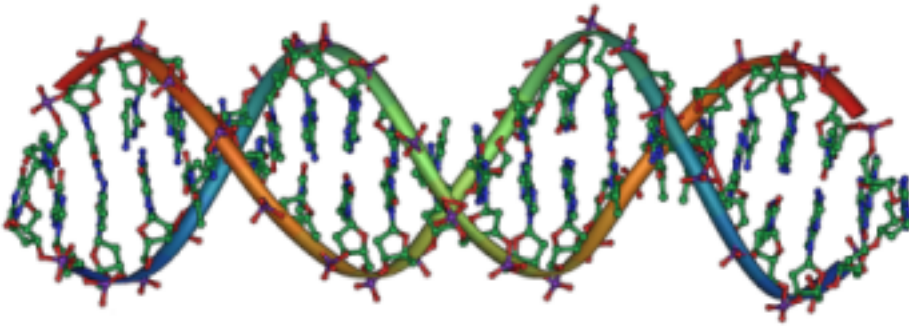
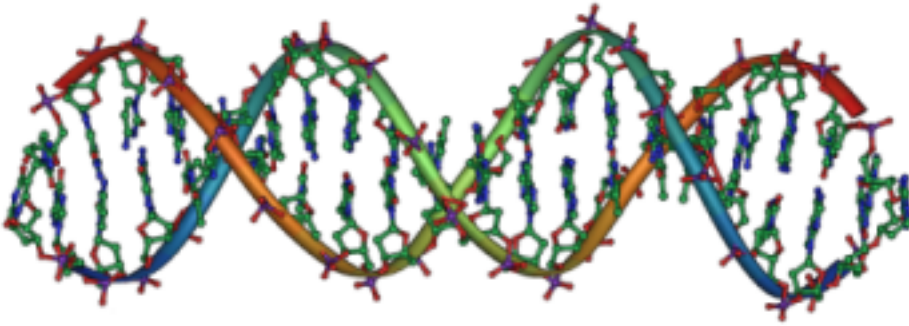


Bio Roll: Users Guide



Version 5.0 Edition

Bio Roll: Users Guide :



Version 5.0 Edition

Published Apr 2008

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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	5.0
Maintained By	Rocks Group
Architecture	i386, x86_64
Compatible with Rocks™	5.0

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		

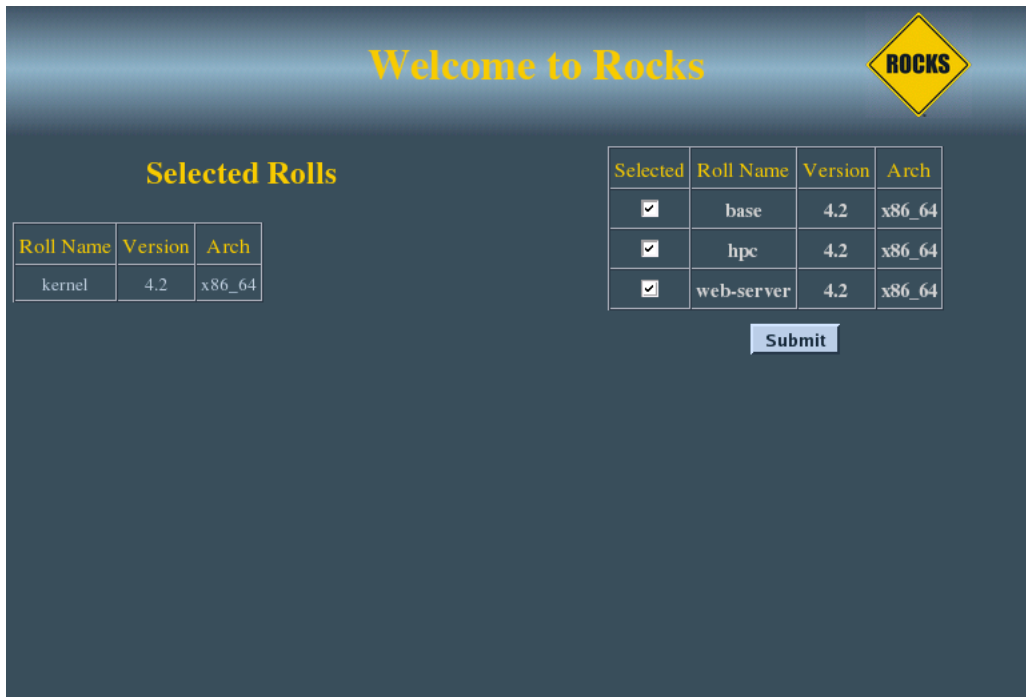
Notes:

- a. You may also substitute your own OS CDs for the Rocks™ OS Roll CDs. In this case you must use all the CDs from your distribution and not use any of the Rocks™ 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 Rocks™ 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://hmmmer.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/>
- 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-Utills
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 [here](#)¹¹. 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 [here](#)¹². 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 matrices 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 separate 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
wgs
-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.nhr  drosoph.nt.nin  drosoph.nt.nsq
-bash-3.1$
```

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

```
[nostramo@xxx ~]$ cat > test.txt
>Test
AGCTTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAGAGTGTCTGATAGCAGC
TTCTGAACCTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGGTCACTAAATACTTTAACCAA
TATAGGCATAGCGCACAGACAGATAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTACGGTGC GGCTGACGCGTACAGGAAACACAGAAAAAAG
CCCGCACCTGACAGTGC GGCTTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTGAA
GTTCGGCGGTACATCAGTGGCAAATGCAGAACGTTTTCTGCGTGTGCCGATATTCTGGAAAGCAATGCC
AGGCAGGGGCGAGGTGGCCACCGTCTCTGCCCCGCCAAAATCACCAACCACCTGGTGGCGATGATTG
AAAAAACCATTAGCGGCCAGGATGCTTTACCCAATATCAGCGATGCCGAACGTATTTTTGCCGAACTTTT
```

- Run the `blastall` program on the test input against the formatted database.

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

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

```
[nostramo@xxx ~]$ blastall -d drosoph.nt -p blastn -i test.txt
BLASTN 2.2.18 [Mar-02-2008]
```

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
```

```
Sequences producing significant alignments:                               Score      E
                                                                           (bits) Value
```

```

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

```

[nostrono@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 v2.0.5.

3.4.2. Using ClustalW

ClustalW can be run at the command line as

```
[nostromo@xxx ~]$ clustalw2
```

```
*****
***** CLUSTAL 2.0.5 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

```
[nostrromo@xxx ~]$ cat > test.txt
>Test
AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAGAGTGTCTGATAGCAGC
TTCTGAACTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGGTCACTAAATACTTTAACCAA
TATAGGCATAGCGCACAGACAGATAAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTAACGGTGCGGGCTGACGCGTACAGGAAACACAGAAAAAAG
CCCGCACCTGACAGTGCAGGGCTTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTGAA
GTTTCGGCGGTACATCAGTGGCAAATGCAGAACGTTTTTCTGCGTGTGCCGATATTCTGGAAAGCAATGCC
AGGCAGGGGCGAGGTGGCCACCGTCTCTCTGCCCCGCCAAAATCACCAACCACCTGGTGGCGATGATTG
AAAAAACCATTAGCGGCCAGGATGCTTTACCCAATATCAGCGATGCCGAACGTATTTTTGCCGAACTTTT
```

- 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/`.

```
[nostrromo@xxx ~]$ fasta35
# fasta35
FASTA searches a protein or DNA sequence data bank
  version 35.03 Feb. 18, 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 - 560 nt
Library: drosoph.nt
..... Done!
122655632 residues in 1170 sequences

      opt      E( )
< 20      0      0:
  22      0      0:          one = represents 3 library sequences
  24      0      0:
  26      0      0:
  28      0      0:
  30      4      2:*=
```

```

32  12    9:==*=
34  35   23:=====*=
36  61   48:=====*=
38  89   79:=====*=
40 109  110:=====*=
42 136  135:=====*=
44 146  149:=====*=
46 152  151:=====*=
48 127  145:=====*=
50 135  132:=====*=
52  99  116:=====*=
54  94   99:=====*=
56  80   83:=====*=
58  66   68:=====*=
60  46   55:=====*=
62  41   44:=====*=
64  42   35:=====*=
66  30   28:=====*=
68  26   22:=====*=
70  19   17:=====*=
72  17   13:=====*=
74  14   10:=====*=
76  7    8:==*=
78  7    6:==*=
80  9    5:==*=
82  3    4:==*
84  0    3:*
86  0    2:*
88  2    2:*      inset = represents 1 library sequences
90  1    1:*
92  0    1:*      :*
94  0    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    0:       *
116 0    0:       *
118 0    0:       *
>120 0    0:       *
122655632 residues in 1611 sequences
Statistics: Expectation_n fit: rho(ln(x))= 7.6446+/-0.00204; mu= 7.1203+/- 0.231
mean_var=233.3955+/-93.485, 0's: 0 Z-trim: 0 B-trim: 0 in 0/54
Lambda= 0.083951
Kolmogorov-Smirnov statistic: 0.0247 (N=27) at 42
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: 8.130
Enter filename for results []: How many scores would you like to see? [20]

The best scores are:
                                opt bits E(1611)
gi|10727961|gb|AE003541.2|AE003541 Drosophila (265536) [r] 171 36.0      1
gi|10728546|gb|AE003447.2|AE003447 Drosophila (304085) [f] 171 36.0      1
gi|7290382|gb|AE003426.1|AE003426 Drosophila m (300193) [f] 159 34.5      2.7
gi|7290880|gb|AE003443.1|AE003443 Drosophila m (302357) [f] 157 34.3      3.2
gi|10727731|gb|AE003838.2|AE003838 Drosophila (263411) [r] 149 33.3      6.3
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
gi|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 32.9      8.8
gi|10726452|gb|AE003691.2|AE003691 Drosophila (226773) [f] 145 32.9      8.8
gi|10727164|gb|AE003603.2|AE003603 Drosophila (294914) [r] 144 32.6      10
gi|7290252|gb|AE003423.1|AE003423 Drosophila m (291976) [r] 144 32.6      10
gi|10727489|gb|AE003803.2|AE003803 Drosophila (282567) [r] 143 32.6      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
gi|10727995|gb|AE003546.2|AE003546 Drosophila (281602) [f] 137 31.9      17
gi|10728551|gb|AE003448.2|AE003448 Drosophila (310364) [f] 137 31.9      17
More scores? [0]
Display alignments also? (y/n) [n]

```

```

560 residues in 1 query sequences
122655632 residues in 1170 library sequences
Scomplib [35.03]
start: Wed Apr 9 10:43:49 2008 done: Wed Apr 9 10:44:41 2008
Total Scan time: 8.130 Total Display time: 0.000

```

Function used was FASTA [version 35.03 Feb. 18, 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 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.
```

```
MrBayes >
```

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

```
[nostromo@xxx ~]$ /opt/openmpi/bin/mpirun -np 4 /opt/Bio/mrbayes/mb /opt/Bio/mrbayes/primates.nex >
[nostromo@xxx ~]$ cat log.txt
```

```
MrBayes v3.1.2
```

```
(Bayesian Analysis of Phylogeny)
```

(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

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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 = 915  
Parsing 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 v3.67.

3.9.2. Further Information

Further information 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 v5.65

3.10.2. Usage

T-coffee is used for standard alignments and alignment combinations. It is installed at `/opt/Bio/t_coffee/` 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/t_coffee/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/t_coffee/example/sample_aln2.fasta
```

```
PROGRAM: T-COFFEE (Version_5.65)
-full_log      S      [0]
-run_name      S      [0]
-mem_mode      S      [0]      mem
-extend        D      [1]      1
-extend_mode   S      [0]      very_fast_triplet
-max_n_pair    D      [0]      10
-seq_name_for_quadruplet S      [0]      all
-compact       S      [0]      default
-clean         S      [0]      no
-do_self       FL     [0]      0
-do_normalise  D      [0]      1000
-template_file S      [0]
-in            S      [0]
-seq           S      [1]      /opt/Bio/t_coffee/example/sample_aln2.fasta
-aln          S      [0]
-method_limits S      [0]
-method        S      [0]
-lib           S      [0]
-profile       S      [0]
-profile1      S      [0]
-profile2      S      [0]
-pdb           S      [0]
-out_lib       W_F    [0]      no
-lib_only      D      [0]      0
-outseqweight  W_F    [0]      no
-dpa           FL     [0]      0
-seq_source    S      [0]      ANY
-cosmetic_penalty D    [0]      -50
-gapopen       D      [0]      0
-gapext        D      [0]      0
-fgapopen      D      [0]      0
-fgapext       D      [0]      0
-nomatch       D      [0]      0
-newtree       W_F    [0]      default
-tree          W_F    [0]      NO
-usetree       R_F    [0]
-tree_mode     S      [0]      nj
-distance_matrix_mode S  [0]      ktup
-distance_matrix_sim_mode S [0]      idmat_sim1
-quicktree     FL     [0]      0
-outfile       W_F    [0]      default
-maximise      FL     [1]      1
-output        S      [0]      clustalw      html
-infile        R_F    [0]
-matrix        S      [0]      default
-tg_mode       D      [0]      1
-profile_mode  S      [0]      cw_profile_profile
-profile_comparison S  [0]      profile
-dp_mode       S      [0]      cfasta_pair_wise
-ktuple        D      [0]      1
```

```

-ndiag          D      [0]    0
-diag_threshold D      [0]    0
-diag_mode      D      [0]    0
-sim_matrix     S      [0]    vasiliky
-transform      S      [0]
-check_type     FL     [0]    0
-type          S      [0]
-outorder      S      [0]    aligned
-inorder       S      [0]    aligned
-seqnos        S      [0]    off
-case          S      [0]    keep
-cpu           D      [0]    0
-maxnseq       D      [0]    1000
-maxlen        D      [0]    -1
-weight        S      [0]    default
-seq_weight    S      [0]    t_coffee
-align         FL     [1]    1
-mocca         FL     [0]    0
-domain        FL     [0]    0
-start         D      [0]    0
-len           D      [0]    0
-scale         D      [0]    0
-mocca_interactive FL  [0]    0
-evaluate_mode S      [0]    t_coffee_fast
-get_type      FL     [0]    0
-clean_aln     D      [0]    0
-clean_threshold D    [1]    1
-clean_iteration D    [1]    1
-clean_evaluate_mode S  [0]    t_coffee_fast
-extend_matrix FL     [0]    0
-prot_min_sim  D      [40]   40
-prot_max_sim  D      [60]   60
-prot_min_cov  D      [0]    0
-pdb_min_sim   D      [30]   30
-pdb_max_sim   D      [100]  100
-pdb_min_cov   D      [50]   50
-pdb_blast_server W_F  [0]    SIB
-prot_blast_server W_F  [0]    SIB
-pdb_db         W_F  [0]    nrl3d
-protein_db     W_F  [0]    nr
-method_log     W_F  [0]    no
-struct_to_use S      [0]
-cache          W_F  [0]    use
-align_pdb_param_file W_F  [0]    no
-align_pdb_hasch_mode W_F  [0]    hasch_ca_trace_bubble
-external_aligner S    [0]    NO
-msa_mode       S      [0]    tree
-one2all        S      [0]
-lalign_n_top   D      [0]    10
-iterate        D      [0]    0
-trim           D      [0]    0
-split         D      [0]    0
-trimfile       S      [0]    default

```

```

-split          D          [0]      0
-split_nseq_thres D        [0]      0
-split_score_thres D       [0]      0
-check_pdb_status D        [0]      0
-clean_seq_name D         [0]      0
-seq_to_keep    S         [0]
-dpa_master_aln S         [0]
-dpa_maxnseq    D         [0]      0
-dpa_min_score1 D         [0]
-dpa_min_score2 D         [0]
-dpa_keep_tmpfile FL      [0]      0
-dpa_debug      D         [0]      0
-multi_thread   S         [0]
-lib_list       S         [0]
-tip            S         [0]      one
-rna_lib        S         [0]
-no_warning     D         [0]      0

```

INPUT FILES

```

Input File (S) /opt/Bio/t_coffee/example/sample_aln2.fasta Format clustal_aln
Input File (M) lalign_id_pair
Input File (M) slow_pair

```

INPUT SEQUENCES: 6 SEQUENCES [PROTEIN]

```

Input File /opt/Bio/t_coffee/example/sample_aln2.fasta Seq 1cms Length 175 type PROTEIN Struct
Input File /opt/Bio/t_coffee/example/sample_aln2.fasta Seq 4pep Length 174 type PROTEIN Struct
Input File /opt/Bio/t_coffee/example/sample_aln2.fasta Seq 4ape Length 178 type PROTEIN Struct
Input File /opt/Bio/t_coffee/example/sample_aln2.fasta Seq 3app Length 174 type PROTEIN Struct
Input File /opt/Bio/t_coffee/example/sample_aln2.fasta Seq 2apr Length 178 type PROTEIN Struct
Input File /opt/Bio/t_coffee/example/sample_aln2.fasta Seq 1cms_1 Length 148 type PROTEIN Struct

```

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:[3]

```
lalign_id_pair [method]
```

```
[Submit Job][TOT= 15][100 %][ELAPSED TIME: 0 sec.]
```

```
[Retrieve Job][TOT= 15][100 %][ELAPSED TIME: 0 sec.]
```

```
slow_pair [method]
```

```
[Submit Job][TOT= 15][100 %][ELAPSED TIME: 0 sec.]
```

```
[Retrieve Job][TOT= 15][100 %][ELAPSED TIME: 0 sec.]
```

Library Total Size: [5133]

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 NEIGHBOR JOINING DENDROGRAM

[MODE=nj] [DONE]

PROGRESSIVE_ALIGNMENT [Tree Based]

```

Group 7: [Group 5 ( 1 seq)] with [Group 4 ( 1 seq)]-->[Score= 50][Len= 179]
Group 8: [Group 7 ( 2 seq)] with [Group 6 ( 1 seq)]-->[Score= 36][Len= 184]
Group 9: [Group 2 ( 1 seq)] with [Group 1 ( 1 seq)]-->[Score= 10][Len= 212]
Group 10: [Group 3 ( 1 seq)] with [Group 9 ( 2 seq)]-->[Score= 26][Len= 217]
Group 11: [Group 10 ( 3 seq)] with [Group 8 ( 3 seq)]-->[Score= 30][Len= 221]

```

CLUSTAL FORMAT for T-COFFEE Version_5.65 [http://www.tcoffee.org], CPU=0.93 sec, SCORE=37, Nseq=6, L

```

3app AASGVATNTPTAN--DEEYITPVTIG--GTTLNL-----NFDTGSA
4ape -STGSATTTPIDS-L-DDAYITPVQIGTPAQTLNL-----DFDTGSS
4pep -----IGDEPLENYL-DTEYFGTIGIGTPAQDFTV-----IFDTGSS
1cms ---GEVASVPLTNYL-DSQYFGKIYLGTPPQEFV-----LFDTGSS
1cms_1 -YTGSLHWVPVT---VQQYW-----QFTVDSVTISGVVACEGGCQAILDTGTS
2apr ---AGVGTVPMTDYGNDIEYYGQVTIGTPGKKFNL-----DFDTGSS

```

```

* * :: :***:

```

```

3app DLWVFSTELPASQQSGHSVYNPSATGK--ELSGYTWSISYGDGSSASGNVFTDSVTVGGV
4ape DLWVFSSETTASEVDGQTIYTPSKSTTAKLLSGATWSISYGDGSSSSGDVYTDTVSVGGI
4pep NLWVPSVYCSSLACSDHNQFNPDDSSSTFEA-TSQELSIYGTGS-MTGILGYDTVQVGGI
1cms DFWVPSIYCKSNACKNHQRFDPKSSSTFQN-LGKPLSIHYGTGS-MQGILGYDTVTVSNI
1cms_1 KLVGPSSD-----I
2apr DLWIASTLCTNCG-SGQTKYDPNQSSTYQA-DGRTWSISYGDGSSASGILAKDNVNLGGL
.: * :

```

```

3app TAHGQAVQAAQQISAQFQQDTNNDG-----LLGLAFSSINTVQPQSQT-----
4ape TVTGQAVESAKKVSSSFTEIDSTIDG-----LLGLAFSTLNTVSPQQKT-----
4pep SDTNQIFGLSETEPGSFLYAPFDG-----ILGLAYPSISA---SGATP-----
1cms VDIQQTVGLSTQEPGDVFTYAEPFDG-----ILGMAYPSLASEYS---IP-----
1cms_1 LNIQQAIGATQNQYGEFIDCDNLSYMPVTVFEINGKMYPLTPSAYT---SQDQGFCTSG
2apr LIKGQTIELAKREAASFAS-GPNDG-----LLGLGFDTITTVRGV--KT-----
* . : ... . : * : :

```

```

3app -FFDTV--KSSLAQPLFAVALK---HQQPGVYDFGFIDSSK

```



```

4ape      -FFDNA--KASLDSPVFTADLG---YHAPGTYNFGFIDTTA
4pep      -VFDNLWDQGLVSQLDFSVYLS-SNDDSGSVLLGGIDSSY
1cms      -VFDNMMNRHLVAQDLFSVYMD--RNGQESMLTLGAIDPSY
1cms_1    FQSENHSQKWILGDVFIREYYS--VFDRANN--LVGLAKAI
2apr      -PMDNLISQGLISRPIFGVYLGKAKNGGGGEYIFGGYDSTK
          :.  :  :  :.  .  :  :

```

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
# TIP 15: -other_pg seq_reformat -in <aln> -action +trim %50 Will reduce the redundancy of your MSA

# Command Line: t_coffee /opt/Bio/t_coffee/example/sample_aln2.fasta [PROGRAM:T-COFFEE]
# T-COFFEE Memory Usage: Current= 6.248 Mb, Max= 8.329 Mb
# T-COFFEE CPU Usage: 930 millisec
# Results Produced with T-COFFEE (Version_5.65)
# 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/t_coffee/doc/`
- T-Coffee Documentation²⁶

3.11. MPI-Blast

3.11.1. About

MPI-Blast is a program from LANL²⁷ 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 2.2.18.

3.11.2. 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.

```
[nostrromo@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 at least 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          ecoli.nt.000.nsq  ecoli.nt.001.nsq  ecoli.nt.002.nsq  ecoli.nt.003.nsq
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.

```
[nostrromo@xxx ~]$ cat > test.txt
>Test
AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAAGAGTGTCTGATAGCAGC
```

```

TTCTGAACTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGGTCACATAAATACTTTAACCAA
TATAGGCATAGCGCACAGACAGATAAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTAACGGTGCGGGCTGACGCGTACAGGAAACACAGAAAAAG
CCCGCACCTGACAGTGCGGGCTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTTGAA
GTTGCGGGGTACATCAGTGGCAAATGCAGAACGTTTTCTGCGTGTTGCCGATATTCTGGAAAGCAATGCC
AGGCAGGGGCGAGGTGGCCACCGTCTCTCTGCCCGGCCAAAATCACCAACCACCTGGTGGCGATGATTG
AAAAAACATTAGCGGCCAGGATGCTTTACCCAATATCAGCGATGCCGAACGTATTTTTGCCGAACTTTT

```

```
[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.

3.11.3. 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

```

#!/bin/bash

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

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

$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_sge.sh
Your job 11 ("mpiblast_sge.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.

3.11.4. Further Information

Further information about using mpiblast can be found at the MPI-Blast home page²⁸.

For support, please join the mpiblast mailing list²⁹

3.12. GROMACS

3.12.1. 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 3.3.1. It is available at <http://www.gromacs.org> under the GNU General Public Licence v2.0.

3.12.2. 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 Page³⁰
- GROMACS Documentation³¹
- GROMACS Online Reference Manual³²
- GROMACS FAQ³³
- Tutorials available on your machines at `/opt/Bio/gromacs/share/tutor`

3.13. Bioperl

3.13.1. About

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

3.13.2. 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 Docs³⁴.

3.13.3. Further Information

Further information about bioperl is available at the Bioperl home page³⁵

3.14. Biopython

3.14.1. About

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

3.14.2. 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 documentation³⁶.

3.14.3. Further Information

Further information about biopython is available at the Biopython home page³⁷

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.cbc.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.lanl.gov/>
28. <http://mpiblast.lanl.gov/>
29. <http://mpiblast.lanl.gov/Support.Lists.html>
30. <http://www.gromacs.org/>
31. <http://www.gromacs.org/gromacs/documentation/documentation.html>
32. [/gromacs/online.html](#)
33. [/gromacs/gmxfaq.html](#)
34. <http://doc.bioperl.org/>
35. <http://www.bioperl.org/>
36. <http://www.biopython.org/documentation/>
37. <http://www.biopython.org/>

Appendix A. Rocks Copyright

Rocks(r)
www.rocksclusters.org
version 5.0 (V)

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```
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```

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```

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```
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```

```
<signature of Ty Coon>, 1 April 1989
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```

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```
<one line to give the program's name and a brief idea of what it does.>  
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```

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```

```
<signature of Ty Coon>, 1 April 1989
Ty Coon, President of Vice
```

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BLAST - open source parallel BLAST

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