Streamlining Access to Reference Datasets

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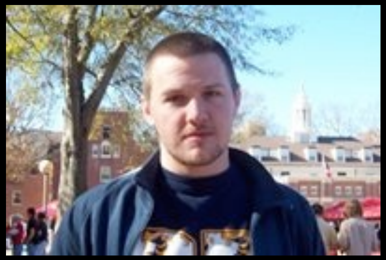
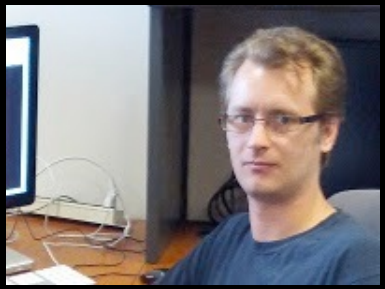


Dannon Baker

Dan Blankenberg



Dave Bouvier

Marten Čech

John Chilton

Dave Clements

Nate Coraor

Carl Eberhard

Jeremy Goecks

Sam Guerler

Jen Jackson

Ross Lazarus

Anton Nekrutenko

Nick Stoler

James Taylor

Greg Von Kuster

http://wiki.galaxyproject.org/GalaxyTeam

Overview

Intro to Built-in Datasets

Some Problems

Data Managers

- What?
- Demo

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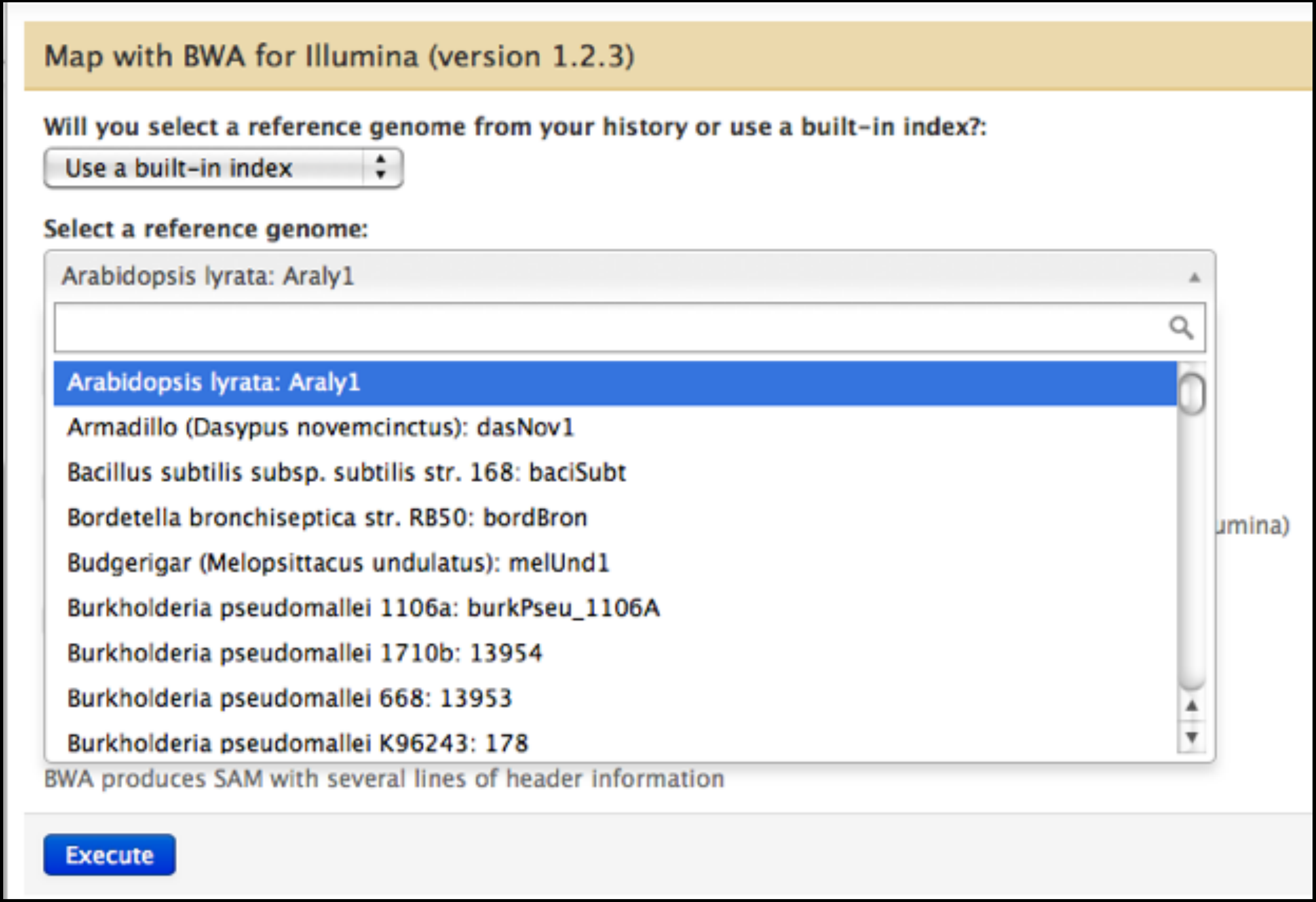
Built-in Datasets

BWA example



Map with BWA for Illumina (version 1.2.3)

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

Use a built-in index

Select a reference genome:

Arabidopsis lyrata: Araly1

- Arabidopsis lyrata: Araly1
- Armadillo (Dasypus novemcinctus): dasNov1
- Bacillus subtilis subsp. subtilis str. 168: baciSubt
- Bordetella bronchiseptica str. RB50: bordBron
- Budgerigar (Melopsittacus undulatus): melUnd1
- Burkholderia pseudomallei 1106a: burkPseu_1106A
- Burkholderia pseudomallei 1710b: 13954
- Burkholderia pseudomallei 668: 13953
- Burkholderia pseudomallei K96243: 178

umina)

BWA produces SAM with several lines of header information

Built-in Datasets

BWA example

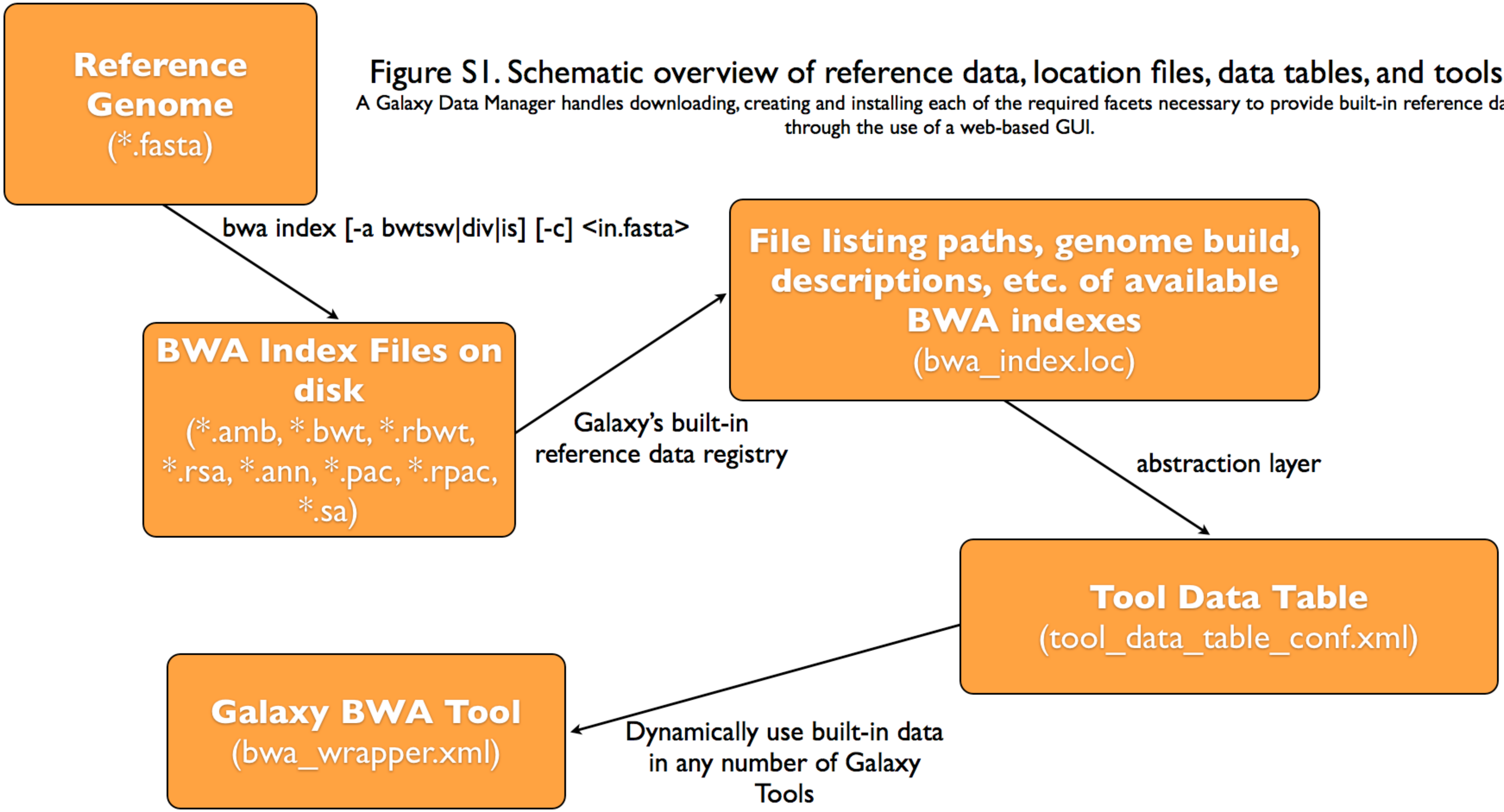


Figure S1. Schematic overview of reference data, location files, data tables, and tools.
A Galaxy Data Manager handles downloading, creating and installing each of the required facets necessary to provide built-in reference data through the use of a web-based GUI.

Reference Genome
(*.fasta)

bwa index [-a bwtsw|div|is] [-c] <in.fasta>

BWA Index Files on disk
(*.amb, *.bwt, *.rbwt, *.rsa, *.ann, *.pac, *.rpac, *.sa)

Galaxy's built-in reference data registry

File listing paths, genome build, descriptions, etc. of available BWA indexes
(bwa_index.loc)

abstraction layer

Tool Data Table
(tool_data_table_conf.xml)

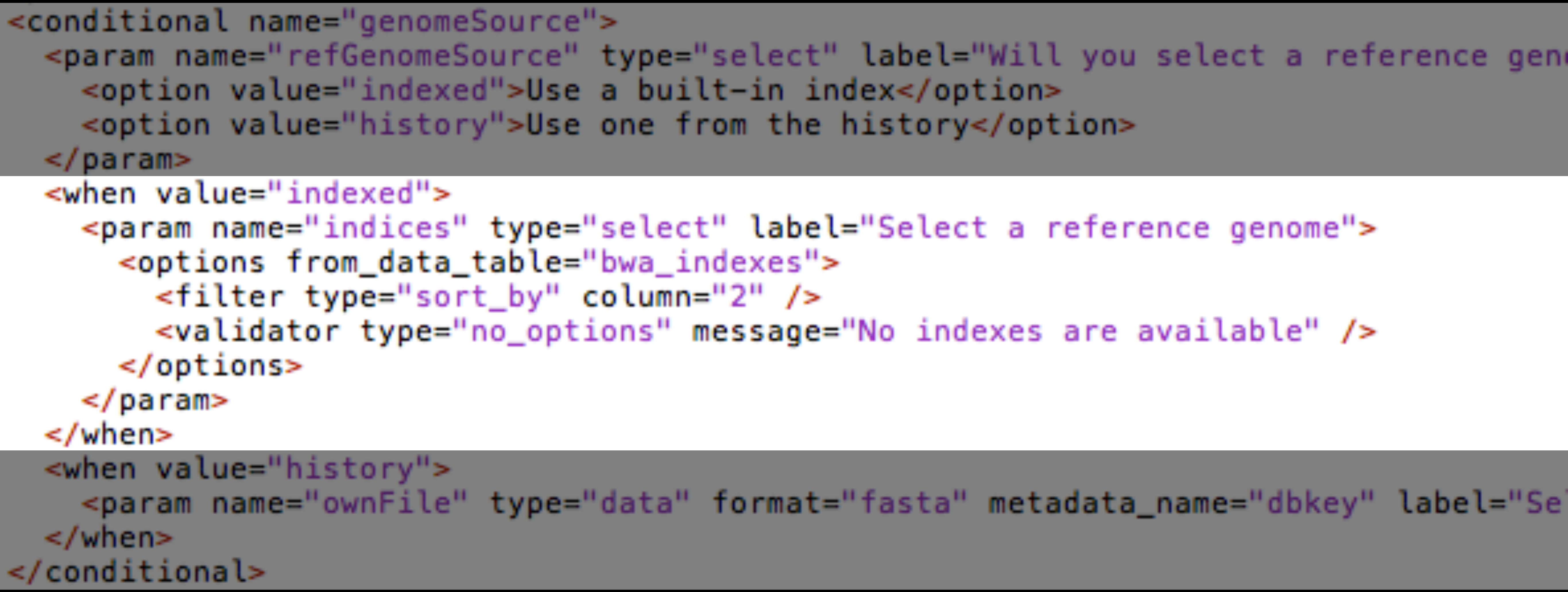
Dynamically use built-in data in any number of Galaxy Tools

Galaxy BWA Tool
(bwa_wrapper.xml)

Blankenberg, et al. Wrangling Galaxy's reference data. Bioinformatics. 2014 Jul 1.;30(13):1917-9.

Built-in Datasets

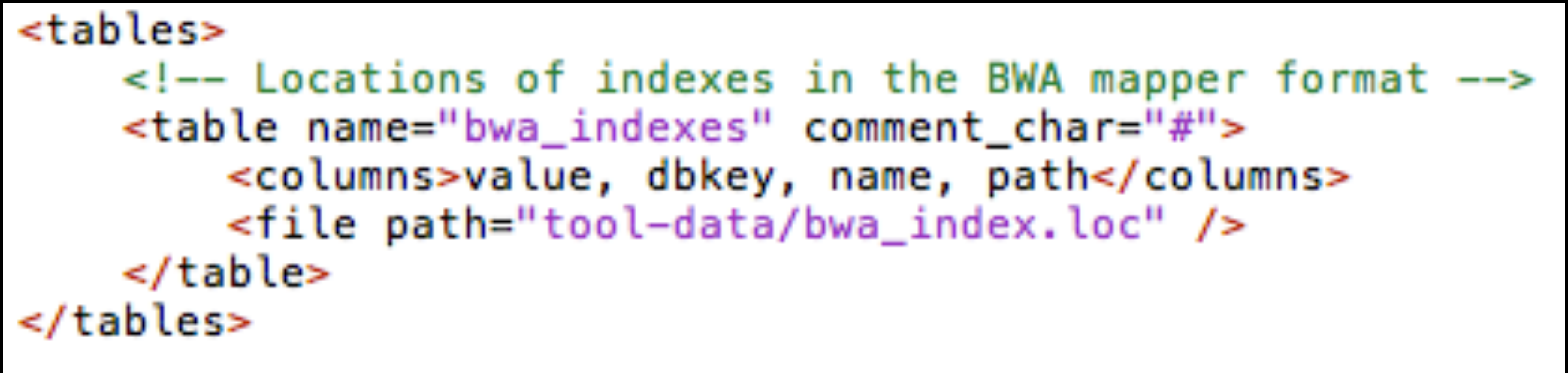
bwa_wrapper.xml



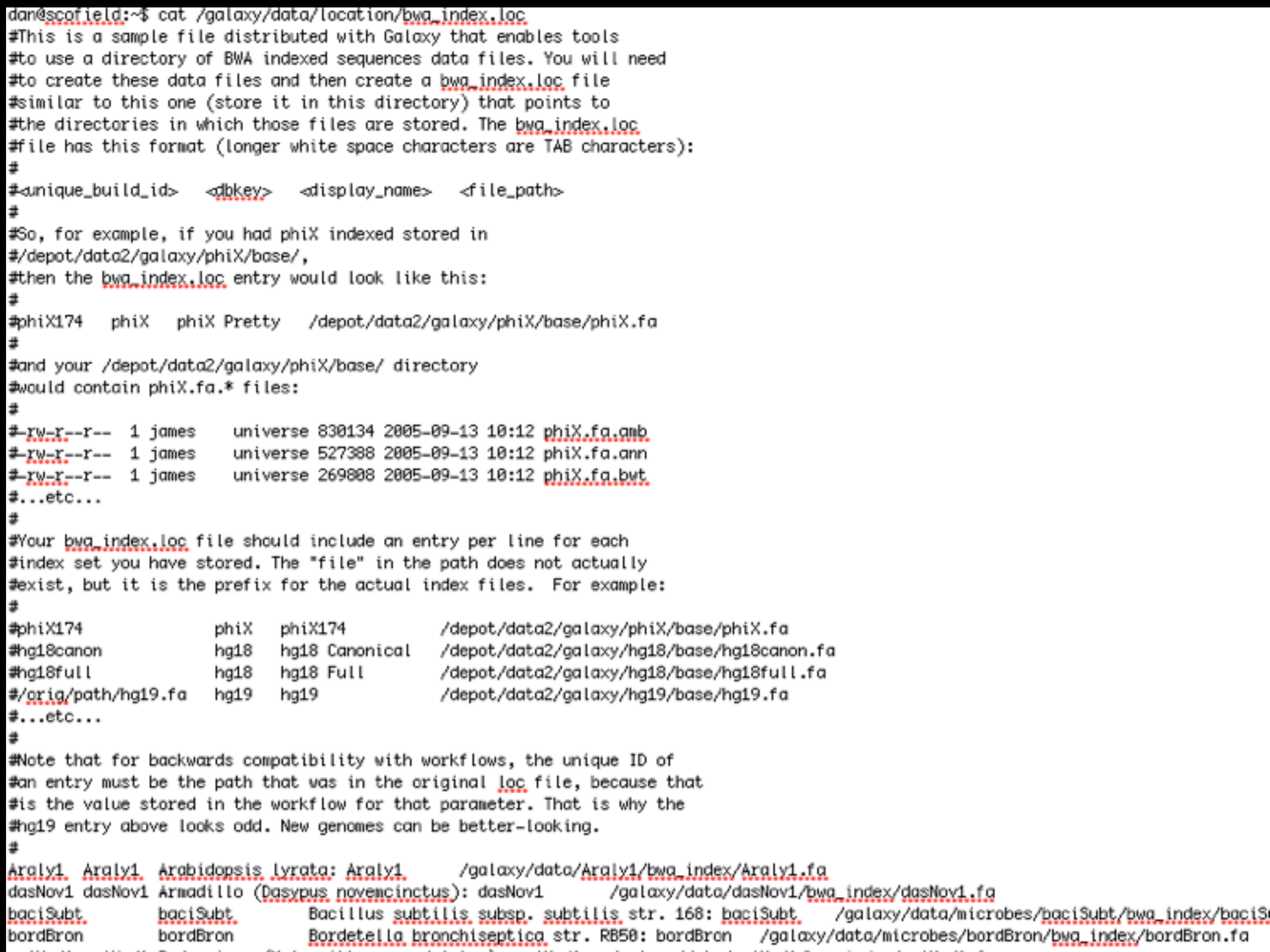
```
<conditional name="genomeSource">
  <param name="refGenomeSource" type="select" label="Will you select a reference gen
    <option value="indexed">Use a built-in index</option>
    <option value="history">Use one from the history</option>
  </param>
  <when value="indexed">
    <param name="indices" type="select" label="Select a reference genome">
      <options from_data_table="bwa_indexes">
        <filter type="sort_by" column="2" />
        <validator type="no_options" message="No indexes are available" />
      </options>
    </param>
  </when>
  <when value="history">
    <param name="ownFile" type="data" format="fasta" metadata_name="dbkey" label="Se
  </when>
</conditional>
```

Built-in Datasets

tool_data_table_conf.xml



```
<tables>
    <!-- Locations of indexes in the BWA mapper format -->
    <table name="bwa_indexes" comment_char="#">
        <columns>value, dbkey, name, path</columns>
        <file path="tool-data/bwa_index.loc" />
    </table>
</tables>
```



```
dan@scofield:~$ cat /galaxy/data/location/bwa_index.loc
#This is a sample file distributed with Galaxy that enables tools
#to use a directory of BWA indexed sequences data files. You will need
#to create these data files and then create a bwa_index.loc file
#similar to this one (store it in this directory) that points to
#the directories in which those files are stored. The bwa_index.loc
#file has this format (longer white space characters are TAB characters):
#
#<unique_build_id>   <dbkey>   <display_name>   <file_path>
#
#So, for example, if you had phiX indexed stored in
#/depot/data2/galaxy/phiX/base/,
#then the bwa_index.loc entry would look like this:
#
#phiX174   phiX   phiX Pretty   /depot/data2/galaxy/phiX/base/phiX.fa
#
#and your /depot/data2/galaxy/phiX/base/ directory
#would contain phiX.fa.* files:
#
#-rw-r--r--  1 james    universe 830134 2005-09-13 10:12 phiX.fa.amb
#-rw-r--r--  1 james    universe 527388 2005-09-13 10:12 phiX.fa.ann
#-rw-r--r--  1 james    universe 269808 2005-09-13 10:12 phiX.fa.bwt
#...etc...
#
#Your bwa_index.loc file should include an entry per line for each
#index set you have stored. The "file" in the path does not actually
#exist, but it is the prefix for the actual index files.  For example:
#
#phiX174              phiX   phiX174          /depot/data2/galaxy/phiX/base/phiX.fa
#hg18canon            hg18   hg18 Canonical   /depot/data2/galaxy/hg18/base/hg18canon.fa
#hg18full             hg18   hg18 Full        /depot/data2/galaxy/hg18/base/hg18full.fa
#/orig/path/hg19.fa   hg19   hg19             /depot/data2/galaxy/hg19/base/hg19.fa
#...etc...
#
#Note that for backwards compatibility with workflows, the unique ID of
#an entry must be the path that was in the original loc file, because that
#is the value stored in the workflow for that parameter. That is why the
#hg19 entry above looks odd. New genomes can be better-looking.
#
Araly1  Araly1  Arabidopsis lyrata: Araly1      /galaxy/data/Araly1/bwa_index/Araly1.fa
dasNov1 dasNov1 Armadillo (Dasypus novemcinctus): dasNov1       /galaxy/data/dasNov1/bwa_index/dasNov1.fa
baciSubt        baciSubt        Bacillus subtilis subsp. subtilis str. 168: baciSubt    /galaxy/data/microbes/baciSubt/bwa_index/baciS
bordBron        bordBron        Bordetella bronchiseptica str. RB50: bordBron   /galaxy/data/microbes/bordBron/bwa_index/bordBron.fa
```

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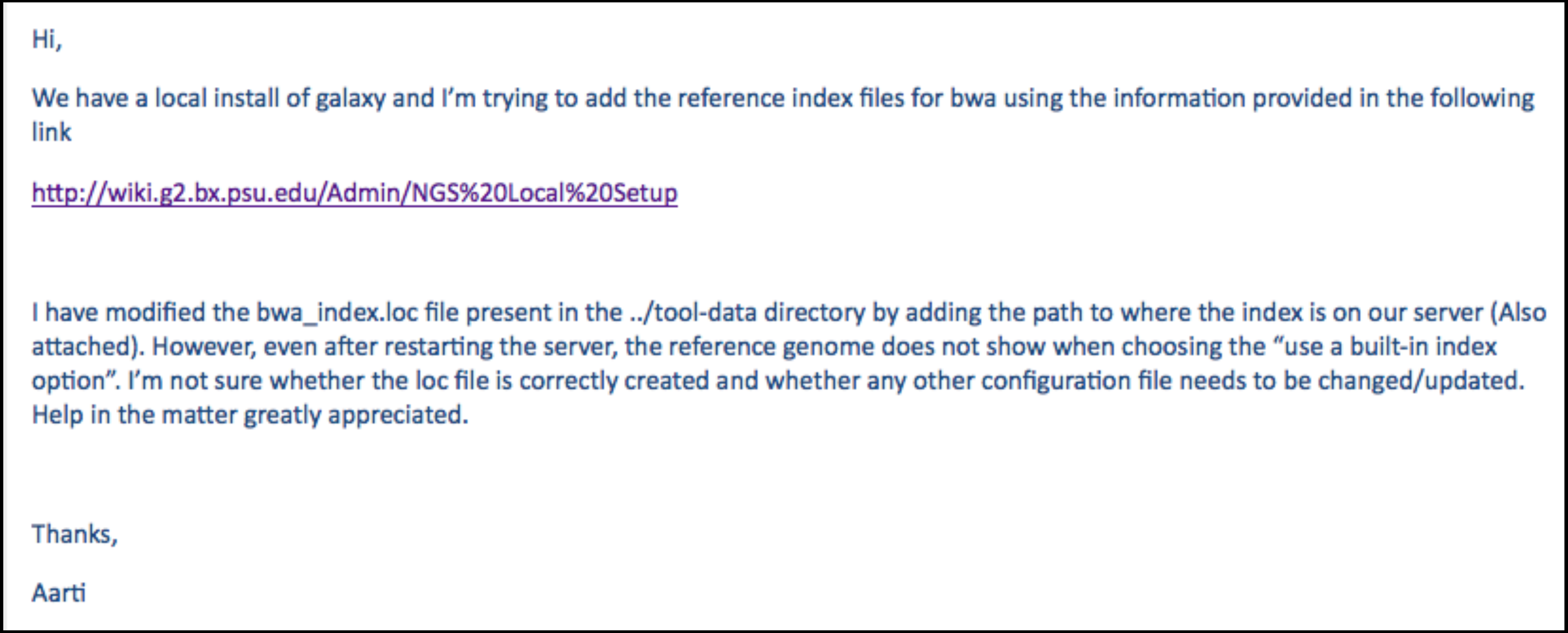
Some Problems

- Time consuming
    - ~30 minutes for workshop to add one BWA index
- Administrator needs to know how to update each type of reference data
    - Format of reference Data
    - Format of Location (.loc) file

Some Problems



Hi,

We have a local install of galaxy and I'm trying to add the reference index files for bwa using the information provided in the following link

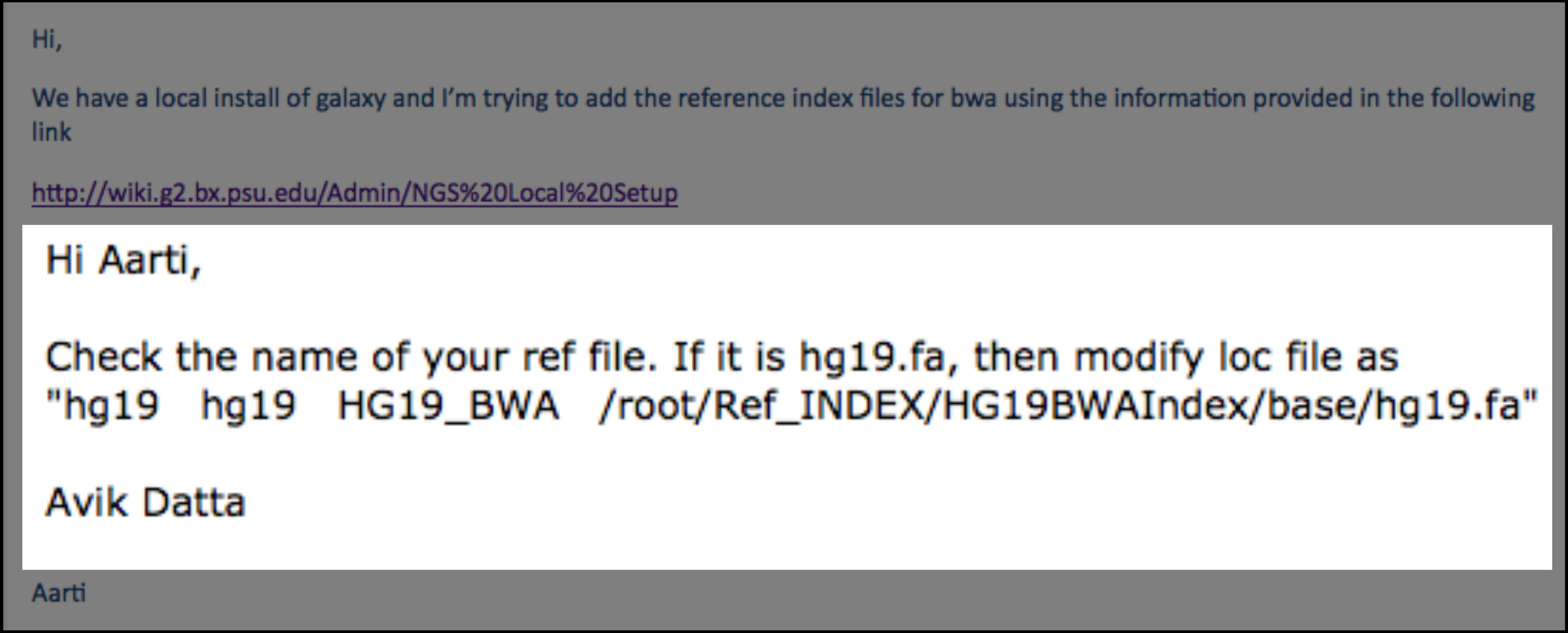
http://wiki.g2.bx.psu.edu/Admin/NGS%20Local%20Setup

I have modified the bwa_index.loc file present in the ../tool-data directory by adding the path to where the index is on our server (Also attached). However, even after restarting the server, the reference genome does not show when choosing the "use a built-in index option". I'm not sure whether the loc file is correctly created and whether any other configuration file needs to be changed/updated. Help in the matter greatly appreciated.

Thanks,

Aarti

Some Problems



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http://wiki.g2.bx.psu.edu/Admin/NGS%20Local%20Setup

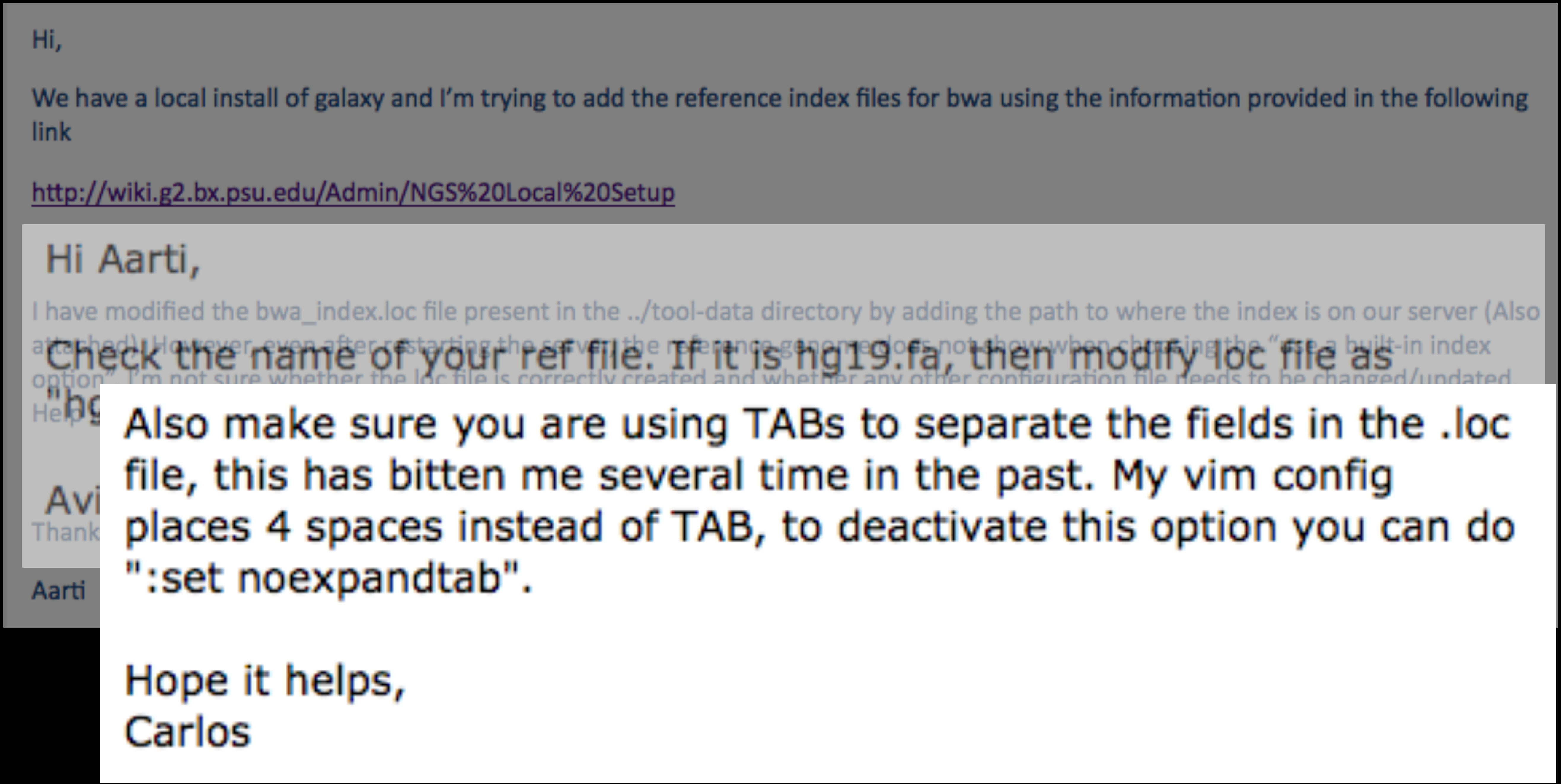
Hi Aarti,

Check the name of your ref file. If it is hg19.fa, then modify loc file as
"hg19   hg19   HG19_BWA   /root/Ref_INDEX/HG19BWAIndex/base/hg19.fa"

Avik Datta

Aarti

Some Problems



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Thank

Aarti

Hi Aarti,

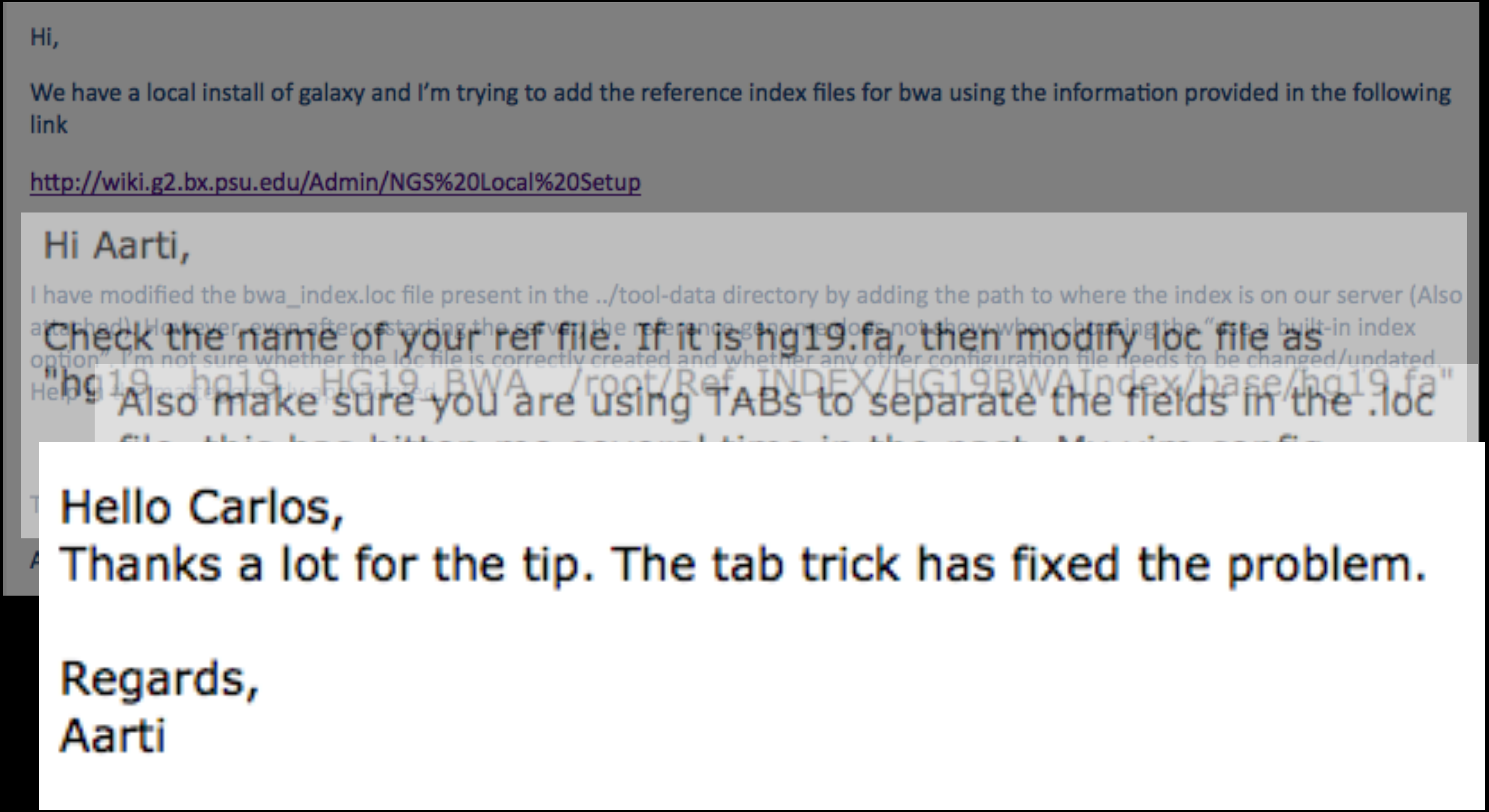
Check the name of your ref file. If it is hg19.fa, then modify loc file as "hg

Avi

Also make sure you are using TABs to separate the fields in the .loc file, this has bitten me several time in the past. My vim config places 4 spaces instead of TAB, to deactivate this option you can do ":set noexpandtab".

Hope it helps,
Carlos

Some Problems



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Hi Aarti,

Check the name of your ref file. If it is hg19.fa, then modify loc file as "hg19 hg19 HG19_BWA /root/Ref_INDEX/HG19BWAIndex/base/hg19.fa"

Also make sure you are using TABs to separate the fields in the .loc file, this has bitten me several time in the past. My vim config

Hello Carlos,
Thanks a lot for the tip. The tab trick has fixed the problem.

Regards,
Aarti

Other concerns

Accessible?

- Manually download genome FASTA files
- Download, compile, run bwa index; which options?

Reproducible?

- Only if the person performing manual steps keeps good notes

Transparent?

- Send email to sysadmin asking for notes

Need to restart Galaxy server when new entries are added

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Data Managers

Allows for the creation of built-in (reference) data

- underlying data
- data tables
- *.loc files

Specialized Galaxy tools that can only be accessed by an admin

Defined locally or installed from ToolShed

Data Managers

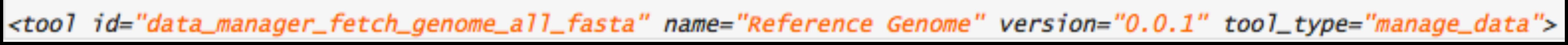
Flexible Framework

- not just Genomic data
- Interactively Run Data Managers through UI
- Workflow compatible
- API

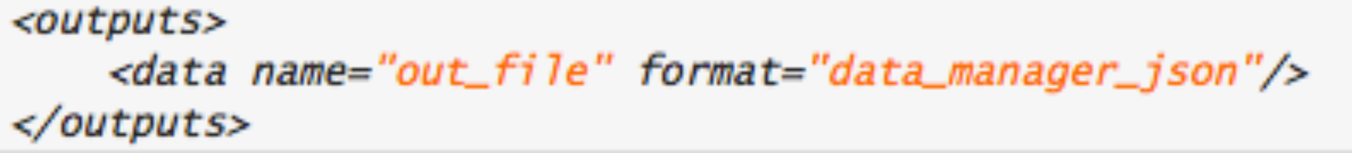
Examples:

- Adding New genome builds (dbkeys)
- Fetching Genome (FASTA) sequences
- Building short read mapper indexes for genomes

Special class of Galaxy tool

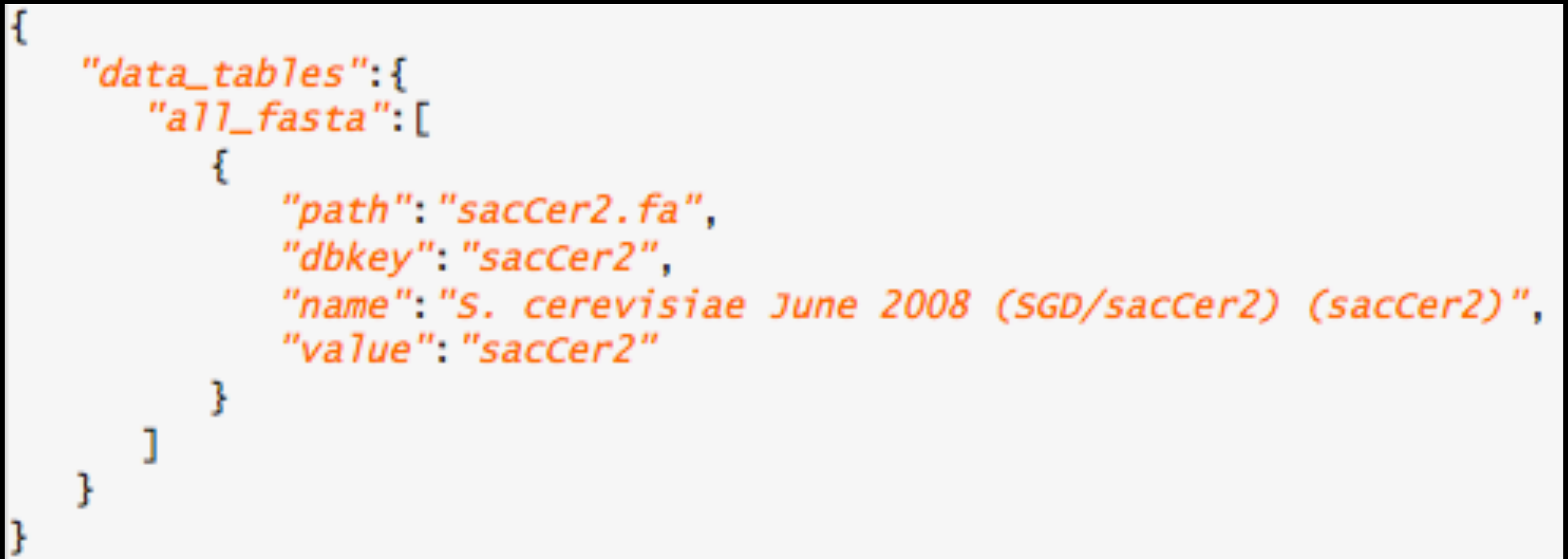


```
<tool id="data_manager_fetch_genome_all_fasta" name="Reference Genome" version="0.0.1" tool_type="manage_data">
```



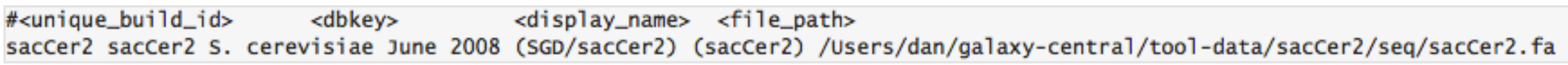
```
<outputs>
    <data name="out_file" format="data_manager_json"/>
</outputs>
```

Writes a JSON description of new data table entries as content of tool output file



```
{
    "data_tables":{
        "all_fasta":[
            {
                "path":"sacCer2.fa",
                "dbkey":"sacCer2",
                "name":"S. cerevisiae June 2008 (SGD/sacCer2) (sacCer2)",
                "value":"sacCer2"
            }
        ]
    }
}
```

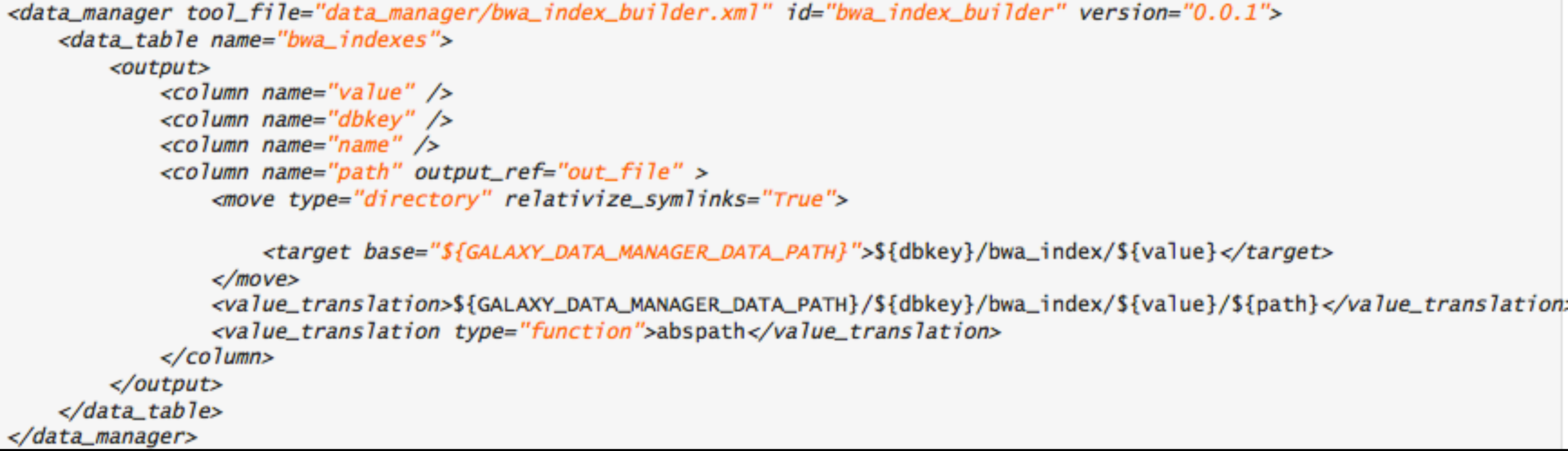
This creates a new entry in the Tool Data Table:



```
#<unique_build_id>      <dbkey>         <display_name>   <file_path>
sacCer2 sacCer2 S. cerevisiae June 2008 (SGD/sacCer2) (sacCer2) /Users/dan/galaxy-central/tool-data/sacCer2/seq/sacCer2.fa
```

Where the sacCer2.fa file was placed by the tool in the output file's extra_files_path

data_manager entry inside <data_managers> tag in data_mananger_conf.xml



```
<data_manager tool_file="data_manager/bwa_index_builder.xml" id="bwa_index_builder" version="0.0.1">
    <data_table name="bwa_indexes">
        <output>
            <column name="value" />
            <column name="dbkey" />
            <column name="name" />
            <column name="path" output_ref="out_file" >
                <move type="directory" relativize_symlinks="True">

                    <target base="${GALAXY_DATA_MANAGER_DATA_PATH}">${dbkey}/bwa_index/${value}</target>
                </move>
                <value_translation>${GALAXY_DATA_MANAGER_DATA_PATH}/${dbkey}/bwa_index/${value}/${path}</value_translation
                <value_translation type="function">abspath</value_translation>
            </column>
        </output>
    </data_table>
</data_manager>
```

informs Galaxy about

- which data tables to expect for new entries
- special handling of provided JSON values and files

Data Managers: Configuration

enable_data_manager_user_view allows non-admin users to view the available data that has been managed

data_manager_config_file defines the local xml file to use for loading the configurations of locally defined data managers

shed_data_manager_config_file defines the local xml file to use for saving and loading the configurations of locally defined data managers

galaxy_data_manager_data_path defines the location to use for storing the files created by Data Managers. When not configured it defaults to the value of tool_data_path

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Data Manager Demo

- Fetch the Genome Sequence for sacCer3
  - UCSC as the source
  - Install fetching tool from ToolShed
  - define new Genome build / dbkey
  - all_fasta & __dbkeys__ tables are populated automatically
- Build BWA indexes for sacCer3
  - Install indexing tool from ToolShed
  - Build indexes
  - bwa_index table is populated automatically
- Align some reads to the newly added reference genome

Data Manager Demo: Full Disclosure

Fresh Install of galaxy-central stable

- Setup Galaxy admin account already
- Configured tool_dependency_dir
- The sequencing reads are a small subset from SRR507778, originally downloaded from EBI SRA.
- Installed BWA mapper

http://gcc2014.dblankenberg.org/

Make Your Own

Documentation

https://wiki.galaxyproject.org/Admin/Tools/DataManagers/

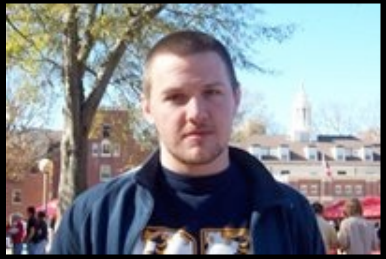
Several examples available in the ToolShed (search for “data_manager”)

Training Day Exercises

https://wiki.galaxyproject.org/Events/GCC2014/TrainingDay/DataManagers

The Galaxy Team

Enis Afgan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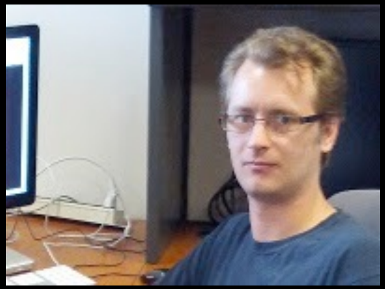
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