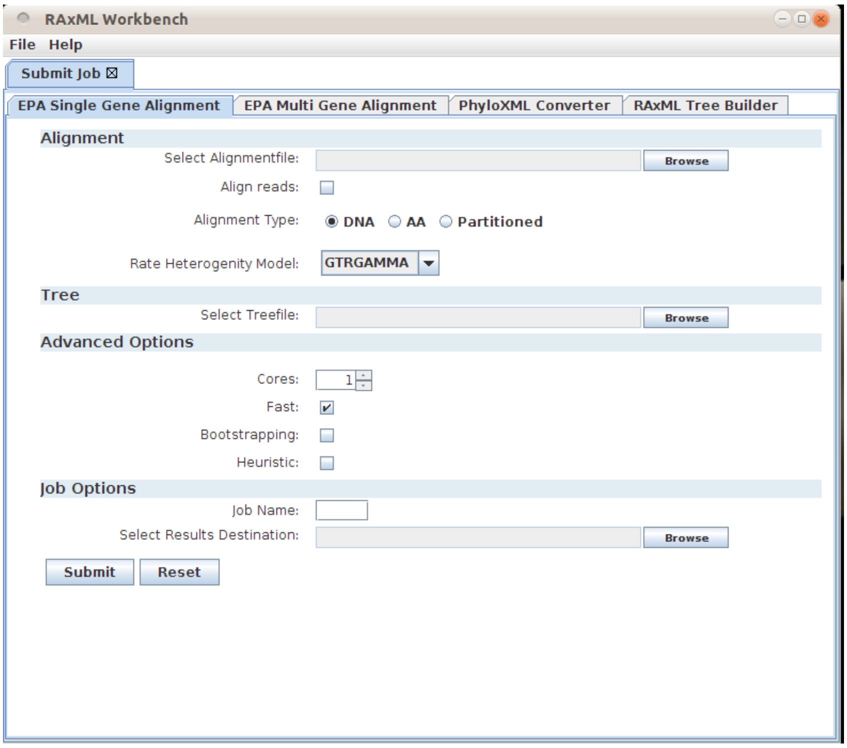
Short documentation for the RAxML Workbench

October 3, 2011

Contents

1 Panel nesting overview

The GUI in figure 1 consists basically of three layers. The first layer is the MainFrame. It holds the menu bar at the top and a penal called *WorkflowPanel* beneath it that



Alignment

Select Alignmentfile:

Align reads: □

Alignment Type: ● DNA ○ AA ○ Partitioned

Rate Heterogenity Model: GTRGAMMA

Tree

Select Treefile:

Advanced Options

Cores: 1

Fast: ☑

Bootstrapping: □

Heuristic: □

Job Options

Job Name:

Select Results Destination:

Figure 1: The start-up presentation of the GUI

administrates all jobs of the user in a TabbedPane. The second layer consists of *Job* objects that can be added and removed from the Workflow's TabbedPane. These Job objects are panels themselves and can be a TabbedPane again, holding the different submission panels, a *WaitingPanel* or a *ResultsPanel*. The last layer are the different submission panels (*SgaFormPanel, MgaFormPanel, PhyloXMLConverterFormPanel and TreeBuilderFormPanel*) which represent the input forms for the submissions, the WaitingPanel that is shown when a job is running, and the ResultsPanel which shows the output files and provides an interface to the treeviewer.

2 The MainFrame

As mentioned before, the MainFrame panel (figure 2) holds a JMenuBar which is shown on the top of the GUI and a WorkflowPanel at the bottom which contains a TabbedPane that holds the Job objects. The actions of the JMenuBar are also controlled in this Panel, like showing the help pdf or exiting the application for example.

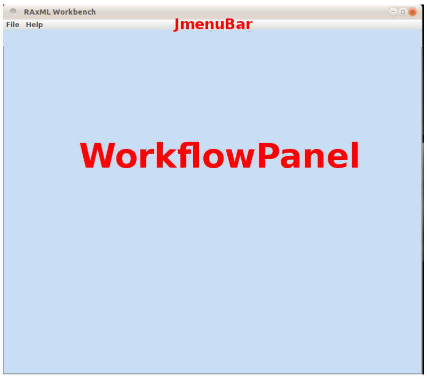


Figure 2: The MainFrame

Figure 3: The WorkflowPanel

3 The WorkflowPanel

The WorkflowPanel (figure 3) administrates the different Job panels stored in its TabbedPane. Jobs can be removed or added.

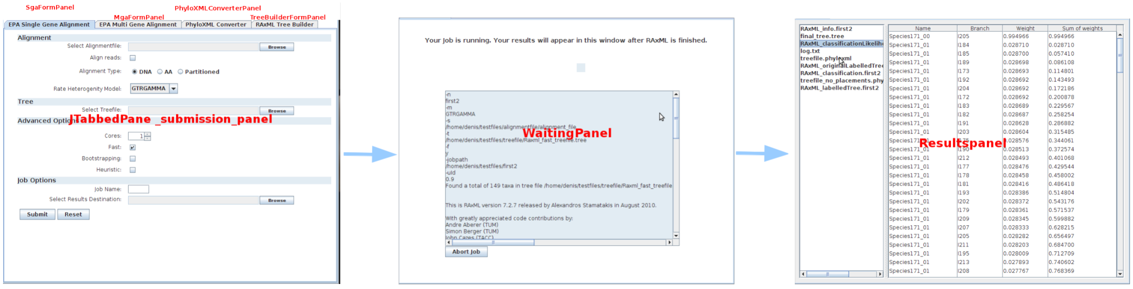
4 The Job (Panel)

This panel provides the different user interfaces available within the GUI. During a submission process, the Job object changes its content multiple times as can be seen in figure 4.

5 The Submission Panels

5.1 SgaFormPanel

This panel contains the complete input form for the EPA single gene submission similar to the EPA webserver one. The inputs are validated and redirected to the Submission object which performs the submission.



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Tree

Select Treefile:

Advanced Options

Cores: 1

Fast: ☑

Bootstrapping: □

Heuristic: □

Job Options

Job Name:

Select Results Destination:

Your Job is running. Your results will appear in this window after RAxML is finished.

```
-n
first2
-m
GTRGAMMA
-s
/home/denis/testfiles/alignmentfile/alignment_file
-t
/home/denis/testfiles/treefile/Raxml_fast_treefile.tree
-f
y
-jobpath
/home/denis/testfiles/first2
-uld
0.9
Found a total of 149 taxa in tree file /home/denis/testfiles/treefile/Raxml_fast_treefile


This is RAxML version 7.2.7 released by Alexandros Stamatakis in August 2010.

With greatly appreciated code contributions by:
Andre Aberer (TUM)
Simon Berger (TUM)
John Cazes (TACC)
```

RAxML_info.first2
final_tree.tree
RAxML_classificationLikelih
log.txt
treefile.phyloxml
RAxML_originalLabelledTree
RAxML_classification.first2
treefile_no_placements.phy
RAxML_labelledTree.first2

Name	Branch	Weight	Sum of weights
Species171_00	I205	0.994966	0.994966
Species171_01	I184	0.028710	0.028710
Species171_01	I185	0.028700	0.057410
Species171_01	I189	0.028698	0.086108
Species171_01	I173	0.028693	0.114801
Species171_01	I192	0.028692	0.143493
Species171_01	I204	0.028692	0.172186
Species171_01	I172	0.028692	0.200878
Species171_01	I183	0.028689	0.229567
Species171_01	I182	0.028687	0.258254
Species171_01	I191	0.028628	0.286882
Species171_01	I203	0.028604	0.315485
Species171_01	I175	0.028576	0.344061
Species171_01	I190	0.028513	0.372574
Species171_01	I212	0.028493	0.401068
Species171_01	I177	0.028476	0.429544
Species171_01	I178	0.028458	0.458002
Species171_01	I181	0.028416	0.486418
Species171_01	I193	0.028386	0.514804
Species171_01	I202	0.028372	0.543176
Species171_01	I179	0.028361	0.571537
Species171_01	I209	0.028345	0.599882
Species171_01	I207	0.028333	0.628215
Species171_01	I205	0.028282	0.656497
Species171_01	I211	0.028203	0.684700
Species171_01	I195	0.028009	0.712709
Species171_01	I213	0.027893	0.740602
Species171_01	I208	0.027767	0.768369

Figure 4: The Job(Panel), the Job panel holds different panels within the submission process. From left to right: At the left, a new Job is opened and the different submission forms are shown. After the submission, the Job changes its content to a WaitingPanel (middle). After the submission has been processed and finished it changes its content again to a ResultsPanel (right).

5.2 MgaFormPanel

This panel contains the complete input form for the EPA multi gene submission similar to the EPA webserver one

5.3 PhyloXMLConverterFormPanel

The PhyloXMLConverterFormPanel provides an user interface for converting classification and treefiles into a phyloXML file that can be read by the treeviewer. It directly calls the convertToPhyloXML java program and performs the submission.

5.4 TreebuilderFormPanel

This allows the user to have a simplified access to the RAxML treebuilder. It performs the submission through the Submission class.

6 WaitingPanel

The Waiting Panel shows a little animation at the top (LoadingAnimation.java) that is supposed to tell the user, that the program is still running and not hung up. Beneath the animation, a textfield showing the outputs of the running programs is shown. This panel allows the user to abort his job. After pressing the abort button, the running process is killed.

7 ResultsPanel

This Panel collects the results file, parses them and decides after that how to represent them. Classification files are represented as tables, phyloXML files are opened within the treeviewer and the rest is shown in a plain text format.

Table 1: bioprogs folder

directory	**content**
`hmmer`	Hmmer
`raxml_pthreads_SSE3`	parallel version of the EPA
`raxml_SSE3`	the SSE3 version of the EPA
`swps3`	The SWPS3 algorithm for the MGA pipeline

8 Constants

The Constants class holds internal parameters that force for example a specific program folder hierarchy and naming. Everything that is somehow ”hard coded” is present in this class. The paths of the external program are also defined there.

8.1 Folder hierarchy

As mentioned before, the folder hierarchy is fixed within the Constants class of the project. Within the `RAxML_Workbench` folder there are supposed to be three directories, `bioprogs, jars, misc` and the executable RAxML_Workbench.jar which includes also the treeviewer. The GUI expects every external non-java program within the bioprogs folder as shown in table 1. Within the `jars` folder the java programs convertToPhyloXML.jar, treecheck.jar and treeMergeLengthsLabels.jar are expected. Also the treeviewer configuration file `_aptx_configuration_file`. The `misc` folder contains the html formatted about page and the help pdf that can be accessed within the GUI.

9 Testing

The GUI contains a test class called *TestRaxmlWorkbench* like the EPA-Webserver, it tests some use cases. When developing, this tests turned out to be very valuable. For this reason they should be performed regularly. The testfiles needed for the testing procedure lie within the project folder `testfiles`. The path of the testfolder is defined within the *Constants* class. The file names etc. are directly defined within the *TestRaxmlWorkbench* class.

10 Bug report

10.1 MGA Pipeline

The multi gene alignment pipeline is not running within the windows version, because there was/is no windows executable of the swps3 algorithm available. If it is available, insert it into the `bioprogs/swps3/` folder as it was done in the linux versions.