FASTQ quality formats
  - FASTQ splitter: on joined paired end reads
  - FASTQ zipper: on paired end reads
  - FASTQ Summary Statistics by column
  - ROCHE-454 DATA
  - Build basic quality distribution
  - Select high quality sequences
  - Combine FASTA and QUAL into FASTQ
  - AS-SOLID DATA
  - Convert SOLID output to fastq
  - Compute quality statistics for SOLID data
  - Draw quality score heatmap for SOLID data
  - GENERIC FASTQ MANIPULATION
  - Filter FASTQ reads by quality score and length
  - FASTQ zipper: by column
  - FASTQ Quality Trimmer: by sliding window
- Common**
  - Metagenomic analysis
  - Human Genome Variation
  - EMBOSS
  - NGS TOOLBOX BETA
  - NGS QC and manipulation
  - ILLUMINA
  - Map with Bowtie for Illumina
  - ROCHE-454
  - Large map short reads against reference sequence
  - Mapalign: compare short reads against Ref-Seq and map databases
  - Peak calling: output BED-SOLID
  - Map with Bowtie for SOLID
  - NGS SAM Tools
  - NGS Indel Analysis
  - NGS RNA Analysis
  - NGS RNA Analysis
  - SNP/INDEL Data: Filters
  - SNP/INDEL Data: LD: Plots
  - SNP/INDEL Statistical Models
- NEW TOOLBOX BETA**
  - NGS QC and manipulation
  - NGS Statistics
  - NGS SAM Tools
    - Filter SAM on bitwise flag values
    - Convert SAM to interval
    - SAM-to-BAM converts SAM format to BAM format
    - BAM-to-SAM converts BAM format to SAM format
    - Merge BAM files merges BAM files together
    - Converts interval from BAM format
    - Filter: filter on coverage and SNPs
    - Filter: filter on coverage and SNPs
    - Repeat: provides simple stats on BAM files
    - Filter: find significant changes in transcript expression, printing and promoter size filtering
    - Filter: Combined Transcripts using tracking file
- NGS SAM Tools**
  - NGS Indel Analysis
  - Filter: index for SAM
  - Extract index from SAM
  - Index Analysis
  - NGS Peak Calling
  - MACS: Model-based Analysis of ChIP-Seq
  - GenTrack: index: on a BED file
  - NGS RNA Analysis
  - RNA-Seq
  - MACS: Model-based Analysis of ChIP-Seq data
  - Cuffdiff: transcript assembly and FPKM/RPKM estimates for RNA-Seq data
  - Cuffdiff: compare assembled transcripts to a reference annotation and track Cuffdiff: transcript assembly multiple experiments
  - Cuffdiff: find significant changes in transcript expression, printing and promoter size filtering
  - Filter: Combined Transcripts using tracking file

## Galaxy Workflows

```

graph TD
    Unknown[Unknown] --> T25[25: hg19chr9.bam]
    T25 --> T26[26: BAM-to-SAM on data 25 converted SAM]
    T26 --> T27[27: MACS peaks on hg19chr9.bam]
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    T31 --> T27
    
    T27 --> T28
    
    T28 --> T29
    
    T29 --> T30
    
    T30 --> T31
    
    T31 --> T27
    
    T27 --> T28
    
    T28 --> T29
    
    T29 --> T30
    
    T30 --> T31
    
    T31 --> T27
    
```



## Galaxy Workflows

## Galaxy Workflows

## Visualization

## Sharing and publishing

### Share or Publish History 'LANA ChIP peaks on hg19'

**Making History Accessible via Link and Publishing It**

This history is currently restricted so that only you and the users listed below can access it. You can:

- Make History Accessible via Link**  
Generates a web link that you can share with other people so that they can view and import the history.
- Make History Accessible and Publish**  
Makes the history accessible via link (see above) and publishes the history to Galaxy's **Published Histories** section, where it is publicly listed and searchable.

**Sharing History with Specific Users**

You have not shared this history with any users.

[Share with a user](#)

[Back to Histories List](#)

## Sharing and publishing

### Share or Publish History 'LANA ChIP peaks on hg19'

**Making History Accessible via Link and Publishing It**

This history is currently accessible via link and published.

Anyone can view and import this history by visiting the following URL:  
<http://galaxy.hpc.ufl.edu/ui/moskatenko/h/iana-chip-peaks-on-hg19>

This history is publicly listed and searchable in Galaxy's **Published Histories** section.

You can:

- Unpublish History**  
Removes this history from Galaxy's **Published Histories** section so that it is not publicly listed or searchable.
- Disable Access to History via Link and Unpublish**  
Disables this history's link so that it is not accessible and removes history from Galaxy's **Published Histories** section so that it is not publicly listed or searchable.

**Sharing History with Specific Users**

The following users will see this history in their history list and will be able to view, import, and run it.

**Email**  
 magitz@ufl.edu

[Share with another user](#)

## Sharing and publishing

### Share or Publish Workflow 'LANA ChIP peaks on hg19'

**Making Workflow Accessible via Link and Publishing It**

This workflow is currently accessible via link and published.

Anyone can view and import this workflow by visiting the following URL:  
<http://galaxy.hpc.ufl.edu/ui/moskatenko/h/iana-chip-peaks-on-hg19>

This workflow is publicly listed and searchable in Galaxy's **Published Workflows** section.

You can:

- Unpublish Workflow**  
Removes this workflow from Galaxy's **Published Workflows** section so that it is not publicly listed or searchable.

**Published Workflows**

search name, annotation, owner, and tag

Name	Annotation	Owner	Community Rating	Community Tags	Last Updated
LANA ChIP peaks on hg19		moskatenko	☆☆☆☆	(chr9) (hg19) (peaks) (iana) (chip)	2 minutes ago

**Published Histories**

search name, annotation, owner, and tag

Name	Annotation	Owner	Community Rating	Community Tags	Last Updated
LANA ChIP peaks on hg19	Peak calling on LANA ChIP-seq data using Human chromosome 9 from hg19 build	moskatenko	☆☆☆☆	(chr9) (hg19) (peaks) (iana) (chip)	4 minutes ago



## Galaxy pages

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

Author: [m1](#)

History: [View](#) [Download](#) [Delete](#) [Share](#)

Rating: ★★★★★

Tags: [Metagenomics](#) [Genomics](#) [Bioinformatics](#)

Created: 2012-06-20 10:00:00

Updated: 2012-06-20 10:00:00

How to use this document

This document is a live copy of supplementary material for the [paper](#). It provides access to the exact analysis and workflow described in the paper, so you can see the workflow, change parameters, or add new data to the analysis. The workflow is available in the [Galaxy history](#) and [Galaxy workflow](#) sections. You can also report bugs, share your own Galaxy workflow and data, or contact the author for more information. A [Galaxy workflow](#) is a reusable workflow that can be used to reproduce the analysis.

How to use the Galaxy history

This is the Galaxy history showing the execution of the pipeline to MEGAN.

How to use the Galaxy workflow

This is the Galaxy workflow showing a generic version of metagenomic data. This corresponds to the "A complete metagenomic pipeline" section of the manuscript and Figure S4.

How to use the Galaxy workflow for general analysis of metagenomic data

This is the Galaxy workflow for general analysis of metagenomic data. This corresponds to the "A complete metagenomic pipeline" section of the manuscript and Figure S4.

How to use the Galaxy workflow for general analysis of metagenomic data

This is the Galaxy workflow for general analysis of metagenomic data. This corresponds to the "A complete metagenomic pipeline" section of the manuscript and Figure S4.

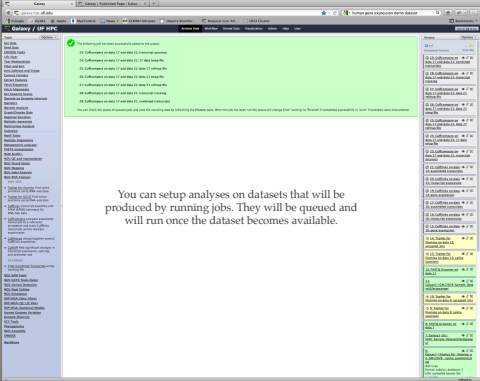
Accessing the Data

Raw data and Galaxy workflow history are available in the [Galaxy history](#) and [Galaxy workflow](#) sections. You can also access the data through the [Galaxy Data Store](#) from where the data can be downloaded through Galaxy or by direct download.


Supplemental Analysis

Comparison between Galaxy pipeline and MEGAN

The analysis pipeline history comparing the results. Individual elements of this history are referred to as history items. 1 and 2 are of an early MEGAN pipeline.



You can setup analyses on datasets that will be produced by running jobs. They will be queued and will run once the dataset becomes available.




## Summary

- ◆ Analyze data without the CLI
- ◆ Visualize the results
- ◆ Publish histories, workflows, and annotated pages
- ◆ Add new tools, get support @ HPC
- ◆ Focus on your science, not minutiae
- ◆ UF Galaxy – coming to a browser near you!


## How to get help

- ◆ Asking for help
  - Support Request Tickets
    - <http://support.hpc.ufl.edu>
    - Use for everything - not just software bugs but for any questions or help requests
    - Searchable database of solutions
  - When you don't have access to web
    - [support@hpc.ufl.edu](mailto:support@hpc.ufl.edu)
    - [om@hpc.ufl.edu](mailto:om@hpc.ufl.edu) (Biological Support)
    - [magitz@ufl.edu](mailto:magitz@ufl.edu) (Bio training and Q/A)



## Documentation

- ◆ UF HPC Encyclopedia
  - <http://wiki.hpc.ufl.edu>
    - Documents on hardware and software resources
    - User guides
    - Sample submission scripts
    - Research-specific sections
  - <http://hpc.ufl.edu/support>
    - Frequently Asked Questions
    - Account set up and maintenance



# Thank you!