#usegalaxy

# Increasing the Utility of Galaxy Workflows

John Chilton (@jmchilton) and the Galaxy Team

http://bit.ly/bosc2015workflows

# The Illusion of Galaxy Workflows

# Galaxy Workflows - Kind of Awesome

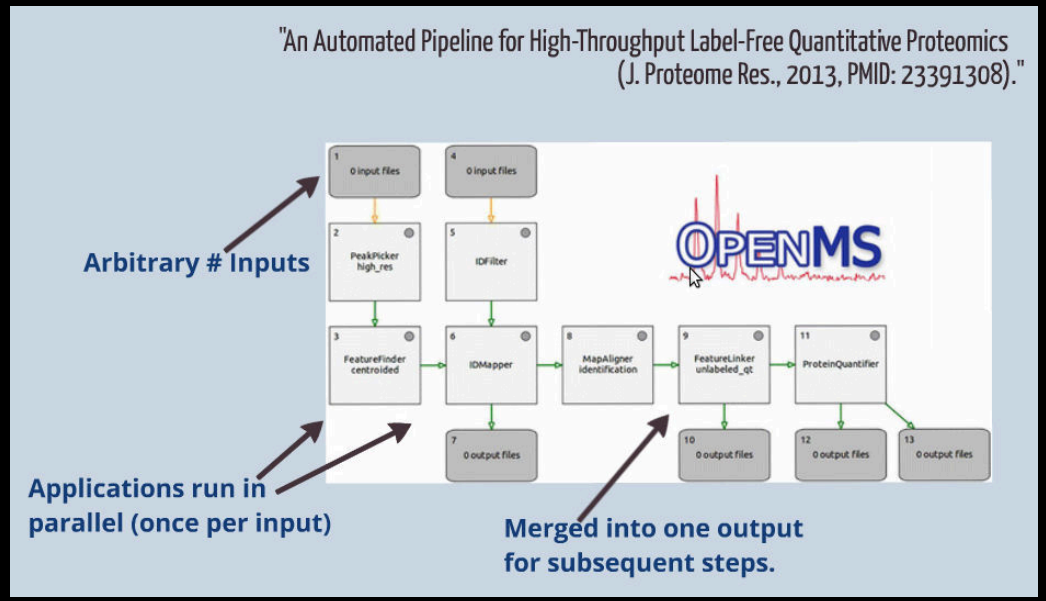
- Designed for biologists, accessibility - easy to build and easy to run.
- Sharable, Publishable
  - e.g. NCBI BLAST+ integrated into Galaxy - Cock et. al. dx.doi.org/10.1101/014043
- Data Flow
  - Blog by Samuel Lampa http://bionics.it/posts/workflows-dataflow-not-task-deps

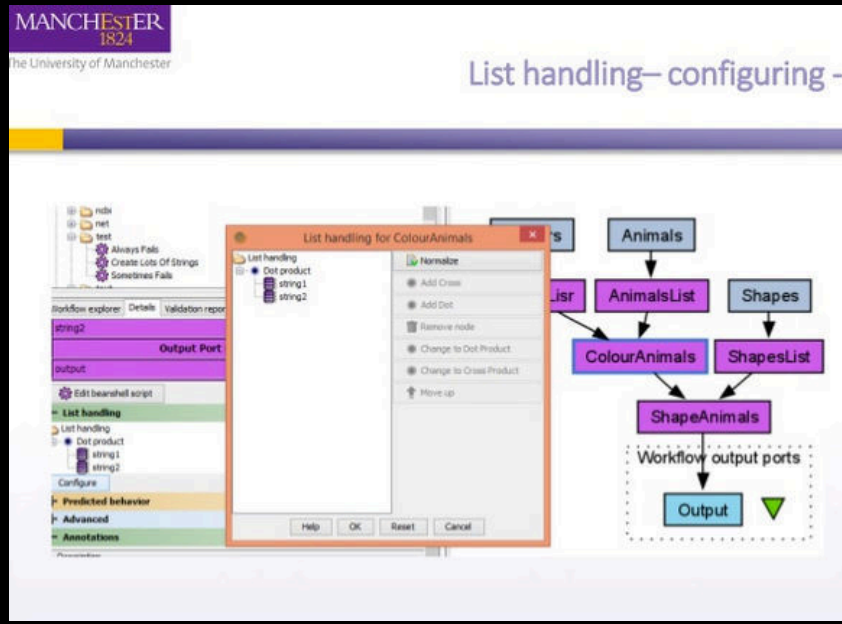
"Best Galaxy feature Galaxy users don't know about."

# The Illusion of Workflows

- Galaxy didn't "schedule" workflows - it would just queue up a bunch of jobs.
  - Therefore Galaxy had no way to conditionally evaluate branches or handle various dynamic functionality one would expect from a workflow.

# Data Flow Limitations




http://www.slideshare.net/mygrid/2014-taverna-tutorial-advanced-taverna

# Addressing These Problems

- Map/reduce style data flow using dataset collections.
- Implemented a workflow engine.

# Collection Types

Currently two supported type pseudo-plugins - “list” and “paired”.

- Lists can contain arbitrary number of named elements
- Pairs contain a “forward” and “reverse” element.

Types can be combined to build nested types - for instance “list:paired” describes a list of paired datasets.

# Upload Some Data...

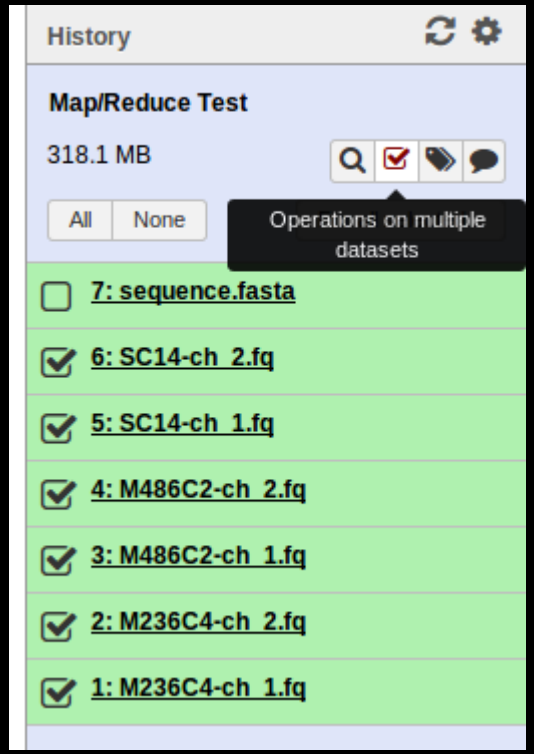
**Download data directly from web or upload files from your disk**

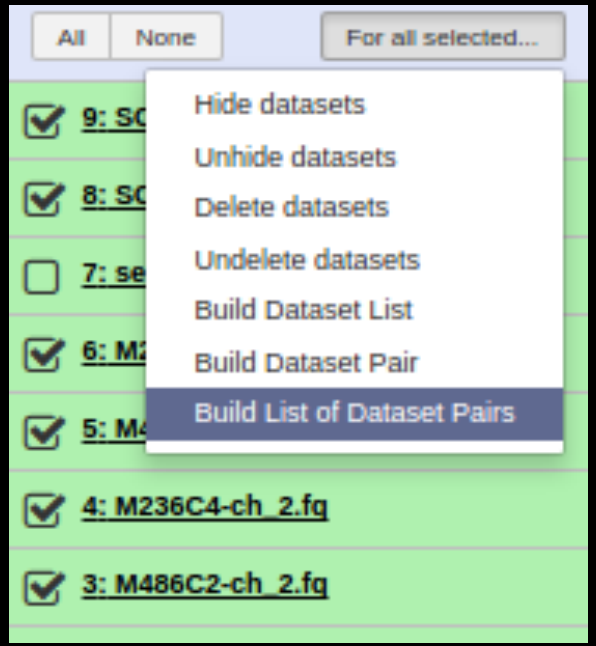
| Name | Size | Type | Genome | Settings | Status |
|---|---|---|---|---|---|
| M236C4-ch_1.fq | **45.4** MB | fastqsanger | unspecified (?) | | 100% |
| M236C4-ch_2.fq | **45.4** MB | fastqsanger | unspecified (?) | | 100% |
| M486C2-ch_1.fq | **46.9** MB | fastqsanger | unspecified (?) | | 100% |
| M486C2-ch_2.fq | **46.9** MB | fastqsanger | unspecified (?) | | 100% |
| SC14-ch_1.fq | **74.4** MB | fastqsanger | unspecified (?) | | 100% |
| SC14-ch_2.fq | **74.4** MB | fastqsanger | unspecified (?) | | 100% |
| sequence.fasta | **16.9** KB | fasta | unspecified (?) | | 100% |

You can Drag & Drop files into this box.

Choose local file | Paste/Fetch data | Start | Pause | Reset | Close

# Select the Pairs



# Create a Collection…

Galaxy

Analyze Data | Workflow | Shared Data | Visualization | Admin | Help | User

**Create a collection of paired datasets**

3 pairs created: all datasets have been successfully paired

**0 unpaired forward** - (0 filtered out)

_1

Choose filters Clear filters

**0 unpaired reverse** - (0 filtered out)

_2

**3 paired** Unpair all

| | | |
|---|---|---|
| M236C4-ch_1.fq → | M236C4-ch | ← M236C4-ch_2.fq |
| M486C2-ch_1.fq → | M486C2-ch | ← M486C2-ch_2.fq |
| SC14-ch_1.fq → | SC14-ch | ← SC14-ch_2.fq |

Remove file extensions from pair names?

Name: Enter a name for your new list

Cancel

Create list

# Collection Mapping (1 / 3)

FASTQ Groomer (version 1.0.4)

**File to groom:**

6: SC14-ch_2.fq

*Tool consumes a FASTQ file.*

**Input FASTQ quality scores type:**

Sanger & Illumina 1.8+

**Advanced Options:**

Hide Advanced Options

Execute

*-List of Paired Datasets*

*-Individual FASTQ datasets.*

**What it does**

This tool offers several conversions options relating to the FASTQ format.

When using *Basic* options, the output will be *sanger* formatted or *cssanger* formatted (when the input is Color Space Sanger).

When converting, if a quality score falls outside of the target score range, it will be coerced to the closest available value (i.e. the minimum or maximum).

History

**Map/Reduce Test**

318.1 MB

8: Paired mt Datasets

7: sequence.fasta

6: SC14-ch_2.fq

5: SC14-ch_1.fq

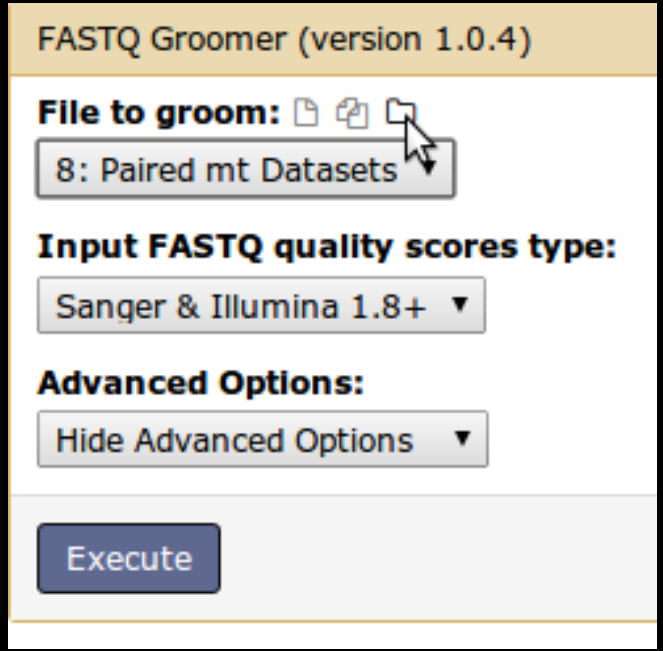
4: M486C2-ch_2.fq

3: M486C2-ch_1.fq

2: M236C4-ch_2.fq

1: M236C4-ch_1.fq

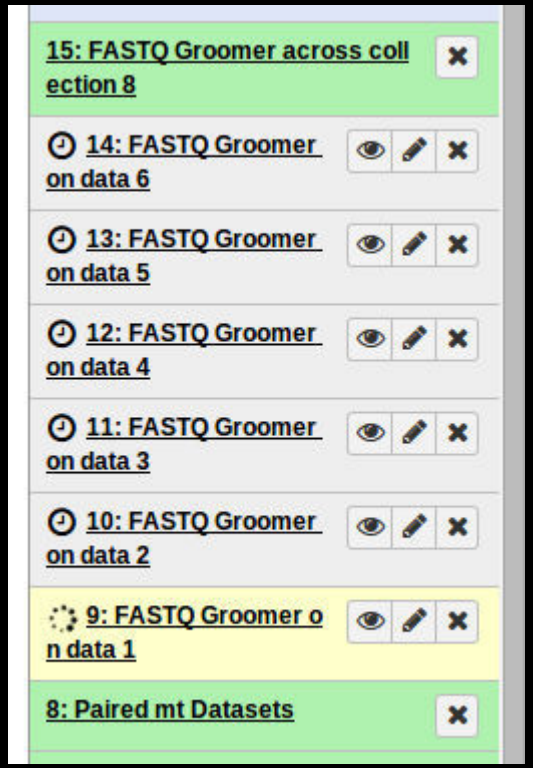
# Collection Mapping (2 / 3)

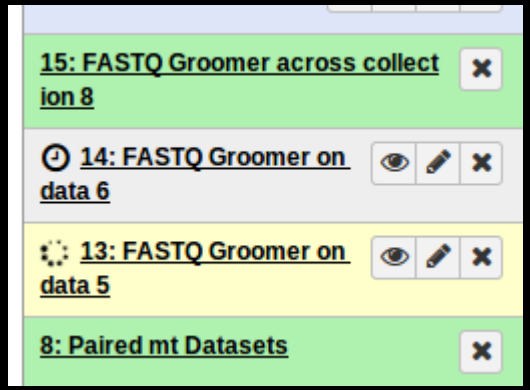



Collection map icon replaces input options with valid collections.

Runs tool over every dataset in list of pairs and produces groomed list of pairs.

# Collection Mapping (3 / 3)





Like hiding workflow datasets, they are visible initially and hidden after completion (only collection remains visible).

Collection always green regardless of contents (stateless).

Need to do better on both points... not scalable enough.

# Sample Tracking: Identifiers + Indices

## Paired mt Datasets

list:paired collection

- Element - 0:M236C4 (paired collection)
  - Element - 0:forward
    - hda - *M236C4-ch_1.fq*
  - Element - 1:reverse
    - hda - *M236C4-ch_2.fq*
- Element - 1:M486C2 (paired collection)
  - Element - 0:forward (hda)
    - hda - M486C2-*ch_1.fq*
  - Element - 1:reverse (hda)
    - hda - M486C2-*ch_2.fq*

...

## FASTQ Groomer across collection 8

list:paired collection

- Element - 0:M236C4 (paired collection)
  - Element - 0:forward
    - hda - *FASTQ Groomer on data 1*
  - Element - 1:reverse
    - hda - *FASTQ Groomer on data 2*
- Element - 1:M486C2 (paired collection)
  - Element - 0:forward (hda)
    - hda - *FASTQ Groomer on data 3*
  - Element - 1:reverse (hda)
    - hda - *FASTQ Groomer on data 4*

...

Mapping over collections - dataset naming is normal, but new collection created with identical tree structure and element identifiers preserved.

# Subcollection Mapping

Bowtie2 (version 0.2)

**Is this library mate-paired?:**

Paired-end Dataset

**FASTQ Paired Dataset:**

Nucleotide-space: Must have Sanger-scaled quality values with ASCII offset 33

**Minimum insert size for valid paired-end alignments:**

0

**Maximum insert size for valid paired-end alignments:**

250

**Write unaligned reads to separate file(s):**

**Will you select a reference genome from your history or use a built-in index?:**

Use one from the history

Built-ins were indexed using default options

**Select the reference genome:**

7: sequence.fasta

History

**Map/Reduce Test**

636.1 MB

15: FASTQ Groomer across collection 8

8: Paired mt Datasets

7: sequence.fasta

6: SC14-ch_2.fq

5: SC14-ch_1.fq

4: M486C2-ch_2.fq

3: M486C2-ch_1.fq

2: M236C4-ch_2.fq

1: M236C4-ch_1.fq

Bowtie 2, Tophat, BWA-mem, Picard, Hitsat, etc... have all been updated to consume paired datasets.

# Subcollection Mapping

Bowtie2 (version 0.2)

**Is this library mate-paired?:**

Paired-end Dataset

**FASTQ Paired Dataset:**

15: FASTQ Groomer across collection 8

Nucleotide-space: Must have Sanger-scaled quality values with ASCII offset 33

**Minimum insert size for valid paired-end alignments:**

0

**Maximum insert size for valid paired-end alignments:**

250

**Write unaligned reads to separate file(s):**

History

**Map/Reduce Test**

636.1 MB

15: FASTQ Groomer across collection 8

8: Paired mt Datasets

7: sequence.fasta

6: SC14-ch_2.fq

5: SC14-ch_1.fq

4: M486C2-ch_2.fq

**Map/Reduce Test**

636.1 MB

19: Bowtie2 across collection 15

18: Bowtie2 on data 7, data 9, and others: aligned reads

17: Bowtie2 on data 7, data 9, and others: aligned reads

16: Bowtie2 on data 7, data 9, and others: aligned reads

15: FASTQ Groomer across collection 8

# Subcollection Mapping (Identifiers)

## Paired mt Datasets

list:paired collection

- Element - 0:M236C4 (paired collection)
  - Element - 0:forward
    - hda - *M236C4-ch_1.fq*
  - Element - 1:reverse
    - hda - *M236C4-ch_2.fq*
- Element - 1:M486C2 (paired collection)
  - Element - 0:forward (hda)
    - hda - M486C2-*ch_1.fq*
  - Element - 1:reverse (hda)
    - hda - M486C2-*ch_2.fq*

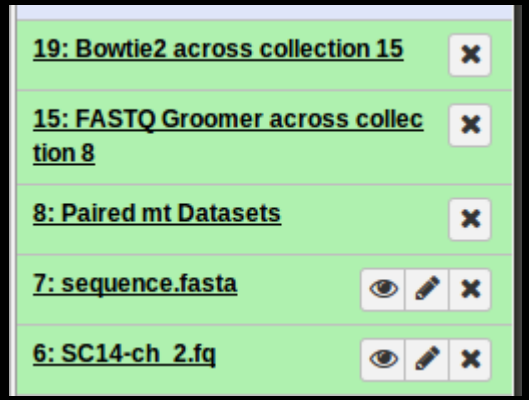
...

## Bowtie 2 across collection 13

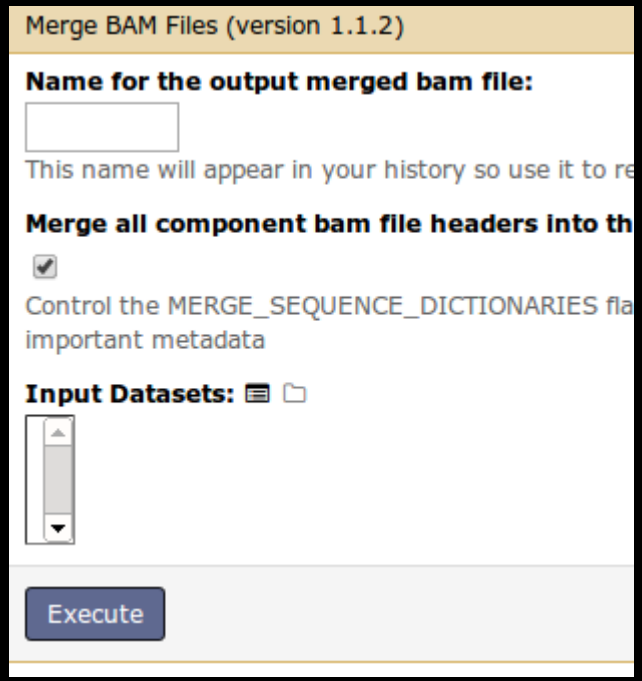
list collection

- Element - 0:M236C4
  - hda - *Bowtie 2 on data 9 and data 10*
- Element - 1:M486C2
  - hda - *Bowtie 2 on data 11 and data 12*

...



# Reducing Collections




Modified *"Merge BAM Files"* tool to use multiple input data parameter instead of two input parameters and a repeat block.

# Reducing Collections


Can dynamically substitute collection for the multiple selection of datasets.

# Extract a Workflow

Dataset Collection Creation

*Dataset collection created in a way not compatible with workflows*

Treat as input dataset

Dataset Collection Creation

*Dataset collection created in a way not compatible with workflows*

**7: M486C2**

Treat as input dataset

Dataset Collection Creation

*Dataset collection created in a way not compatible with workflows*

**8: Paired mt Datasets**

Treat as input dataset

FASTQ Groomer

Include "FASTQ Groomer" in workflow

**13: FASTQ Groomer across collection 8**

Bowtie2

Include "Bowtie2" in workflow

**16: Bowtie2 across collection 13**

Merge BAM Files

Include "Merge BAM Files" in workflow

**17: NewBam.bam**

**18: NewBam_Merge BAM Files.log**

flagstat

Include "flagstat" in workflow

**19: flagstat on data 17**

19: flagstat on data 17

18: NewBam_Merge BAM Files.log

17: NewBam.bam

16: Bowtie2 across collection 13

13: FASTQ Groomer across collection 8

8: Paired mt Datasets

7: M486C2

6: M236C4

5: sequence.fasta

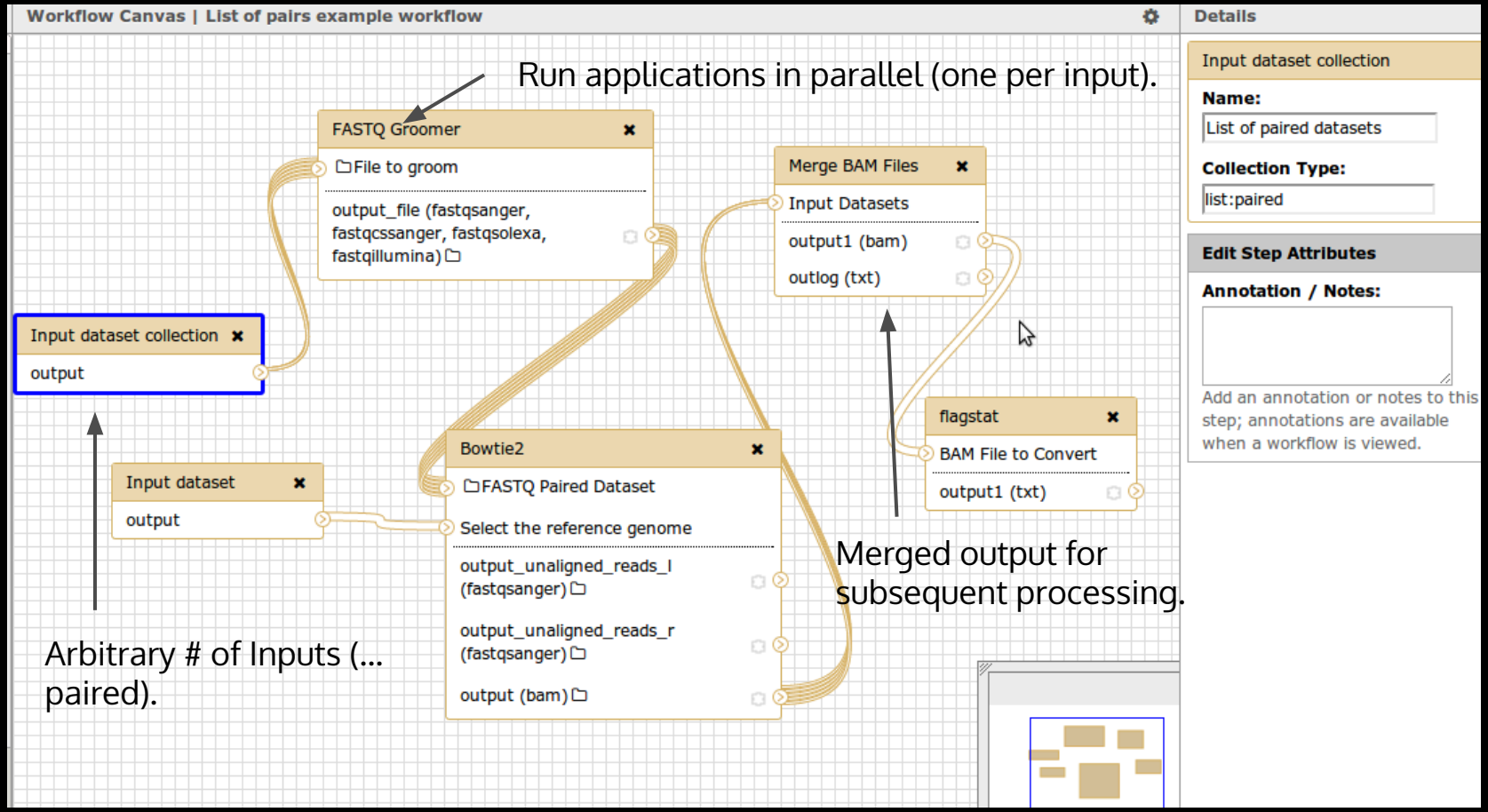
4: M486C2-ch_2.fq

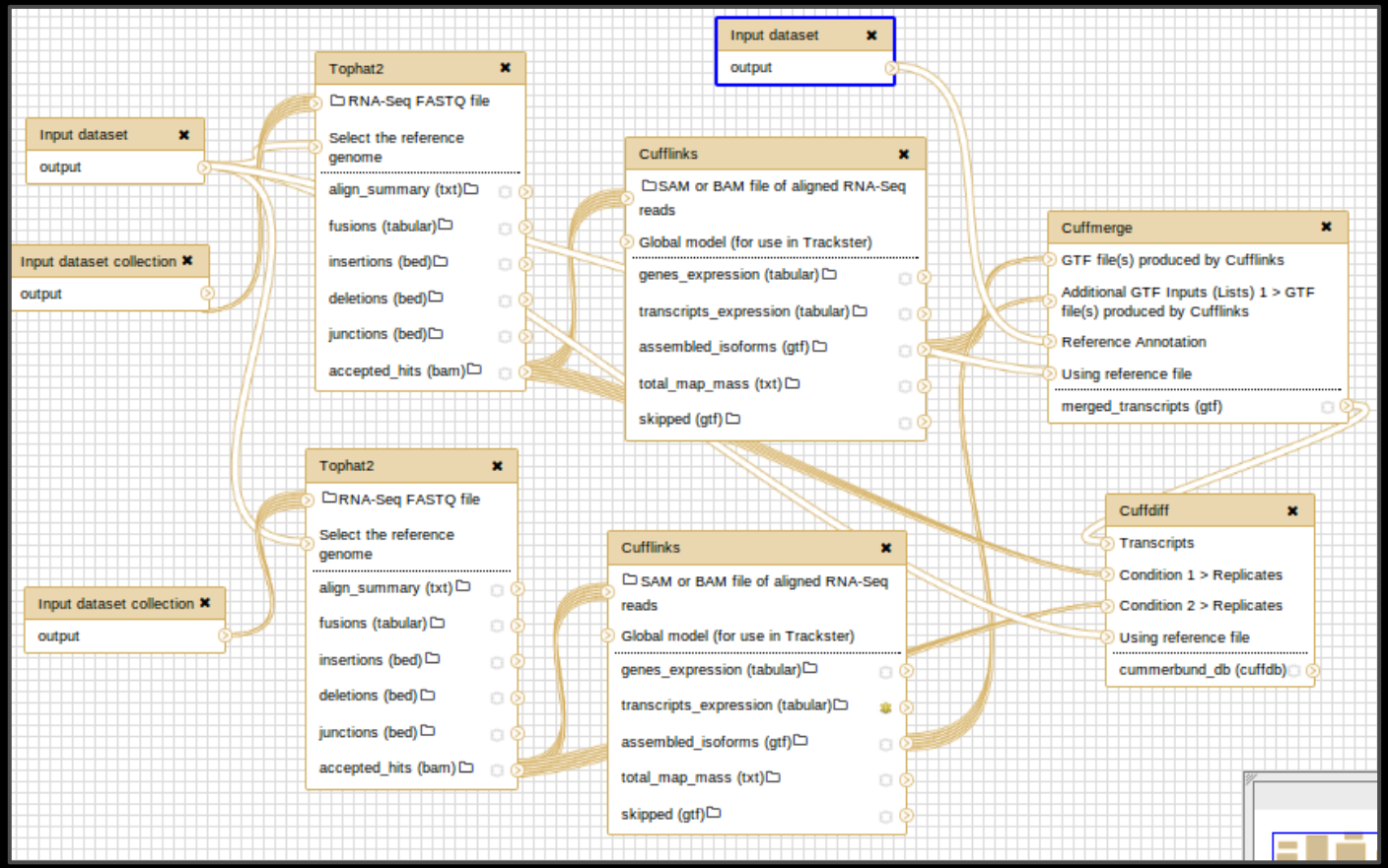
3: M486C2-ch_1.fq

2: M236C4-ch_2.fq

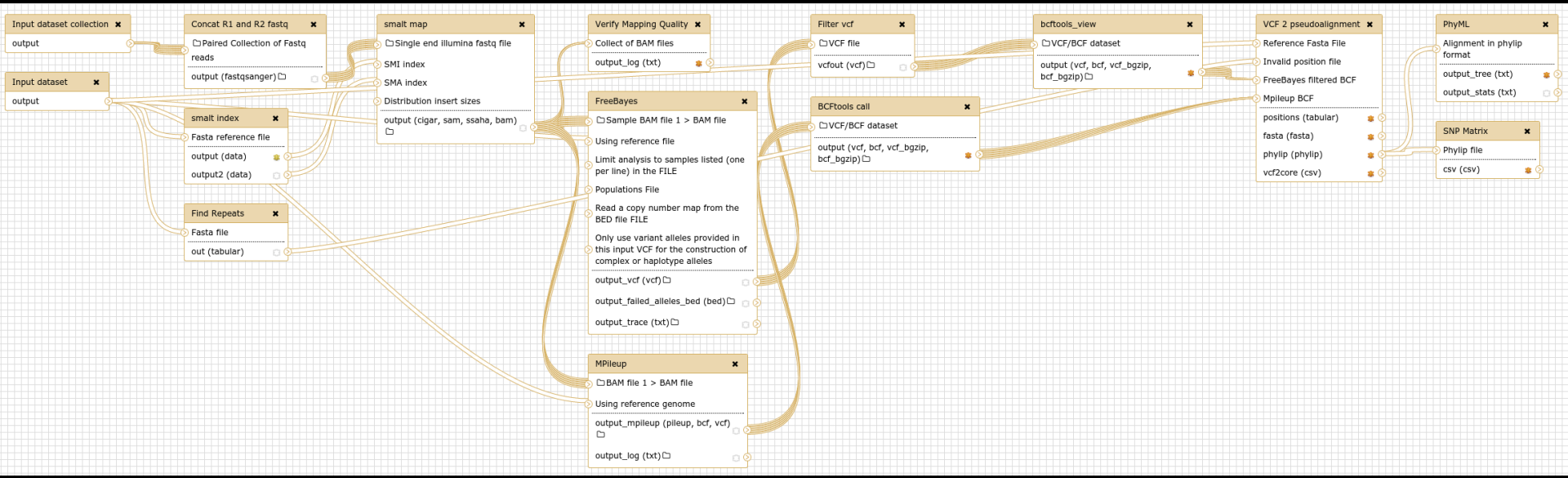
1: M236C4-ch_1.fq

# More Powerful Workflows






RNA-Seq workflow based using the Tuxedo suite.

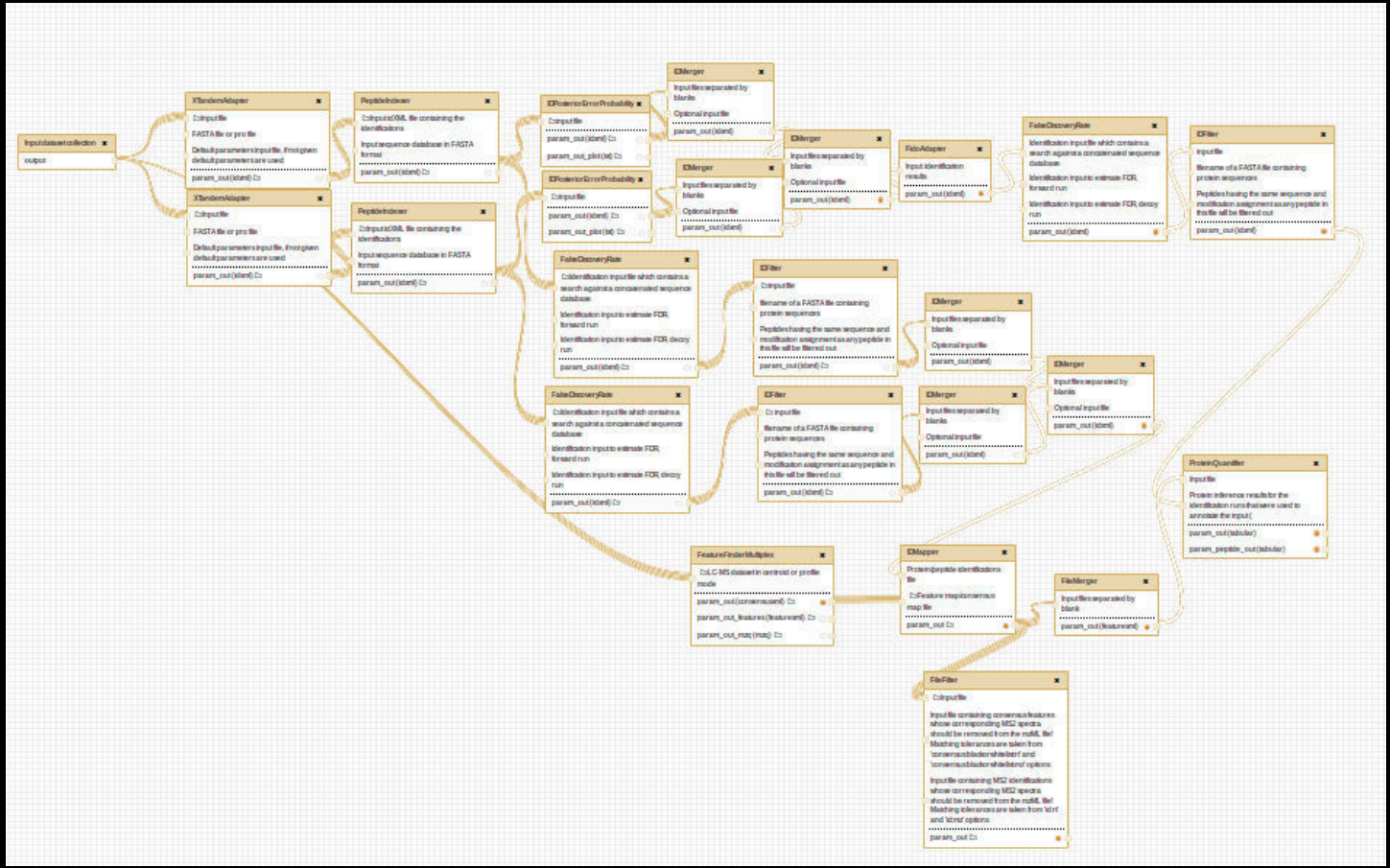



Core phylogenomics SNP pipeline by Aaron Petkau, Gary Van Domselaar, Philip Mabon, and Lee Katz. Used to assist in outbreak response for food-born illness by the public health agency of Canada. Process hundreds of paired strains at a time.

http://bit.ly/gcc2015irida

Protein identification of mass spectrometry data using Open MS.
Tools and workflow by Torsten Houwaart

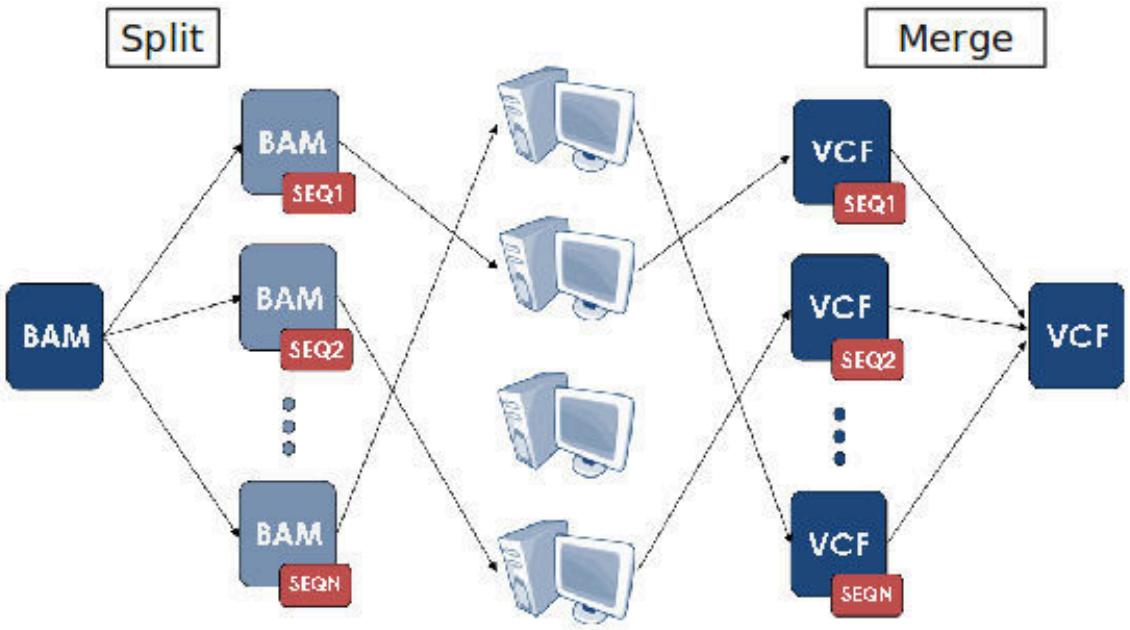
http://bit.ly/gcc2015rna



# Banner Year for Tool Development

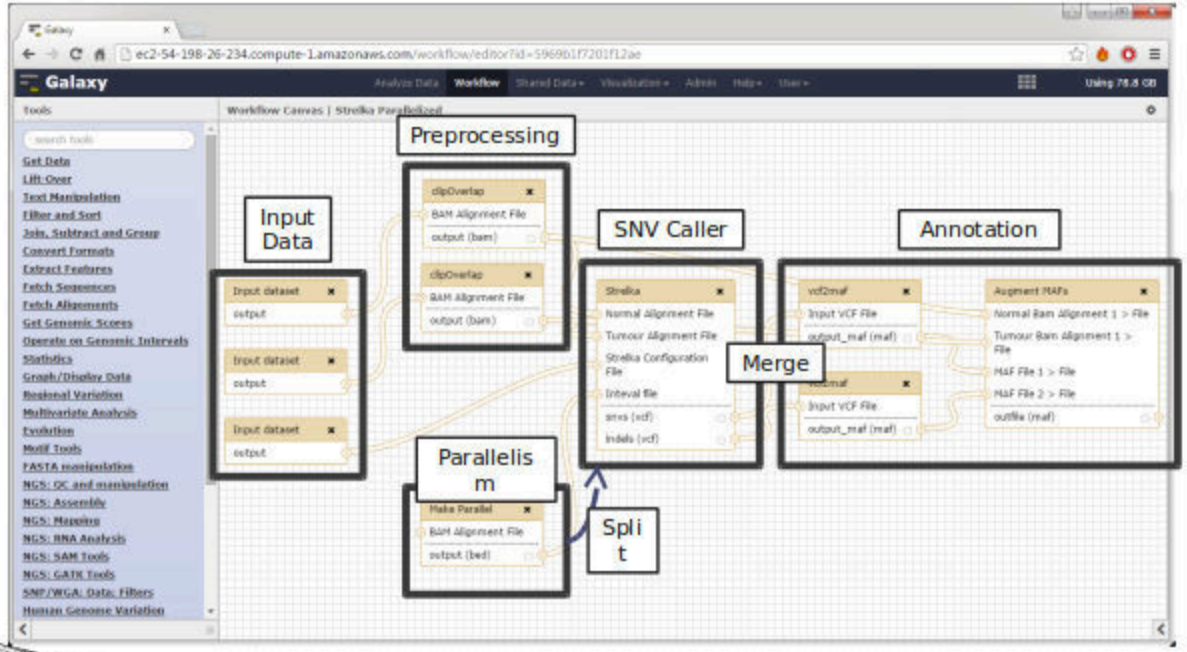
- In 2015, we have a had a real focus on tool development - new & updated tools for many areas including RNA-seq and metagenomics - with collection compatibility being a large focus.
- Support for collection aware read-group handling for BWA, Bowtie 2, Picard.

# Parallelization in Galaxy



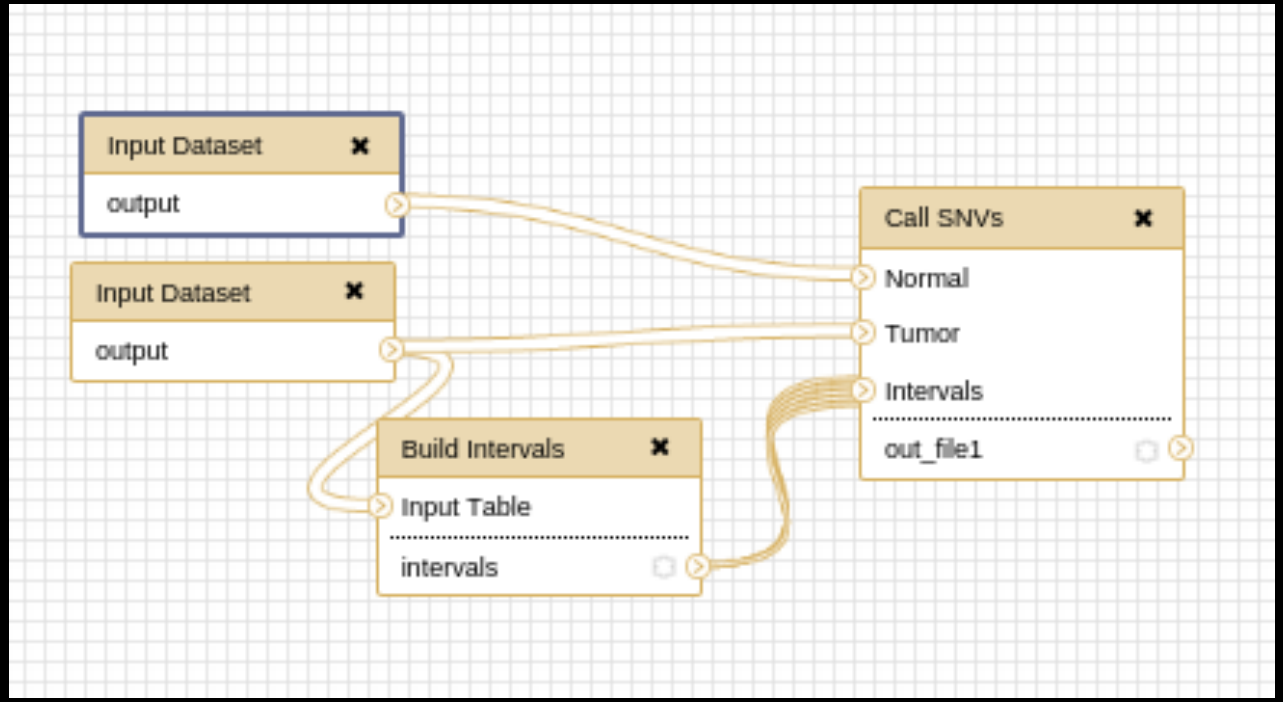

http://bit.ly/gcc2015cancergenomics
Marco Albuquerque, et. al.

# Somatic SNV Workflow




http://bit.ly/gcc2015cancergenomics

Marco Albuquerque, et. al.

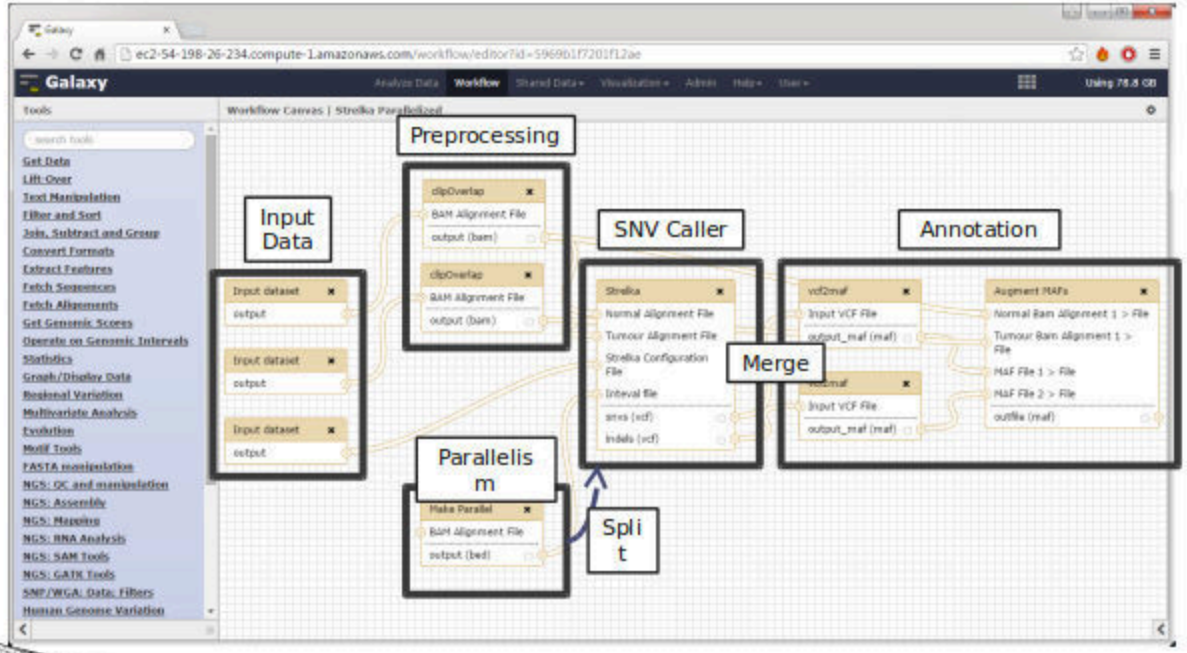

Input Dataset
output
Input Dataset
output
Build Intervals
Input Table
intervals
Call SNVs
Normal
Tumor
Intervals
out_file1

# Workflow - Rewrite

- Stateful models allowing re-evaluating workflows over time. Large or complex workflows will now be evaluated in the background.
- Plugin framework for describing how scheduling occurs.

... groundwork for future enhancements - still must build new UI elements and modules (loops, conditionals) to maximize the utility of this...

# Somatic SNV Workflow



# More output collections.

Similar approach by Kyle Ellrott @ UCSC.

Usig biobambam to split a bam file, mapping with BWA, and then merging the results.

https://github.com/ucscCancer/pcawg_tools/tree/master/tools/pcap_tools

## “Implicit” Connections between Steps

Steps can wait arbitrarily on other steps without needing to specify an explicit input-to-output “data flow”.

Use for admin workflows to populate reference data.

See talk by Dan Blankenberg at the 2015 GCC - Less Click, More Quick. http://bit.ly/gcc2015lessclick

# Toward 10,000 samples (beyond collections)

- Optimize database interactions, tool execution.
- Move workflow scheduling into own process, optimize.
- Differentiate between cluster failures and tool failures.
  - Retry later on cluster failures.
  - Retry on different cluster or with different resource params on failures.
- Optimize disk usage - streaming
- More diverse and bigger compute and storage
  - Separate metadata calculation out into its own “job”
  - XSEDE
  - More portable dependency management (docker, Homebrew, tool shed installs without galaxy)

The Galaxy Team

# Thanks!


With special thanks to **Carl Eberhard** - for building UI powering this work.

The Galaxy Community for building awesome stuff with Galaxy and pushing the platform forward - especially **Philip Mabon**.

# Should I CWL?

- Definitely - but it is *not* the best way to reach the large Galaxy community today.
- CWL is not in Galaxy today and may never be.
- CWL tools and workflows might never provide user experience of Galaxy native.
- Tool authors should #usegalaxy.

# Extra Content

# Bam Splitting Workflow

Add a BAM splitting workflow example.

- biobambam split
- bwa-mem
- reheader merge

# Splitting a BAM File

Something as simple as splitting a BAM file though is a real problem. The number and nature of one job cannot be determined until the previous one completed.

**MergeSamFiles** merges multiple SAM/BAM datasets into one (Galaxy Tool Version 1.126.0)

**Select SAM/BAM dataset or dataset collection**

No sam or bam dataset available.

Dataset collection

If empty, upload or import a SAM/BAM dataset

**Merge the sequence dictionaries of the datasets being merged**

Yes No

MERGE_SEQUENCE_DICTIONARIES; default=False

**Assume the input file is already sorted**

Yes No

ASSUME_SORTED; default=False

**Comment**

Insert Comment

You can provide multiple comments

**Select validation stringency**

Lenient

Setting stringency to SILENT can improve performance when processing a BAM file in which variable-length d
not otherwise need to be decoded.

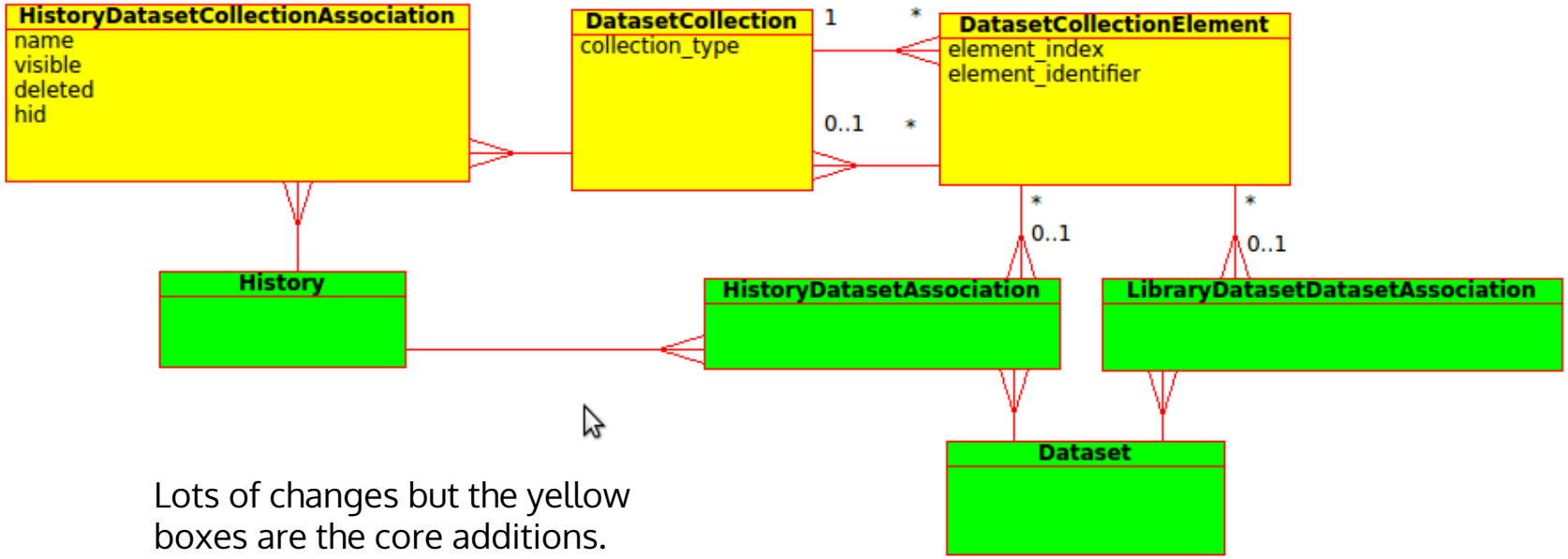
Execute

# Handful of Reduction Tools...

A handful of reduction tools need to be updated (so will tools consuming pairs). Using multiple input data parameters instead of repeat parameters will still allow these tools to work with uncollected dataset.

repeat blocks - while cumbersome - allow duplicated entries & control of order. Multiple input data parameters should be enhanced to have same control.

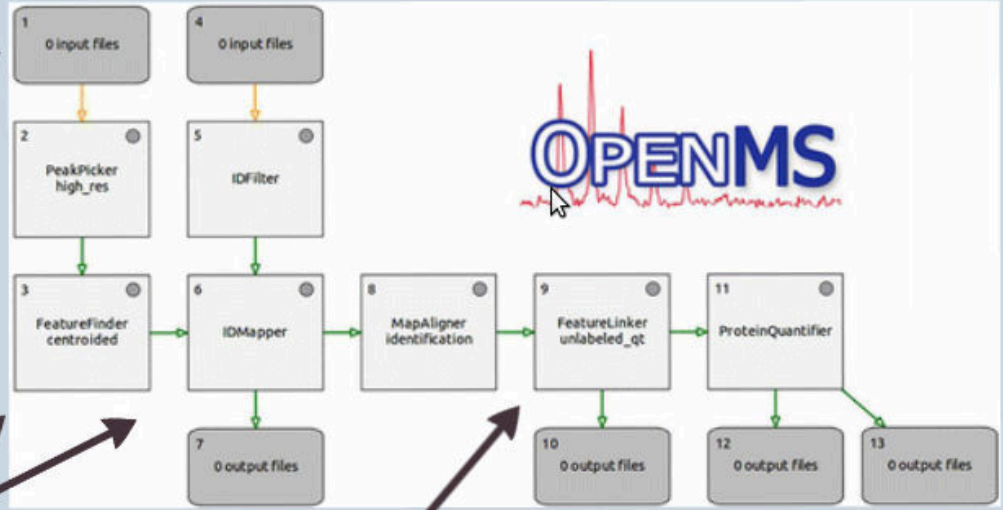
# Models




Lots of changes but the yellow boxes are the core additions.

# John @ GCC 2012, 2013 - Workflows... not good enough!

"An Automated Pipeline for High-Throughput Label-Free Quantitative Proteomics (J. Proteome Res., 2013, PMID: 23391308)."

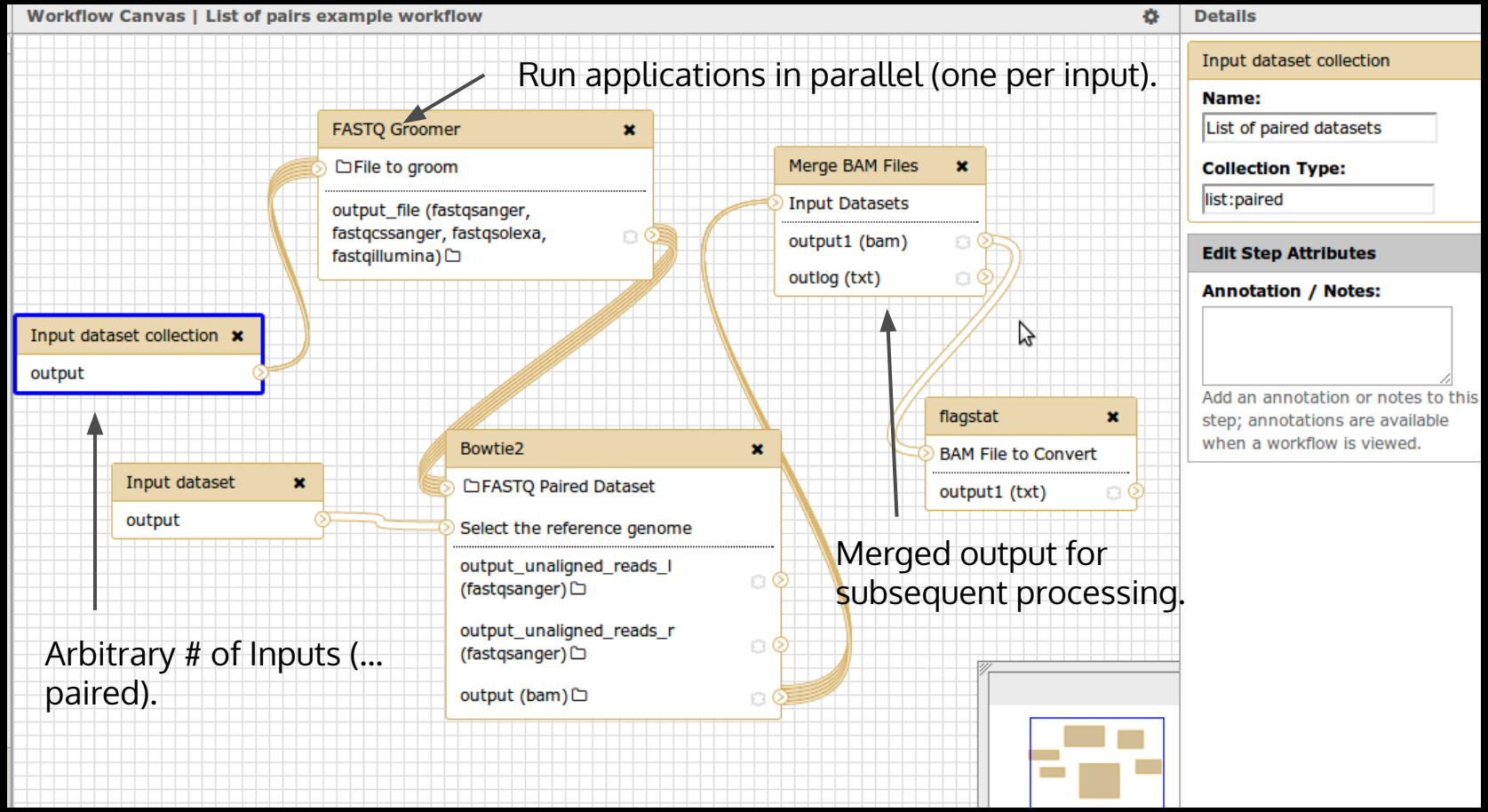



Arbitrary # Inputs

Applications run in parallel (once per input)

Merged into one output for subsequent steps.

# More Powerful Workflows



# API First Development

Initial work focused on building an API for creating and *using* dataset collections.

Upshot - API is richer than UI currently (especially in stable).

bioblend contains high-level functionality for creating and "viewing" collections in different ways.

# Tool Parameters - Cheetah-isms

Common paired data idiom:

```
bowtie $collect_param.forward $collect_param.reverse
```

Common list data idiom:

```
#for $f in $collect_param# $f #end for#
```

-or-

```
#for $name in $collect_param.keys()# $f[$name] #end for#
```

Nested data:

```
#for $f in $collect_param# $f.is_collection ...
```

# Tool Parameters - Testing

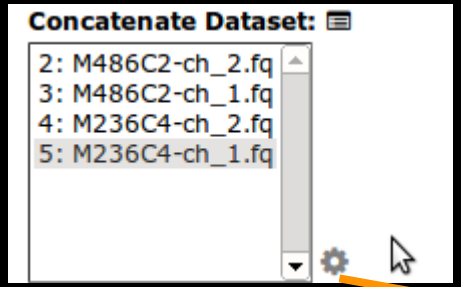
```
<test>
  <param name="collect_param">
    <collection type="paired">
      <element name="forward" value="simple_line.txt" />
      <element name="reverse" value="simple_line_alternative.txt" />
    </collection>
  </param>

  ...
```

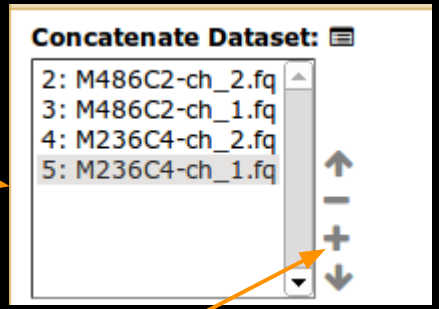
# Plan: Multiple-Data Improvements

Enhance multiple input data parameters to allow control of order and repeated entries.

All the ease of multiple data inputs with actually greater versatility than placing simple data inputs into repeat blocks.




Mock Up




An advanced “add to selection” modal would provide interesting room to grow - options for importing library datasets, digging into collections, etc....

# Plans - Other

- https://trello.com/c/WodW2sLb
- Subcollection mapping over multiple data parameters.
- Fix history import/export for data collections.
- Implicit conversion
- Allow batch input of collections to workflows

# Tool Parameters - Tool XML

```
<param name="collect_param1" type="data_collection"
        format="bam" collection_type="paired" />
```

Optional - filter collections by contained formats.

Optional - filter collections by collection_type.

# TODO:

- Screenshots of building up workflow from scratch?

Extra Slides (post presentation)…

- Comparison with multiple file datasets.

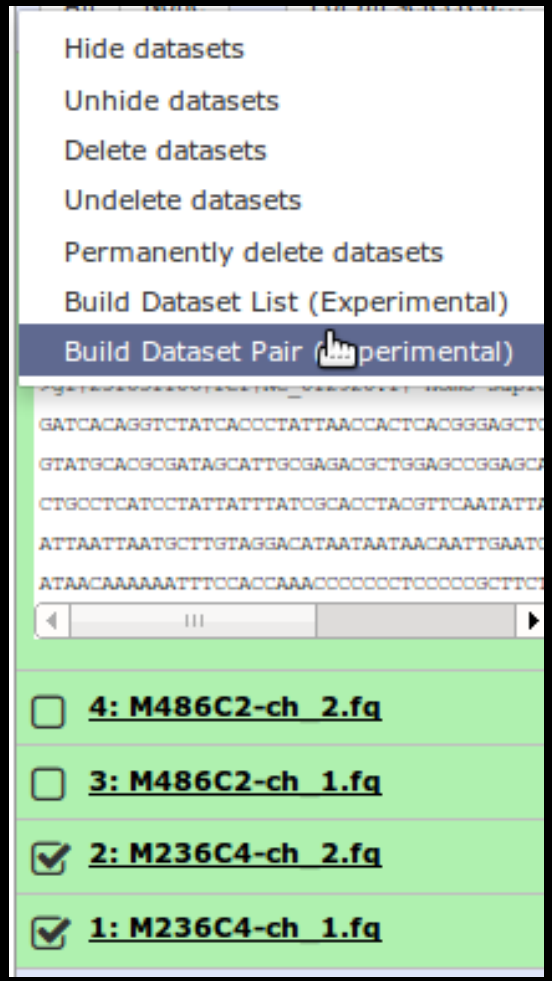
REDO Initial Screenshots with Correct History Name on Bigger Monitor.

# Building Collections…

```
>>> from bioblend import galaxy
>>> gi = galaxy.GalaxyInstance(url="localhost:8080",
                                key="db53bb4500dfaeda25ceb378069b722b")
>>> hist = gi.histories.get_histories(name="Map/Reduce Test")[0]
>>> gi.histories.show_history(hist["id"], contents=True, deleted=False)
>>> pair1_id = [d for d in gi.histories.show_history(hist["id"], contents=True)
                if d["hid"] == 5][0]["id"]
>>> pair2_id = [d for d in gi.histories.show_history(hist["id"], contents=True)
                if d["hid"] == 6][0]["id"]
>>> gi.histories.update_dataset_collection(hist["id"], pair1_id, name="M236C4")
>>> gi.histories.update_dataset_collection(hist["id"], pair2_id, name="M486C2")
```

bioblend contains support for creating, reading, updating (name, annotations, etc…), and deleting history dataset collections.

https://github.com/afgane/bioblend/commit/f8d40b687be4c699d608e930c59726793922fa0a



# Collection Mapping (1 / 3)

FASTQ Groomer (version 1.0.4)

**File to groom:**

4: M486C2-ch_2.fq

*Tool consumes a FASTQ file.*

**Input FASTQ quality scores type:**

Sanger & Illumina 1.8+

**Advanced Options:**

Hide Advanced Options

Execute

*-List of Paired Datasets*
*-Paired Datasets*
*-Individual FASTQ datasets.*

**What it does**

This tool offers several conversions options relating to the FASTQ format.

When using *Basic* options, the output will be *sanger* formatted or *cssanger* formatted (when the input is Color Space Sanger).

When converting, if a quality score falls outside of the target

History

**Map/Reduce Test**

519.8 MB

8: Paired mt Datasets

7: M486C2

6: M236C4

5: sequence.fasta

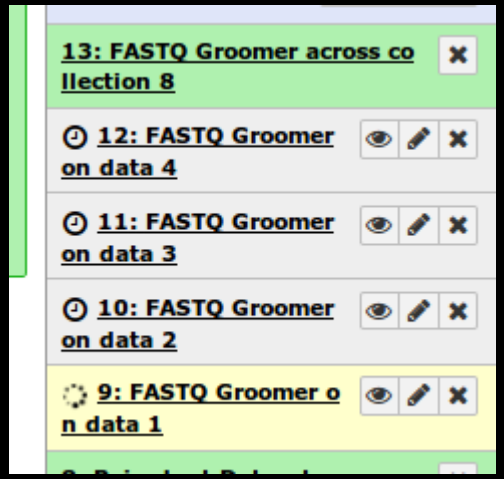
4: M486C2-ch_2.fq

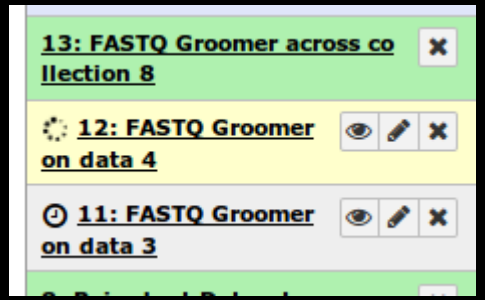
3: M486C2-ch_1.fq

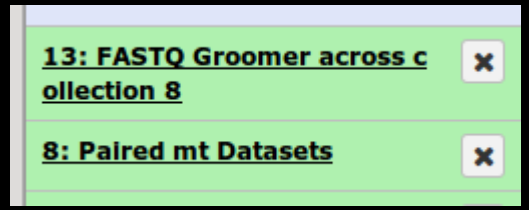
2: M236C4-ch_2.fq

1: M236C4-ch_1.fq

# Collection Mapping (3 / 3)



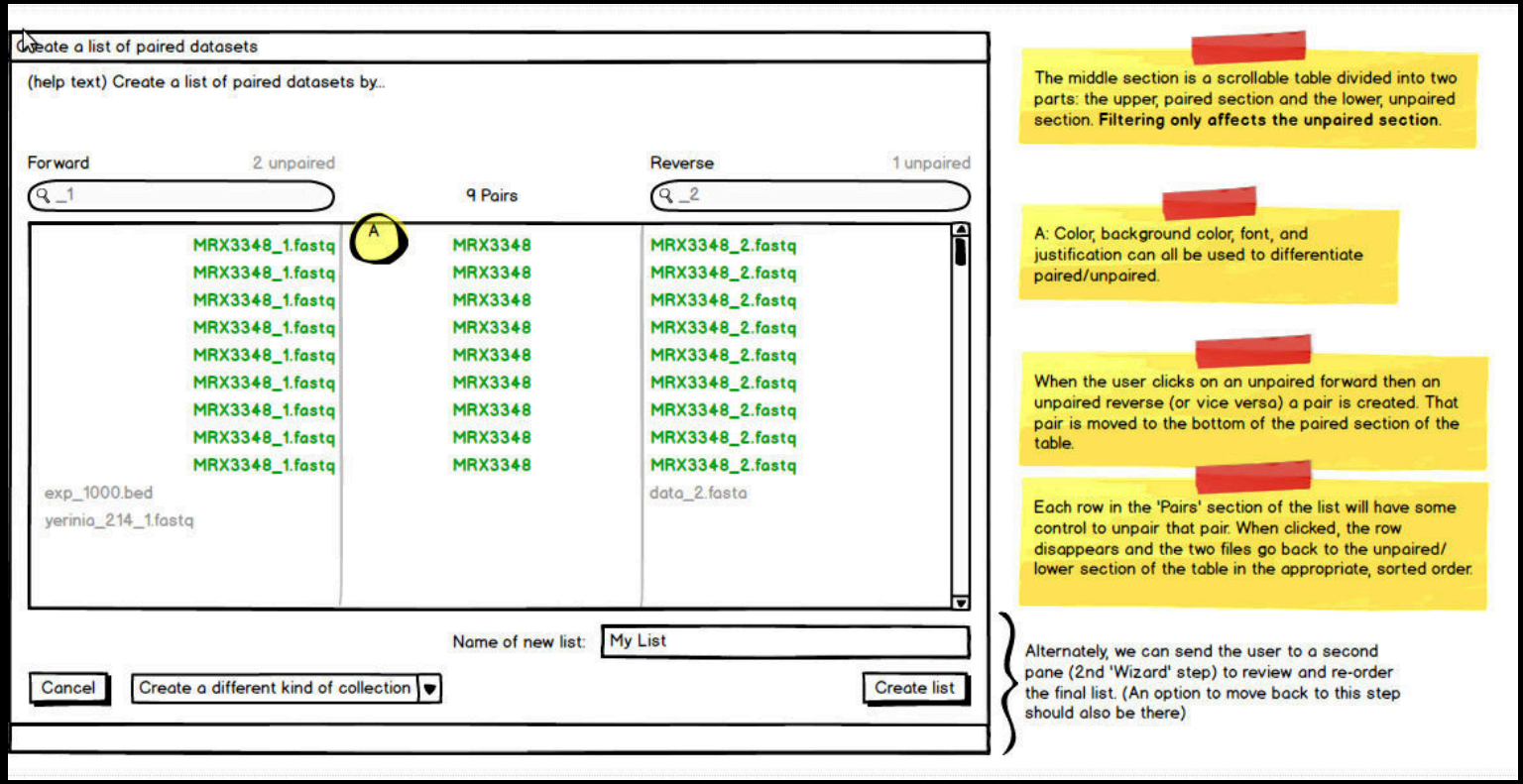

Like hiding datasets in workflow execution, datasets are visible running or queued and they are hidden after (and only collection is visible).

Collection is always green regardless of contents - is currently stateless.

Need to do a better job on both points - this is not too scalable - but it was an easy quick win.

# Plans - UI for Creating Collections

https://trello.com/c/CIIdaxl2 Mockup @ mybalsamiq



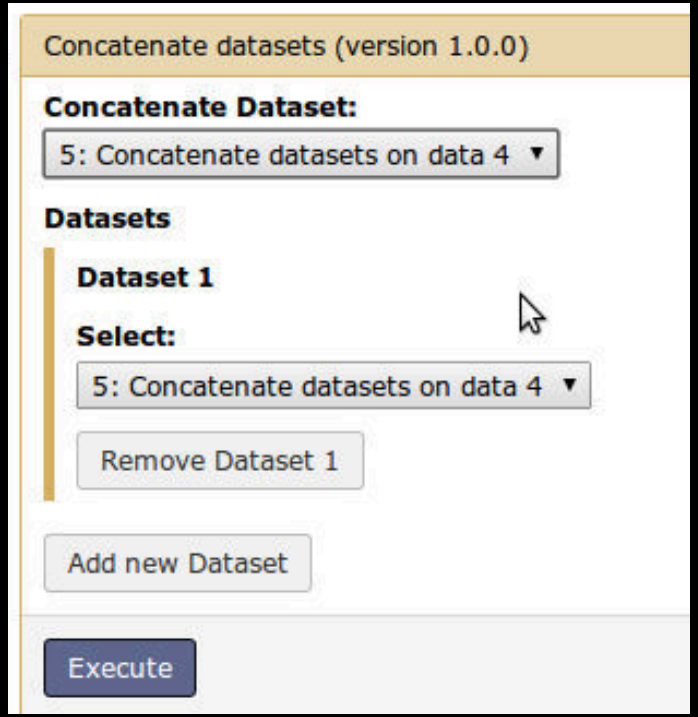
# Why not repeat replacements?

In its most simple form - allowing replacement of one repeat block with a collection - this feature would be gross to implement - it would add a lot of complexity to already complex parts of Galaxy.

… and it would not work with any tools.

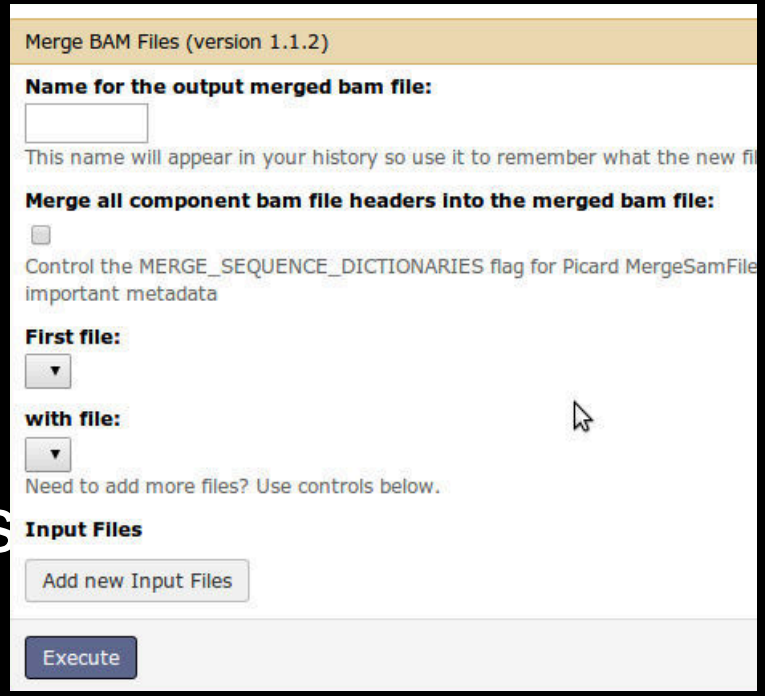
# Concatenate (Easiest Reduction)

Not just a repeat, would need to be able to dynamically replace input + repeat to work with this. That will be ugly and will have implications all over.



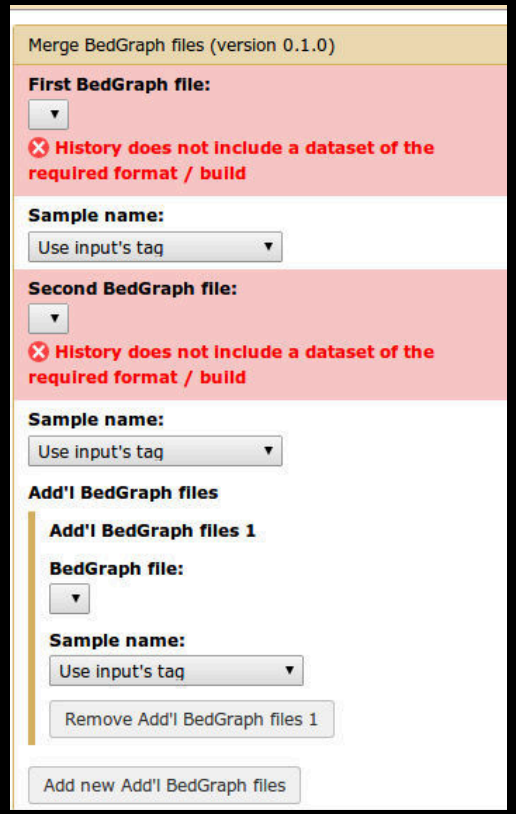
# Merging Bams

Second most common reduction - has two inputs and a repeat. So we need to be able to dynamically replace any number inputs and a repeat. Hmm….



# Merging BedGraph

Found another reduction tool on main. Multiple inputs, multiple extra options. How could this reasonably allow collection replacement at the infrastructure level.

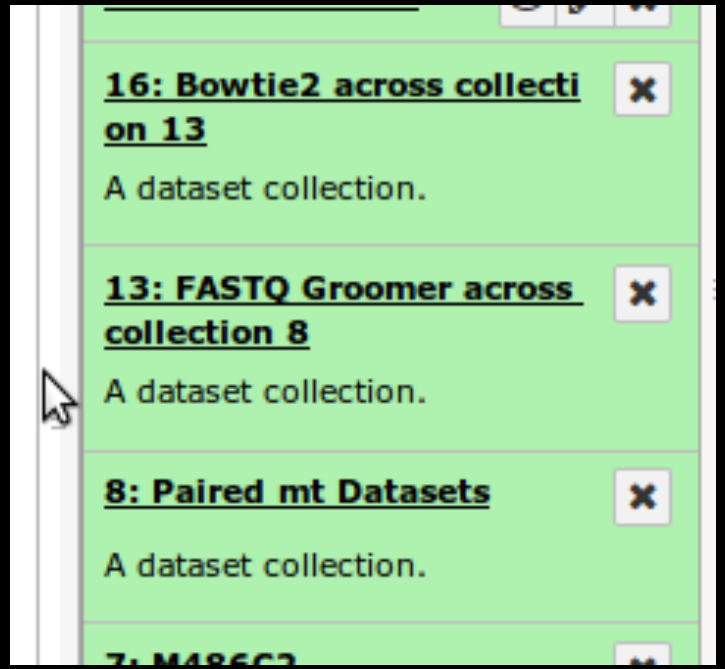


# Plans - More Options in History Panel

https://trello.com/c/hnmWWKlB

Currently can hide, delete, and see name.

Cannot rename, rerun, see type, see contents, see/add annotations, see/add tags, download, etc...



# Plans - UI for Uploading Collections

https://trello.com/c/ZAXwWOZ2

Incorporate collection builder when uploading files (or vise versa).

# Plans - UI for Viewing Collections

https://trello.com/c/PVdbbpQS

# Plans - Store Collections in Data Libraries

https://trello.com/c/3axmjaxE

# Plans - Improved Reductions

https://trello.com/c/lp5YmA1O

Improvements to multiple data parameters described earlier and/or ability to reduce across repeat statements.

# Plans - Filtering Collections

https://trello.com/c/ryKJrsYc

Main Goal: Filter out the failed datasets and keep going.

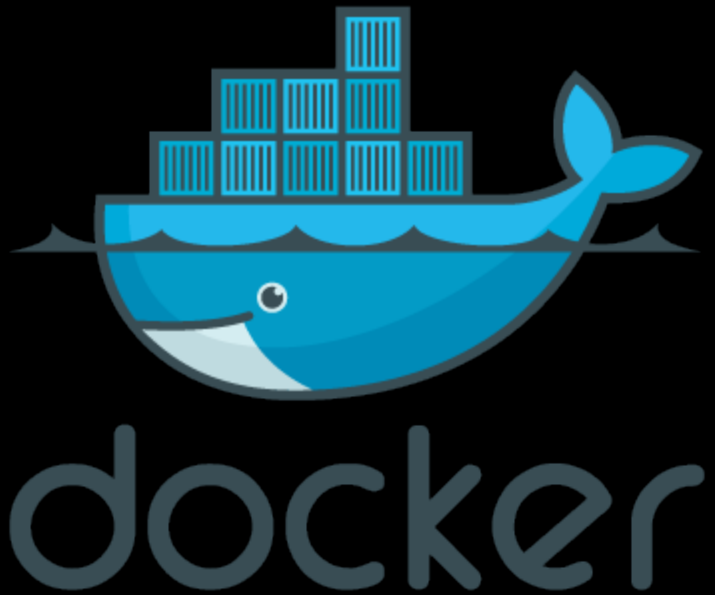
Would like more general filters - filter on metadata (*file size*, *number of sequences*, etc...)

Needs to be trackable so can extract and execute in workflows. May require delayed workflow evaluation.

# Plans - Rerun Tools / Resuming Workflows

https://trello.com/c/lxVJy7fs

# Docker… Docker… Docker...




https://github.com/jmchilton/gcc2014_demo