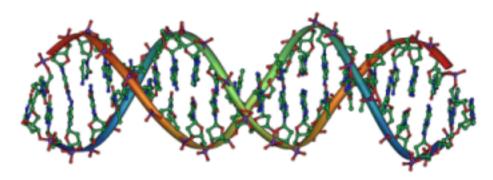
Bio Roll: Users Guide



Version 5.2 Edition

Bio Roll: Users Guide:



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Preface

Bio-Informatics is the use of techniques from applied mathematics, informatics, statistics, and computer science to solve biological problems. Major research efforts in the field include sequence alignment, gene finding, genome assembly, protein structure alignment, protein structure prediction, prediction of gene expression and protein-protein interactions, and the modeling of evolution.

To address the requirements of these efforts, a wide spectrum of bio-informatics tools are available. These tools, while powerful, are packaged according to the individual tastes of the developers.

The Bio-informatics Roll is a collection of some of the most common bio-informatics tools that are being used by the community today. This roll is being developed in an attempt to standardize and ease packaging and installation of these tools.

Chapter 1. Overview

Table 1-1. Summary

Name	bio
Version	5.2
Maintained By	Rocks Group
Architecture	i386, x86_64
Compatible with Rocks TM	5.2

Table 1-2. Roll Compatibility

Roll	Requires a	Optional b	Conflicts
alpha		X	
area51		X	
base	X		
bio	X		
condor		X	
ganglia		X	
grid		X	
hpc	X		
java	X		
kernel	X		
os (disk 1)	X		
os (disk 2)	X		
os (disk 3)		X	
os (disk 4)		X	
os (disk 5)		X	
os (disk 6)		X	
os (disk 7)		X	
pbs		X	
service-pack		X	
sge		X	
viz		X	
web-server	X		
xen		X	

Roll	Requires a	Optional ь	Conflicts

Notes:

- a. You may also substitute your own OS CDs for the RocksTM OS Roll CDs. In this case you must use all the CDs from your distribution and not use any of the RocksTM OS Roll CDs.
- b. Only Rolls that have been verified as compatible with this Roll are listed. Other Rolls will likely work, but have not been tested by the maintainer of this Roll.

Chapter 2. Installing

2.1. On a New Server

The bio Roll should be installed during the initial installation of your server (or cluster). This procedure is documented in section 1.2 of the RocksTM usersguide. You should select the bio Roll from the list of available rolls when you see a screen that is similar to the one below.



2.2. On an Existing Server

The bio Roll may also be added onto an existing server (or frontend). For sake of discussion, assume that you have an iso image of the roll called bio.iso. The following procedure will install the Roll, and after the server reboots the Roll should be fully installed and configured.

```
$ su - root
# rocks add roll bio.iso
# rocks enable roll bio
# rocks-dist dist
# kroll bio | bash
# init 6
```

Chapter 3. Using

3.1. List of packages present in the Bio Roll

The Bio Roll contains a suite of Bio-informatics applications, most commonly in use by the bio-informatics community. The list of applications is as follows:

- HMMER From Washington University at St. Louis http://hmmer.wustl.edu/
- NCBI BLAST From National Center for Biotechnology Information www.ncbi.nlm.nih.gov/BLAST/2
- MpiBLAST From Los Alamos National Laboratory http://mpiblast.lanl.gov/
- · biopython www.biopython.org
- ClustalW From the European BioInformatics Institute http://www.ebi.ac.uk/clustalw/
- MrBayes From School of Computational Science at the Florida State University http://mrbayes.csit.fsu.edu/
- T_Coffee From Information Genomique et Structurale at Centre National de la Recherche Scientifique The T-Coffee Home Page⁷
- Emboss From European Molecular Biology Institute http://emboss.sourceforge.net/
- Phylip From the Dept. of Biology at the University of Washington http://evolution.genetics.washington.edu/phylip.html
- fasta From the University of Virginia http://fasta.bioch.virginia.edu/
- Glimmer From Center for Bioinformatics and Computational Biology at the University of Maryland http://www.cbcb.umd.edu/software/glimmer/
- TIGR Assembler From the J. Craig Venter Institute http://www.jcvi.org/cms/research/software/
- · All the perl utilities mentioned below are from CPAN
- · perl-bioperl
- · perl-bioperl-run
- · perl-bioperl-gui
- · perl-bioperl-db

All the packages that appear below are dependencies and are already present in the base and OS Rolls. They are installed automatically during system installation.

foundation-python	gd-devel	perl-HTML-Tagset	perl-Scalar-List-Utils
foundation-python-extras	perl-Data-Stag	perl-IO-String	perl-SOAP-Lite
ReportLab	perl-Digest-MD5	perl-IO-stringy	perl-Storable
flex	perl-File-Temp	perl-libnet	perl-Text-Shellwords
xorg-x11-devel	perl-GD	perl-libwww-perl	perl-XML-DOM
readline	perl-GD-SVG	perl-MIME-Base64	perl-XML-Twig
readline-devel	perl-Graph	perl-Module-Signature	perl-XML-Writer
gd	perl-HTML-Parser	perl-PathTools	

3.2. HMMER

3.2.1. About

HMMER is an implementation of profile HMM methods for sensitive database searches using multiple sequence alignments as queries.

The version of HMMER that is distributed with this version of Rocks was obtained from here¹¹. The version as of code freeze is v2.3.2 and is distributed by WU, St.Louis under the GNU General Public License v2.0.

3.2.2. Usage

HMMER is setup in the /opt/Bio/hmmer directory. The HMMER execution environment is setup automatically by the login scripts. The environment contains HMMER_DB variable which points to the directory containing the hmmer databases. By default, this is set to /share/bio/hmmer/db/.

HMMER has many modes of execution. Please run

\$ man hmmer

for a description of all the executables that come with HMMER.

You may also refer to the Users Guide present here¹². This guide is also available on your rocks installation at /opt/Bio/hmmer/Userguide.pdf

There is also a tutorial available on your cluster at /opt/Bio/hmmer/tutorial/. The description of how to use the tutorial is given in the Userguide.pdf file.

3.3. NCBI BLAST

3.3.1. About

BLAST, or Basic Local Alignment Search Tool, is a collection of tools that are used to search for and find regions of local similarity between sequences. The program compares nucleotide or protein sequences to sequence databases, and calculates the statistical significance of the matches. This software suite has been released free to the public by the National Centre for Biotechnology Information.

3.3.2. Usage

BLAST can be used for protein-protein comparisons or nucleotide-nucleotide comparisons. Before an example of the usage is presented, we must first define some environmental variables.

• \$BLASTDB - This is the variable which points to the Blast Database. This is set to /share/bio/ncbi/db/. This directory should contain the databases that you would want to search. BLAST by default checks this location and

the current working directory for the presence of the databases. This variable is set during login by system login scripts, and may be changed by the user to point to her preferred location in her startup scripts.

• \$BLASTMAT - This variable points to the location where the BLAST scoring matricies are present. It is set to /opt/Bio/ncbi/data Again, they may be changed to point to a desired location on a per-user basis.

BLAST requires the presence of 2 datasets. One dataset is the input sequence that you want to search for, and the other dataset is the database that you want to search against.

Use the following procedure to run blast

Download the BLAST database that you want to blast against. The databases can be obtained from the NCBI ftp site at ftp://ftp.ncbi.nlm.nih.gov/blast/db/. Note that the databases available here are preformatted. Unformatted databases can be obtained in FASTA format at ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/¹⁴. The databases may also be obtained by running the /opt/Bio/ncbi/doc/blast/update_blastdb.pl script. Run the script without any parameters to view usage.

Note that it is recommended that the blast databases be downloaded to the \$BLASTDB location. As not everybody has write access to this location, a seperate user called biouser is created who can write to this location. The users of the system may su to this user using the following command.

```
[nostromo@xxx ~]$ sudo su - biouser
-bash-3.00$ cd $BLASTDB
-bash-3.00$ /opt/Bio/ncbi/doc/blast/update_blastdb.pl --showall
Connected to NCBI
env_nr
env_nt
est
est_human
est_mouse
est others
gss
htgs
human_genomic
nr
nt
other_genomic
pataa
patnt
pdbaa
pdbnt
refseq_genomic
refseq_protein
refseq_rna
sts
swissprot
taxdb
-bash-3.00$ /opt/Bio/ncbi/doc/blast/update_blastdb.pl patnt
Connected to NCBI
Downloading patnt.tar.gz... done.
-bash-3.1$ tar xzf patnt.tar.gz
```

• The above method downloads formatted databases. You can also download unformatted databases from ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/. If you've used the update_db.pl tool or downloaded the databases from ftp://ftp.ncbi.nlm.nih.gov/blast/db/, then DO NOT run formatdb.

Run the formatdb command to format the database to the BLAST format. For this example, we'll use the Drosophila Melanogaster (fruitfly) nucleotide database

```
-bash-3.1$ wget -q ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/drosoph.nt.gz
-bash-3.1$ gunzip drosoph.nt.gz
-bash-3.1$ formatdb -p F -V T -i drosoph.nt
-bash-3.1$ ls drosoph.nt*
drosoph.nt drosoph.nt.nin drosoph.nt.nsq
-bash-3.1$
```

• After the database is formatted, create a test input file.

• Run the blastall program on the test input against the formatted database.

```
[nostromo@xxx ~]$ blastall --help
```

BLASTN 2.2.18 [Mar-02-2008]

gives a list of all the options that you can use to run the blastall program.

[nostromo@xxx ~]\$ blastall -d drosoph.nt -p blastn -i test.txt

```
Reference: Altschul, Stephen F., Thomas L. Madden, Alejandro A. Schaffer, Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997), "Gapped BLAST and PSI-BLAST: a new generation of protein database search programs", Nucleic Acids Res. 25:3389-3402.
```

```
Query= Test
(560 letters)

Database: drosoph.nt
1170 sequences; 122,655,632 total letters

Searching......done
```

Score E
Sequences producing significant alignments: (bits) Value

```
qi|10729531|qb|AE002936.2|AE002936 Drosophila melanoqaster genom...
                                                                          0.86
gi|10728232|gb|AE003493.2|AE003493 Drosophila melanogaster genom...
                                                                     36 0.86
qi|10726497|qb|AE003698.2|AE003698 Drosophila melanogaster genom...
                                                                     36 0.86
qi|10726398|qb|AE003681.2|AE003681 Drosophila melanogaster genom...
                                                                    36 0.86
qi|10729308|qb|AE002665.2|AE002665 Drosophila melanoqaster genom...
                                                                         3.4
qi|10729264|qb|AE002615.2|AE002615 Drosophila melanogaster genom...
                                                                     34 3.4
qi|7298233|qb|AE003648.1|AE003648 Drosophila melanoqaster qenomi...
                                                                   34 3.4
qi|7297628|qb|AE003628.1|AE003628 Drosophila melanogaster genomi...
                                                                    34 3.4
gi|10728546|gb|AE003447.2|AE003447 Drosophila melanogaster genom...
                                                                     34 3.4
qi|7290819|qb|AE003441.1|AE003441 Drosophila melanoqaster qenomi...
                                                                     34 3.4
qi|10728461|qb|AE003431.2|AE003431 Drosophila melanoqaster genom...
                                                                     34 3.4
qi|10728241|qb|AE003495.2|AE003495 Drosophila melanogaster genom...
                                                                     34 3.4
qi|7292554|qb|AE003484.1|AE003484 Drosophila melanogaster genomi...
                                                                     34 3.4
qi|10727872|qb|AE003525.2|AE003525 Drosophila melanogaster genom...
                                                                     34 3.4
qi|10727399|qb|AE003587.2|AE003587 Drosophila melanoqaster genom...
                                                                     34 3.4
qi|10727114|qb|AE003673.2|AE003673 Drosophila melanoqaster genom...
                                                                    34 3.4
qi|10726705|gb|AE003740.2|AE003740 Drosophila melanogaster genom...
                                                                   34 3.4
```

The above example shows how to search for the test input in a drosophila nucleotide database, and a snippet of the output file.

3.3.3. Running Blast with SGE

This section gives a very simple example of running BLAST through the provided batch system SGE.

· Create a simple submission script called blast_sge.sh containing the following -

```
#!/bin/bash
#
#$ -cwd
#$ -S /bin/bash
#$ -j y

export BLASTDB=/share/bio/ncbi/db/
export BLASTMAT=/opt/Bio/ncbi/data/

export PATH=$PATH:/opt/Bio/ncbi/bin

blastall -d drosoph.nt -p blastn -i $HOME/test.txt -o $HOME/result.txt
```

Run

```
[nostromo@xxx ~]$ qsub blast_sge.sh
Your job 10 ("blast_sge.sh") has been submitted
```

• The output of the Blast job is similar to the one given above and will be stored in \$HOME/result.txt

3.3.4. Further Information

For further information about BLAST and its usage, please refer to the following sources

- THE NCBI Blast website http://www.ncbi.nlm.nih.gov/BLAST/15
- BLAST Help page on your cluster BLAST Help Page¹⁶
- BLAST Program selection Guide http://www.ncbi.nlm.nih.gov/blast/BLAST_guide.pdf¹⁷

3.4. ClustalW

3.4.1. About

ClustalW is a multiple sequence alignment program. The version included with this distribution is v2.0.10.

3.4.2. Using ClustalW

ClustalW can be run at the command line as

[nostromo@xxx ~]\$ clustalw2

```
******** CLUSTAL 2.0.10 Multiple Sequence Alignments *******
```

- 1. Sequence Input From Disc
- 2. Multiple Alignments
- 3. Profile / Structure Alignments
- 4. Phylogenetic trees
- S. Execute a system command
- H. HELP
- X. EXIT (leave program)

Your choice:

Choosing the option 'H' brings up the help on clustalW.

3.4.3. Further Information

Further information on the usage of ClustalW can be obtained from clustalw.doc(MS Word Document) available at /opt/Bio/clustalw/doc/clustalw.doc on the frontend of your cluster.

3.5. EMBOSS

3.5.1. About

EMBOSS is the European Molecular Biology Open Software Suite, a set of tools that are used for sequence analysis by the Molecular Biology community (EMBnet).

3.5.2. Further Information

Information about using EMBOSS is available at http://emboss.sourceforge.net/. You may also register at their mailing list here¹⁹.

3.6. Glimmer

3.6.1. About

Glimmer is a system for finding genes in microbial DNA, especially the genomes of bacteria, archaea, and viruses. Glimmer was developed at the Centre for BioInformatics and Computational Biology. The version that is distributed with Rocks is Glimmer v3.02.

3.6.2. Using Glimmer

Glimmer is installed at /opt/Bio/glimmer/. Glimmer is run in 2 stages.

- Glimmer is trained on a particular training set of similar species to recognize genes
- Glimmer is then run on an input DNA sequence to find genes

3.6.3. Further Information

Further information about the usage of Glimmer can be found in the release notes of the software, available here²⁰. This file is also available on the frontend of your cluster at /opt/Bio/glimmer/glim302notes.pdf

3.7. Fasta

3.7.1. About Fasta

FASTA is a program used to search in large Protein or DNA sequence data banks. It was developed at the University of Virginia by William R. Pearson, and D.J. Lippman.

3.7.2. Usage

FASTA is installed in /opt/Bio/fasta/. FASTA is run in a similar manner to NCBI Blast.

· First create a test query file

• The next step is to search for this against a database sequence. For this, we can download a DNA or protein sequence database or use the ones that are provided by the program. For this example, we will use the ones present along with the fasta program in /opt/Bio/fasta/.

```
[nostromo@xxx ~]$ fasta35
FASTA searches a protein or DNA sequence data bank
version 35.04 Oct. 7, 2008
Please cite:
W.R. Pearson & D.J. Lipman PNAS (1988) 85:2444-2448
test sequence file name: test.txt
library file name: drosoph.nt
ktup? (1 to 6) [6]
Query: test.txt
 1>>>Test - 560 nt
Library: drosoph.nt
..... Done!
122655632 residues in 1170 sequences
      opt
               E()
< 20
              0:
       0
 22
              0:
                           one = represents 3 library sequences
 24
       0
              0:
 26
              0:
 28
       0
              0 •
 30
       3
              2:*
```

```
32
    12
         9:==*=
 34
     37
         23:=====*====
 36
    59
         48:=====*===*
 38
    90
        79:=====*==
 40
        110:======*
    110
        135:======*
 42
    133
 44
    147
        149:===========
 46
    151
        151:===========
        50
    131
        132:=====*
 52
    102
        54
    92
        99:======= *
       83:=====*
 56
   80
 58
    68
       68:========*
 60
        55:========
    43
         44:======*
 62
    44
 64
    42
        35:=======*==
    30
       28:=====*
 68
    25
        22:=====*=
 70
    20
         17:====*=
 72
    18
         13:===*=
 74
    14
        10:===*=
 76
         8:==*
     7
 78
         6:=*=
 80
      9
          5:=*=
 82
     3
         4:=*
 84
     0
         3:*
 86
     0
         2:*
 88
     2
                  inset = represents 1 library sequences
         2:*
 90
     1
         1:*
         1:*
 92
     0
                  : *
 94
         1:*
                 : *
 96
     2
         1:*
                  : *=
 98
     0
          0:
100
     0
         0:
102
     0
         0:
104
     0
         0:
106
     0
         0:
108
     0
         0:
110
     0
         0:
112
     0
         0:
114
         0:
     Ω
116
      0
          0:
118
      0
          0:
>120
      0
          0:
122902592 residues in 1611 sequences
Statistics: Expectation_n fit: rho(ln(x)) = 7.6751+/-0.00204; mu= 6.7759+/- 0.231
mean_var=233.8700+/-93.821, 0's: 0 Z-trim: 0 B-trim: 0 in 0/53
Lambda= 0.083866
Kolmogorov-Smirnov statistic: 0.0247 (N=27) at 38
Algorithm: FASTA (3.5 Sept 2006) [optimized]
Parameters: +5/-4 matrix (5:-4) ktup: 6
join: 52, opt: 37, open/ext: -12/-4, width: 16
```

```
Scan time: 10.680
Enter filename for results []: How many scores would you like to see? [20]
The best scores are:
                                                          opt bits E(1611)
qi|10727961|qb|AE003541.2|AE003541 Drosophila (265536) [r] 171 36.0
                                                                            1
qi|10728546|qb|AE003447.2|AE003447 Drosophila
                                              (304085) [f]
                                                             171 36.0
                                                                            1
gi|7290382|gb|AE003426.1|AE003426 Drosophila m (300193) [f]
                                                             159 34.5
                                                                          2.8
qi|7290880|qb|AE003443.1|AE003443 Drosophila m (302357) [f]
                                                            157 34.3
                                                                          3.3
gi|10727731|gb|AE003838.2|AE003838 Drosophila (263411) [r]
                                                                          6.4
gi|7291133|gb|AE003450.1|AE003450 Drosophila m (300732) [f]
                                                            148 33.2
                                                                          6.9
gi|7300931|gb|AE003741.1|AE003741 Drosophila m (233313) [r]
                                                             151 33.2
                                                                          7.1
qi|10726402|gb|AE003682.2|AE003682 Drosophila (224400) [f]
                                                            147 33.1
                                                                          7.5
gi|10728339|gb|AE003512.2|AE003512 Drosophila (301457) [f]
                                                            147 33.1
                                                                          7.5
gi|10728273|gb|AE003500.2|AE003500 Drosophila (327446) [f]
                                                            145 32.8
                                                                          8.9
qi|10726452|gb|AE003691.2|AE003691 Drosophila (226773) [f]
                                                             145 32.8
                                                                          8.9
gi|10727164|gb|AE003603.2|AE003603 Drosophila (294914) [r]
                                                            144 32.6
                                                                           10
qi|7290252|qb|AE003423.1|AE003423 Drosophila m (291976) [r]
                                                            144 32.6
                                                                           10
qi|10727489|qb|AE003803.2|AE003803 Drosophila (282567) [r]
                                                                           10
gi|10727489|gb|AE003803.2|AE003803 Drosophila (282567) [r]
                                                            143 32.5
                                                                           11
gi|10727339|gb|AE003577.2|AE003577 Drosophila (267662) [f]
                                                            142 32.3
                                                                           13
gi|7292734|gb|AE003488.1|AE003488 Drosophila m (302797) [f]
                                                            140 32.2
                                                                           13
gi|7298684|gb|AE003667.1|AE003667 Drosophila m (263704) [r]
                                                            139 31.9
                                                                           17
qi|10727995|gb|AE003546.2|AE003546 Drosophila (281602) [f]
                                                                           17
                                                            137 31.9
qi|10728551|gb|AE003448.2|AE003448 Drosophila (310364) [f]
                                                            137 31.9
                                                                           18
More scores? [0]
Display alignments also? (y/n) [n]
560 residues in 1 query
                          sequences
122655632 residues in 1170 library sequences
Scomplib [35.04]
start: Wed Dec 10 19:45:41 2008 done: Wed Dec 10 19:46:04 2008
Total Scan time: 10.680 Total Display time: 0.000
Function used was FASTA [version 35.04 Oct. 7, 2008]
```

3.7.3. Further Information

Further information about the usage of fasta can be obtained from /opt/Bio/fasta/fasta3x.doc present on the frontend of your installation.

More information is also available at the FASTA home page²¹.

For support, you are encouraged to join the FASTA mailing list at http://list.mail.virginia.edu/mailman/listinfo/fasta_list

3.8. MrBayes

3.8.1. About

MrBayes is a program used for bayesian inference of phylogeny. MrBayes is cowritten by John Huelsenbeck and Fredrik Ronquist.

The version of MrBayes included with this version of Rocks is MPI enabled, and can be used in either parallel or serial modes of execution.

3.8.2. Usage

MrBayes >

MrBayes uses the NEXUS file format for input. To use MrBayes in interactive mode, just type mb at the command line

```
[nostromo@xxx mrbayes]$ mb
MrBayes v3.1.2
                      (Bayesian Analysis of Phylogeny)
                             (Parallel version)
                         (1 processors available)
                                     by
                  Fredrik Ronquist and John P. Huelsenbeck
                       School of Computational Science
                           Florida State University
                            ronquist@csit.fsu.edu
                 Section of Ecology, Behavior and Evolution
                       Division of Biological Sciences
                     University of California, San Diego
                           johnh@biomail.ucsd.edu
              Distributed under the GNU General Public License
               Type "help" or "help <command>" for information
                     on the commands that are available.
```

To use MrBayes in the parallel version, you'll need to use it in non-interactive mode. It can be invoked as shown.

(Parallel version)
(4 processors available)

by

John P. Huelsenbeck and Fredrik Ronquist

Section of Ecology, Behavior and Evolution
Division of Biological Sciences
University of California, San Diego
johnh@biomail.ucsd.edu

School of Computational Science Florida State University ronquist@csit.fsu.edu

Distributed under the GNU General Public License

Type "help" or "help <command>" for information on the commands that are available.

Executing file "/opt/Bio/mrbayes/primates.nex" UNIX line termination Longest line length = 915Parsing file Expecting NEXUS formatted file Reading data block Allocated matrix Matrix has 12 taxa and 898 characters Data is Dna Data matrix is not interleaved Gaps coded as -Setting default partition (does not divide up characters). Taxon 1 -> Tarsius_syrichta Taxon 2 -> Lemur_catta Taxon 3 -> Homo_sapiens Taxon 4 -> Pan Taxon 5 -> Gorilla Taxon 6 -> Pongo Taxon 7 -> Hylobates Taxon 8 -> Macaca_fuscata Taxon 9 -> M_mulatta Taxon 10 -> M_fascicularis Taxon 11 -> M_sylvanus Taxon 12 -> Saimiri_sciureus Setting output file names to "/opt/Bio/mrbayes/primates.nex.run<i>.<p/t>" Successfully read matrix Exiting data block Reached end of file

```
Tasks completed, exiting program because mode is noninteractive

To return control to the command line after completion of file processing,
set mode to interactive with 'mb -i <filename>' (i is for interactive)
or use 'set mode=interactive'
```

[nostromo@xxx ~]\$

3.8.3. Further Information

A wealth of information about MrBayes is available at the MrBayes Home Page²² and at the MrBayes Wiki²³

3.9. Phylip

3.9.1. About

Phylip - Phylogeny Inference Package - is a package of programs for inferring phylogenies or evolutionary trees. The version distributed with Rocks is v3.68.

3.9.2. Further Information

Furtherinformation about Phylip is available at the Phylip home page²⁴.

3.10. T_Coffee

3.10.1. About

T Coffee is a multiple sequence alignment package. The version included with this distribution of Rocks is v7.04

3.10.2. Usage

T-coffee is used for standard alignments and alignment combinations. It is installed at /opt/Bio/tcoffee/ on the Rocks distribution. To use T-Coffee, just type t_coffee at the command line for a list of all possible parameters that can be used. T-coffee recognizes formats such as fasta, clustalw, blast, etc. Example input files are available at /opt/Bio/tcoffee/example/

A simple sequence alignment example is shown below about. It is run against a sample fasta file present in the example directory. Parts of the output are deleted for the sake of brevity. Where missing, output is substituted by ellipses (.....)

[nostromo@xxx ~]\$ t_coffee /opt/Bio/tcoffee/example/sample_aln2.fasta

```
PROGRAM: T-COFFEE (Version_7.04)
-full_log
                 S
                          [0]
-run_name
                 S
-mem_mode
                 S
                          [0]
                                  mem
-extend
                 D
                          [1]
                 S
                          [0]
                                  very_fast_triplet
-extend_mode
                 D
-max_n_pair
                          [0]
-seq_name_for_quadruplet
                                  S
                                           [0]
                                                    all
-compact
                 S
                          [0]
                                  default
-clean
                 S
                          ۲01
                                  no
-do_self
                 FL
                                  0
                          [0]
-do_normalise
                 D
                          [0]
                                  1000
-template_file S
                          [0]
-remove_template_file
                                   [0]
                                           0
                          D
-profile_template_file
                          S
                                   [0]
-in
                          [0]
-seq
                 S
                          [1]
                                  /opt/Bio/tcoffee/example/sample_aln2.fasta
-aln
                          [0]
-method_limits
                 S
                          [0]
                 S
-method
                          [0]
-lib
                 S
                          [0]
                 S
                          [0]
-profile
-profile1
                 S
                          [0]
-profile2
                 S
                          [0]
-pdb
                 S
                          [0]
-relax_lib
                 D
                          [0]
                                  1
-filter_lib
                 D
                          [0]
                                  0
-shrink_lib
                 D
                          F 0 1
-out_lib
                 W_F
                          [0]
                                  no
-out_lib_mode
                          [0]
                                  primary
                 S
                          [0]
-lib_only
                 D
-outseqweight
                 W_F
                          [0]
                                  no
                 FL
                          [0]
                                  0
-dpa
-seq_source
                 S
                          [0]
                                  ANY
-cosmetic_penalty
                          D
                                   [0]
                                           0
                          [0]
                                  0
-gapopen
                 D
                 D
                          [0]
                                  0
-gapext
                 D
                                  0
                          [0]
-fgapopen
-fgapext
                 D
                          [0]
-nomatch
                 D
                          [0]
-newtree
                 W_F
                          [0]
                                  default
-tree
                 W_F
                          [0]
-usetree
                 R_F
                          [0]
-tree_mode
                 S
                          [0]
                                  пj
                          S
                                   [0]
-distance_matrix_mode
                                           ktup
-distance_matrix_sim_mode
                                           [0]
                                                    idmat_sim1
-quicktree
                 FL
                                  0
                          [0]
-outfile
                 W_F
                          [0]
                                  default
-maximise
                 FL
                          [1]
                          [0]
                                                    html
-output
                 S
                                  clustalw
-infile
                 R F
                          [0]
```

```
-matrix
                 S
                          [0]
                                  default
-tg_mode
                 D
                          [0]
-profile_mode
                 S
                          [0]
                                   cw_profile_profile
-profile_comparison
                                           profile
                                  linked_pair_wise
-dp_mode
                 S
                          [0]
                 D
-ktuple
                          [0]
-ndiag
                 D
                          [0]
                                  0
-diag_threshold D
                          [0]
                                  0
-diag_mode
                 D
                          [0]
                          [0]
-sim_matrix
                 S
                                  vasiliky
-transform
                 S
                          [0]
-outorder
                 S
                          [0]
                                  input
                 S
                                   aligned
-inorder
                          [0]
-seqnos
                 S
                          [0]
                                  off
                 S
                          [0]
-case
                                  keep
                 D
-cpu
                          [0]
                                  1000
                 D
                          [0]
-maxnseq
-maxlen
                 D
                          [0]
                                  -1
-weight
                 S
                          [0]
                                  default
-seq_weight
                 S
                          [0]
                                  t_coffee
-align
                 FL
                          [1]
                                  1
-mocca
                                  0
                 FL
                          [0]
-domain
                 FL
                          [0]
                                  0
                          [0]
                                  0
-start
                 D
-len
                 D
                          [0]
                                  0
-scale
                 D
                          [0]
                                  0
-mocca_interactive
                          FL
                                   [0]
-method_evaluate_mode
                          S
                                   [0]
                                           default
                                   t_coffee_fast
-evaluate_mode S
                          [0]
-get_type
                 FL
                          [0]
-clean_aln
                          [0]
                                  0
-clean_threshold
                          D
                                   [1]
                                           1
-clean_iteration
                          D
                                   [1]
                                           t_coffee_fast
-clean_evaluate_mode
                                   [0]
-extend_matrix FL
                                  0
                          [0]
-prot_min_sim
                                  0
-prot_max_sim
                 D
                          [90]
                                   90
-prot_min_cov
                 D
                          [0]
                                  0
                 D
                          [35]
                                  35
-pdb_min_sim
                 D
                          [100]
                                  100
-pdb_max_sim
-pdb_min_cov
                          [50]
                                  50
                          W_F
                                   [0]
                                           EBI
-pdb_blast_server
-blast
                 W_F
                          [0]
                                  EBI
-blast_server
                 W_F
                          [0]
-pdb_db
                 W_F
                          [0]
                                  pdb
-protein_db
                 W_F
                          [0]
                                  uniprot
                 W_F
                          [0]
-method_log
                                  no
-struc_to_use
                 S
                          [0]
-cache
                 W_F
                          [0]
                                  use
-align_pdb_param_file
                          W_F
                                   [0]
-align_pdb_hasch_mode
                          W_F
                                   [0]
                                           hasch_ca_trace_bubble
-external_aligner
                          S
                                   [0]
                                           NO
-msa_mode
                          [0]
                                  tree
```

```
-one2all
              S
                      [0]
-lalign_n_top
              D
                      [0]
                              10
-iterate
              D
                      [0]
                              Ω
-trim
              D
                      [0]
                      [0]
-split
              D
                              Ω
-trimfile
              S
                      [0]
                             default
-split
              D
                      [0]
                      D
                                     0
-split_nseq_thres
                              [0]
-split_score_thres
                      D
                              [0]
                                     0
-check_pdb_status
                      D
                              [0]
                                     0
-clean_seq_name D
                      [0]
                      [0]
-seq_to_keep
             S
-dpa_master_aln S
                      [0]
                      [0]
                              0
-dpa_maxnseq
-dpa_min_score1 D
                      [0]
-dpa_min_score2 D
                      [0]
-dpa_keep_tmpfile
                      FL
                              [0]
                                     0
-dpa debug
                      [0]
-multi_thread S
                      [0]
-lib_list
              S
                      [0]
-tip
              S
                      [0]
                              one
-rna_lib
              S
                      [0]
                      [0]
-no_warning
             D
-run_local_script
                              [0]
                                     0
                      D
-email
                      [0]
                              no
INPUT FILES
       Input File (S) /opt/Bio/tcoffee/example/sample_aln2.fasta Format clustal_aln
       Input File (M) proba_pair
INPUT SEQUENCES: 6 SEQUENCES [PROTEIN]
 Input File /opt/Bio/tcoffee/example/sample_aln2.fasta Seq 4pep Length 174 type PROTEIN Struct U
 Input File /opt/Bio/tcoffee/example/sample_aln2.fasta Seq 4ape Length 178 type PROTEIN Struct U
 Input File /opt/Bio/tcoffee/example/sample_aln2.fasta Seq 3app Length 174 type PROTEIN Struct U
 Input File /opt/Bio/tcoffee/example/sample_aln2.fasta Seq 2apr Length 178 type PROTEIN Struct U
 Input File /opt/Bio/tcoffee/example/sample_aln2.fasta Seq 1cms_1 Length 148 type PROTEIN Struct U
COMPUTE PAIRWISE SIMILARITY [dp_mode: ] [distance_matrix_mode: ktup][Similarity Measure: idmat_sim1]
       Seq: 1cms
       Seq: 1cms_1
       Seq: 2apr
       Seq: 3app
       Seq: 4ape
       Seq: 4pep
READ/MAKE LIBRARIES: [2]
       proba_pair [method]
               [Submit
                        Job][TOT= 15][100 %][ELAPSED TIME:
                                                             1 sec.]
```

```
[Retrieve Job] [TOT= 15] [100 %] [ELAPSED TIME: 0 sec.]
MANUAL PENALTIES: gapopen=0 gapext=0
       Library Total Size: [6175]
Library Relaxation: [6175] ---> [5092]
       #### File Type=
                        WEIGHT Format= tc_weight Name= no | NOT PRODUCED [WARNING:T-COFFEE:Vers
WEIGHTED MODE:t_coffee
         1cms 1.00
       1cms 1 1.10
         2apr 1.00
         3app 0.96
         4ape 0.95
         4pep 0.99
MAKE GUIDE TREE
       [MODE=nj][DONE]
PROGRESSIVE_ALIGNMENT [Tree Based]
               7: [Group 6 ( 1 seq)] with [Group 1 ( 1 seq)]-->[Score= 92][Len= 176]
       Group
               8: [Group 5 ( 1 seq)] with [Group 4 ( 1 seq)] --> [Score= 83] [Len= 179]
       Group
              9: [Group 8 ( 2 seq)] with [Group 3 ( 1 seq)]-->[Score= 74][Len= 186]
             10: [Group 9 ( 3 seq)] with [Group 7 (
                                                            2 seq)]-->[Score= 77][Len= 186]
       Group
       Group
             11: [Group
                           2 ( 1 seq) with [Group 10 ( 5 seq)]-->[Score= 24][Len= 209]
CLUSTAL FORMAT for T-COFFEE Version_7.04 [http://www.tcoffee.org] [MODE: ], CPU=1.21 sec, SCORE=72,
1cms
              GE---VASVPLTNY-----LDSQYFGKIYLGTPPQEFTVLFDTGSSDFWVPSIYCKSNA
              ----IGDEPLENY-----LDTEYFGTIGIGTPAODFTVIFDTGSSNLWVPSVYCSSLA
4pep
4ape
              S-TGSATTTPID-S-----LDDAYITPVQIGTPAQTLNLDFDTGSSDLWVFSSETTASE
3app
              AASGVATNTPTA-----NDEEYITPVTIGG--TTLNLNFDTGSADLWVFSTELPASQ
              AG---VGTVPMTDY----GNDIEYYGQVTIGTPGKKFNLDFDTGSSDLWIASTLCTN-C
2apr
              Y-TGSLHWVPVTVQQYWQFTVDSVTISGVVVACEG-GCQAILDTGTSKLVGPSSD----
1cms_1
                                       : :.
                                                    :***::.: *
              CKNHQRFDPRKSSTFQ-NLGKPLSIHYGTGS-MQGILGYDTVTVSNIVDIQQTVGLSTQE
1cms
4pep
              CSDHNQFNPDDSSTFE-ATSQELSITYGTGS-MTGILGYDTVQVGGISDTNQIFGLSETE
4ape
              VDGQTIYTPSKSTTAKLLSGATWSISYGDGSSSSGDVYTDTVSVGGLTVTGQAVESAKKV
3app
              QSGHSVYNPSATG-KE-LSGYTWSISYGDGSSASGNVFTDSVTVGGVTAHGQAVQAAQQI
2apr
              GSGQTKYDPNQSSTYQ-ADGRTWSISYGDGSSASGILAKDNVNLGGLLIKGQTIELAKRE
               -----ILNIQQAIGATQNQ
1cms_1
1cms
              PGDVFTYAEFD-----GILGMAYPSLASEY-----SIPVFDNM-MNRHLVA----
4pep
              PGSFLYYAPFD-----GILGLAYPSISASG-----ATPVFDNL-WDQGLVS---
              SSSFTEDSTID-----GLLGLAFSTLNTVSPTQ----QKTFFDNA---KASLD----
4ape
              SAOFOODTNND-----GLLGLAFSSINTVOPOS----OTTFFDTV---KSSLA---
3app
```

```
AASFAS-GPND-----GLLGLGFDTITTVRG-----VKTPMDNL-ISQGLIS----
2apr
1cms 1
             YGEFDIDCDNLSYMPTVVFEINGKMYPLTPSAYTSODOGFCTSGFOSENHSOKWILGDVF
                                 : * : :
                                                     . ::. : :
              -ODLFSVYMDRN-G-OESMLTLGAIDPSY
1cms
4pep
              -QDLFSVYLSSN-DDSGSVVLLGGIDSSY
4ape
              -SPVFTADLGY---HAPGTYNFGFIDTTA
3app
             -QPLFAVALKH---QQPGVYDFGFIDSSK
              -RPIFGVYLGKAKNGGGGEYIFGGYDSTK
2apr
1cms_1
             IREYYSVFDR-----ANNLVGLAKAI
OUTPUT RESULTS
       #### File Type= GUIDE_TREE Format= newick Name= sample_aln2.dnd
       #### File Type= MSA Format= clustalw Name= sample_aln2.aln
       #### File Type=
                           MSA Format= html Name= sample_aln2.html
# TIP : See The Full Documentation on www.tcoffee.org
# Command Line: t_coffee /opt/Bio/tcoffee/example/sample_aln2.fasta [PROGRAM:T-COFFEE]
# T-COFFEE Memory Usage: Current= 6.204 Mb, Max= 11.590 Mb
# T-COFFEE CPU Usage: 1210 millisec
# Results Produced with T-COFFEE (Version_7.04)
# T-COFFEE is available from http://www.tcoffee.org
```

3.10.3. Further Information

Further information about t_coffee is available at -

- The T-coffee home page²⁵
- On your cluster head node at /opt/Bio/tcoffee/doc/
- T-Coffee Documentation²⁶

3.11. TIGR Assembler v2

3.11.1. About

The TIGR Assembler is a tool to assemble large shotgun sequencing projects. The version included with this distribution of Rocks is v2

3.11.2. Usage

TIGR is used for assembling large shotgun DNA sequences. It is installed at /opt/Bio/tigr on the Rocks Distribution. To use TIGR, just type TIGR_Assembler at the command line for a list of all possible parameters that can be used.

3.11.3. Further Information

Further information is available at the JCVI TIGR Assembler page²⁷

3.12. MPI-Blast

3.12.1. About

MPI-Blast is a program from LANL²⁸ which parallelizes the NCBI Blast algorithms using Message Passing Interface library. The version of MPI-Blast included with Rocks is v1.5.0-pio patched and compiled against NCBI Blast 2.2.19.

3.12.2. Usage

MPI-Blast is used in a similar manner to NCBI-Blast. MPI-Blast uses the same variables that are available for NCBI-Blast.

There are 3 steps to running MPI-Blast.

Download a FASTA database to \$BLASTDB. For this example we will download the ecoli nucleotide database.

```
[nostromo@xxx ~]$ sudo su - biouser
-bash-3.00$ cd $BLASTDB
-bash-3.00$ wget ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/ecoli.nt.gz
--17:06:23-- ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/ecoli.nt.gz
          => 'ecoli.nt.gz'
Resolving ftp.ncbi.nlm.nih.gov... 165.112.7.10
Connecting to ftp.ncbi.nlm.nih.gov|165.112.7.10|:21... connected.
Logging in as anonymous ... Logged in!
==> SYST ... done.
                   ==> PWD ... done.
==> TYPE I ... done. ==> CWD /blast/db/FASTA ... done.
==> PASV ... done. ==> RETR ecoli.nt.gz ... done.
Length: 1,438,199 (1.4M) (unauthoritative)
100%[========>] 1,438,199
610.14K/s
17:06:27 (607.91 KB/s) - 'ecoli.nt.gz' saved [1438199]
```

 Format the database using mpiformatdb as follows. A good rule is to format the database to atleast 4 processors, as follows

```
-bash-3.00$ gunzip ecoli.nt.gz
```

```
-bash-3.00$ ls
ecoli.nt
-bash-3.00$ mpiformatdb --nfrags=4 -i ecoli.nt -pF --quiet
Reading input file
Done, read 58882 lines
Reordering 400 sequence entries
Breaking ecoli.nt into 4 fragments
Executing: formatdb -p F -i /tmp/reorderncq8B1 -N 4 -n /share/bio/ncbi/db/ecoli.nt -o T
Removed /tmp/reorderncq8B1
Created 4 fragments.
Changing permissions of /share/bio/ncbi/db//ecoli.nt.mbf
-bash-3.00$ ls
                 ecoli.nt.000.nsq ecoli.nt.001.nsq ecoli.nt.002.nsq ecoli.nt.003.nsq
ecoli.nt
ecoli.nt.000.nhr ecoli.nt.001.nhr ecoli.nt.002.nhr ecoli.nt.003.nhr ecoli.nt.mbf
ecoli.nt.000.nin ecoli.nt.001.nin ecoli.nt.002.nin ecoli.nt.003.nin ecoli.nt.nal
ecoli.nt.000.nnd ecoli.nt.001.nnd ecoli.nt.002.nnd ecoli.nt.003.nnd formatdb.log
ecoli.nt.000.nni ecoli.nt.001.nni ecoli.nt.002.nni ecoli.nt.003.nni
ecoli.nt.000.nsd ecoli.nt.001.nsd ecoli.nt.002.nsd ecoli.nt.003.nsd
ecoli.nt.000.nsi ecoli.nt.001.nsi ecoli.nt.002.nsi ecoli.nt.003.nsi
```

· Now, as a normal user, create a test sequence file and run mpiblast on the sequence against the formatted database.

```
[nostromo@xxx ~]$ cat > test.txt
>Test
AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAAGAGTGTCTGATAGCAGC
TTCTGAACTGGTTACCTGCCGTGAGTAAATTAAAATTTTATTGACTTAGGTCACTAAATACTTTAACCAA
TATAGGCATAGCGCACAGACAGATAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
```

[nostromo@xxx mpiblast]\$ /opt/openmpi/bin/mpirun -np 4 /opt/Bio/mpiblast/bin/mpiblast -d ecoli.nt

After mpirun terminates, result.txt contains the result of your computation.

3.12.3. Running MPI Blast and SGE

This section gives a brief overview of running MPI Blast with SGE

Create a simple SGE submission scripts called mpiblast_sge.sh with the following contents

```
#$ -cwd
#$ -j y
#$ -S /bin/bash

export MPI_DIR=/opt/openmpi/
export BLASTDB=/share/bio/ncbi/db/
export BLASTMAT=/opt/Bio/ncbi/data/
```

#!/bin/bash

```
$MPI_DIR/bin/mpirun -np $NSLOTS \
  /opt/Bio/mpiblast/bin/mpiblast \
  -d ecoli.nt -i $HOME/test.txt \
  -p blastn -o $HOME/result.txt
```

Run

```
[nostromo@xxx ~]$ qsub -pe orte 4 mpiblast_sqe.sh
Your job 11 ("mpiblast_sqe.sh") has been submitted
```

• The results of your computation will be present in \$HOME/result.txt

Please note that an MPI blast job requires atleast 3 processors to run. The argument for mpirun specifying the number of processors should be factor of the number of pieces the blast database was divided into. If you're running on a cluster with 2 processors, SGE, by default, will not schedule a job which requires more than 2 slots to run.

3.12.4. Further Information

Further information about using mpiblast can be found at the MPI-Blast home page²⁹.

For support, please join the mpiblast mailing list³⁰

3.13. GROMACS

3.13.1. About

GROMACS - Groningen MAchine for Chemical Simulation - is a software suite meant for molecular dynamics simulation.

The version of GROMACS included with the distribution is version 4.0.2. It is available at http://www.gromacs.org under the GNU General Public Licence v2.0.

3.13.2. Usage

GROMACS is setup in /opt/Bio/gromacs directory. The version included in this distribution is compiled with mpi support. OpenMPI v1.2.6 is used as the MPI library.

To get more help on using GROMACS, please refer to the following resources:

- GROMACS Home Page³¹
- GROMACS Documentation³²
- GROMACS Online Reference Manual³³

- GROMACS FAQ³⁴
- · Tutorials available on your machines at /opt/Bio/gromacs/share/tutor

3.14. Bioperl

3.14.1. About

Bioperl is a set of perl modules for Bio-informatics computation.

3.14.2. Usage

Bioperl modules can be used to supplement already existing applications such as t_coffee, clustalw, and blast. For information on how to use the library, please refer to the API Docs³⁵.

3.14.3. Further Information

Further information about bioperl is available at the Bioperl home page³⁶

3.15. Biopython

3.15.1. About

Biopython is a set of python modules for Bio-informatics computation.

3.15.2. Usage

Biopython modules can be used to supplement already existing applications such as blast. For information on how to use the library, please refer to the biopython documentation³⁷.

3.15.3. Further Information

Further information about biopython is available at the Biopython home page³⁸

Notes

- 1. http://hmmer.wustl.edu/
- 2. http://www.ncbi.nlm.nih.gov/BLAST/
- 3. http://mpiblast.lanl.gov/
- 4. www.biopython.org
- 5. http://www.ebi.ac.uk/clustalw/
- 6. http://mrbayes.csit.fsu.edu/
- 7. http://www.igs.cnrs-mrs.fr/~cnotred/Projects_home_page/t_coffee_home_page.html
- 8. http://emboss.sourceforge.net/
- 9. http://evolution.genetics.washington.edu/phylip.html
- 10. http://fasta.bioch.virginia.edu/
- 11. http://hmmer.wustl.edu/
- 12. ftp://ftp.genetics.wustl.edu/pub/eddy/hmmer/CURRENT/Userguide.pdf
- 13. ftp://ftp.ncbi.nlm.nih.gov/blast/db/
- 14. ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/
- 15. http://www.ncbi.nlm.nih.gov/BLAST/
- 16. /blast/docs/
- 17. http://www.ncbi.nlm.nih.gov/blast/BLAST_guide.pdf
- 18. http://emboss.sourceforge.net/
- 19. http://emboss.sourceforge.net/support/
- 20. http://www.cbcb.umd.edu/software/glimmer/glim302notes.pdf
- 21. http://fasta.bioch.virginia.edu/
- 22. http://mrbayes.csit.fsu.edu/index.php
- 23. http://mrbayes.scs.fsu.edu/wiki/index.php/Manual
- 24. http://evolution.genetics.washington.edu/phylip.html
- 25. http://igs-server.cnrs-mrs.fr/~cnotred/Projects_home_page/t_coffee_home_page.html
- 26. http://igs-server.cnrs-mrs.fr/~cnotred/Documentation/t coffee/t coffee doc.htm
- 27. http://www.jcvi.org/cms/publications/listing/abstract/article/tigr-assembler-a-new-tool-for-assembling-large-shotgun-sequencing-projects/
- 28. http://www.lanl.gov/
- 29. http://mpiblast.lanl.gov/
- 30. http://mpiblast.lanl.gov/Support.Lists.html
- 31. http://www.gromacs.org/
- 32. http://www.gromacs.org/gromacs/documentation/documentation.html
- 33. /gromacs/online.html

- 34. /gromacs/gmxfaq.html
- 35. http://doc.bioperl.org/
- 36. http://www.bioperl.org/
- 37. http://www.biopython.org/documentation/
- 38. http://www.biopython.org/

Appendix A. Rocks Copyright

Rocks(r)
www.rocksclusters.org
version 5.2 (Chimichanga)

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