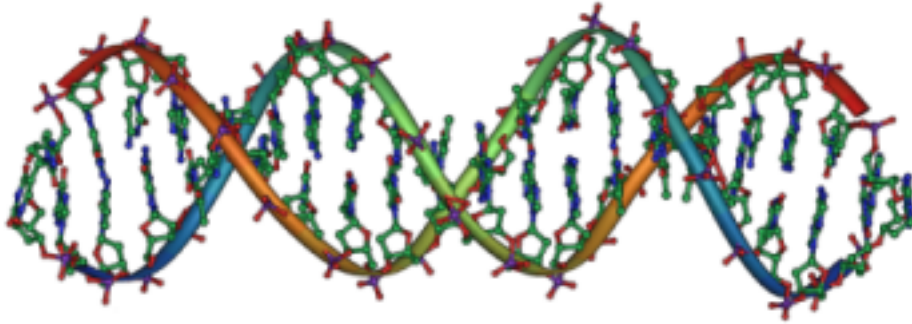
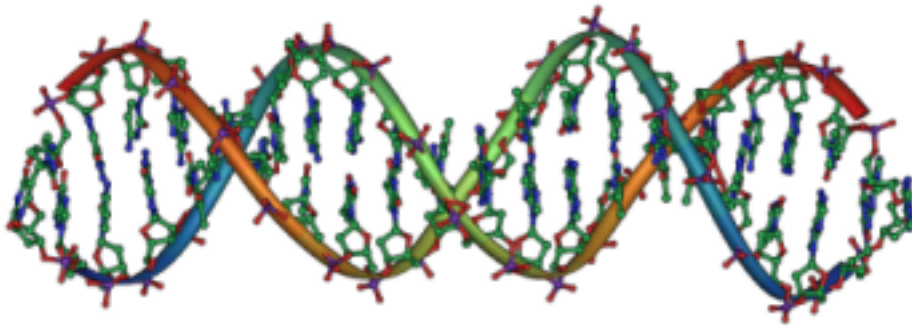


Bio Users Guide



6.1 Edition

Bio Users Guide :



6.1 Edition

Published Nov 27 2012

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Table of Contents

Preface	v
1. Overview	1
2. Installing	2
2.1. On a New Server	2
2.2. On an Existing Server.....	2
3. Using	3
3.1. List of packages present in the Bio Roll	3
3.2. HMMER.....	3
3.3. NCBI BLAST.....	4
3.4. ClustalW.....	7
3.5. EMBOSS.....	8
3.6. Glimmer	8
3.7. Fasta.....	8
3.8. MrBayes	11
3.9. Phylip	13
3.10. T_Coffee.....	14
3.11. TIGR Assembler v2	19
3.12. MPI-Blast	19
3.13. GROMACS	22
3.14. Bioperl.....	22
3.15. Biopython	23
A. Rocks® Copyright	25
B. Third Party Copyrights and Licenses	26
B.1. Biopython	26
B.2. Clustal W	26
B.3. EMBOSS	26
B.4. FASTA	32
B.5. Glimmer.....	32
B.6. GROMACS.....	34
B.7. HMMER	40
B.8. mpiBlast.....	46
B.9. Mr.Bayes.....	48
B.10. NCBI.....	53
B.11. Perl Modules.....	53
B.12. Phylip.....	55
B.13. T_Coffee	56
B.14. TIGR Assembler.....	62

List of Tables

1-1. Summary.....	1
1-2. Compatibility.....	1

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	6.1
Maintained By	Rocks Group
Architecture	i386, x86_64
Compatible with Rocks®	6.1

The bio roll has the following requirements of other rolls. Compatibility with all known rolls is assured, and all known conflicts are listed. There is no assurance of compatibility with third-party rolls.

Table 1-2. Compatibility

Requires	Conflicts
Base	
HPC	
Kernel	
OS	
Web Server	

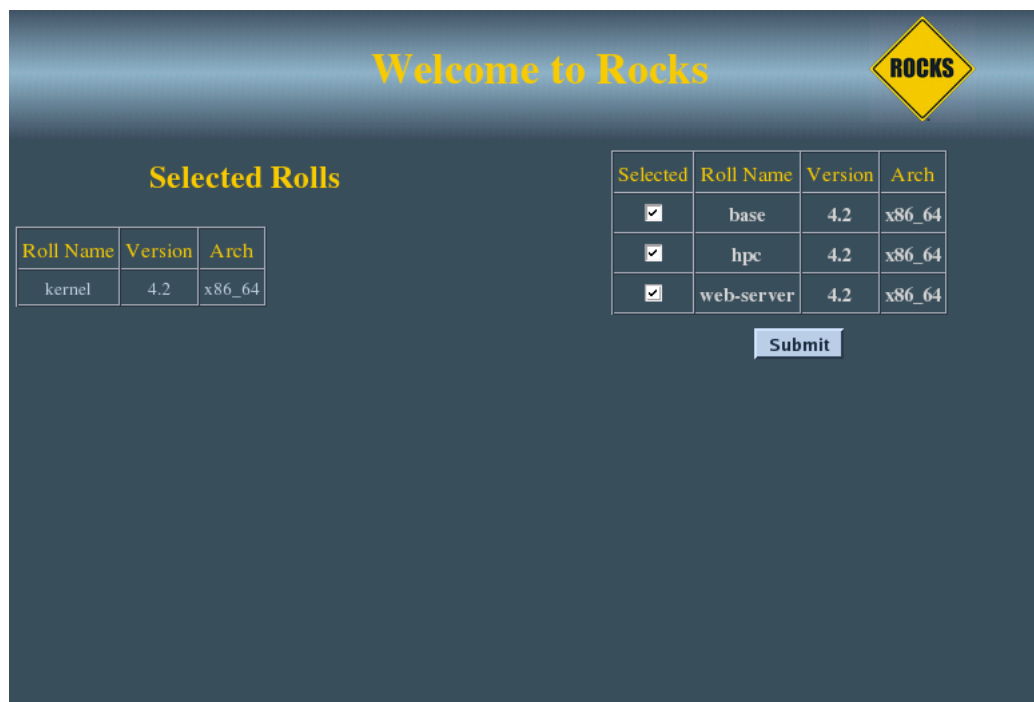


This roll has been released independent of the corresponding Rocks® release. It therefore requires the complete **OS** roll and will not function correctly if using only the **Jumbo** or incomplete set of **OS** CDRoms.

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
# cd /export/rocks/install
# rocks create distro
# rocks run roll 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 - <http://hmm.janelia.org/>
- 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-ext
- perl-bioperl-run
- 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	flex	readline-devel
foundation-python-extras	xorg-x11-devel	gd
ReportLab	readline	gd-devel

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 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 `$HOME/bio/hmmer/db/`.

HMMER has many modes of execution. For a description of all the executables that come with HMMER, please refer to the current HMMER online userguide¹². 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.

- `$BLASTDB` - This is the variable which points to the Blast Database. This is set to `$HOME/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 a BLAST database that you want to run the comparison against. The databases can be obtained from the NCBI ftp site at `ftp://ftp.ncbi.nlm.nih.gov/blast/db/`.



The databases available on the site mentioned above are pre-formatted.

It is recommended that the blast databases be stored at the \$BLASTDB location.

Visit <ftp://ftp.ncbi.nlm.nih.gov/blast/db/> in your browser to see a list of available preformatted databases.

Download one of these on to your cluster using wget.

```
[nostromo@xxx ~]$ wget -q ftp://ftp.ncbi.nlm.nih.gov/blast/db/nt.08.tar.gz
[nostromo@xxx ~]$ gunzip -c nt.08.tar.gz | ( cd $BLASTDB/ && tar -xf -)
```

- The above method downloads a formatted database, and untars it into \$BLASTDB.

Unformatted databases can be obtained in FASTA format at <ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/>¹⁵.

Visit <ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/>¹⁶ in your web browser



If you've 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

```
[nostromo@xxx ~]$ cd $BLASTDB
[nostromo@xxx ~]$ wget -q ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/drosoph.nt.gz
[nostromo@xxx ~]$ gunzip drosoph.nt.gz
[nostromo@xxx ~]$ formatdb -p F -V T -i drosoph.nt
[nostromo@xxx ~]$ ls drosoph.nt*
drosoph.nt  drosoph.nt.nhr  drosoph.nt.nin  drosoph.nt.nsq
[nostromo@xxx ~]$ cd $HOME
```

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

```
[nostromo@xxx ~]$ cat > test.txt
>Test
AGCTTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAGAGTGTCTGATAGCAGC
TTCTGAACCTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGGTCACATAAATACTTTAACC
TATAGGCATAGCGCACAGACAGATAAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTAACGGTGCGGGCTGACGCGTACAGGAAACACAGAAAAAAG
CCCGCACCTGACAGTGC GGCTTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTGAA
GTTTCGGCGGTACATCAGTGGCAAATGCAGAACGTTTTCTGCGTGTGCGGATATTCTGAAAAGCAATGCC
AGGCAGGGGCGAGGTGGCCACCGTCTCTGCCCCGCCAAAATCACCAACCCTGGTGGCGATGATTG
AAAAAACCATTAGCGGCCAGGATGCTTTACCAATATCAGCGATGCCGAACGTATTTTTGCGGAACCTTT
```

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

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

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
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 genom... 34 3.4
gi|7297628|gb|AE003628.1|AE003628 Drosophila melanogaster genom... 34 3.4
gi|10728546|gb|AE003447.2|AE003447 Drosophila melanogaster genom... 34 3.4
gi|7290819|gb|AE003441.1|AE003441 Drosophila melanogaster genom... 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 genom... 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=$HOME/bio/ncbi/db/
export BLASTMAT=/opt/bio/ncbi/data/

/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/>¹⁷
- BLAST Help page on your cluster BLAST Help Page¹⁸
- BLAST Program selection Guide - http://www.ncbi.nlm.nih.gov/blast/BLAST_guide.pdf¹⁹

3.4. ClustalW

3.4.1. About

ClustalW is a multiple sequence alignment program. The version included with this distribution is v2.0.12.

3.4.2. Using ClustalW

ClustalW can be run at the command line as

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

```
*****
***** CLUSTAL 2.0.12 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).

The version of EMBOSS included with this version of Rocks is 6.1.0

3.5.2. Further Information

Information about using EMBOSS is available at <http://emboss.sourceforge.net/>. You may also register at their mailing list [here](#)²¹.

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 [here](#)²². 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

```
[nostrono@xxx ~]$ cat > test.txt
>Test
AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAGAGTGTCTGATAGCAGC
TTCTGAACTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGGTCACTAAATACTTTAACCAA
TATAGGCATAGCGCACAGACAGATAAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTAACGGTGCGGGCTGACGCGTACAGGAAACACAGAAAAAAG
CCCGCACCTGACAGTGC GGCTTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTGAA
GTTTCGGCGGTACATCAGTGGCAAATGCAGAACGTTTTCTGCGTGTGCGGATATTCTGGAAAGCAATGCC
AGGCAGGGGCGAGGTGGCCACCGTCTCTGCCCCGCCAAAATCACCAACCACCTGGTGGCGATGATTG
AAAAAACCATTAGCGGCCAGGATGCTTTACCCAATATCAGCGATGCCGAACGTATTTTTGCGGAACTTTT
```

- 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/`.

```
[nostrono@xxx ~]$ fasta35
# 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      0:          one = represents 3 library sequences
  24      0      0:
  26      0      0:
  28      0      0:
  30      3      2:*
  32     12      9:==*=
  34     37     23:====*====
  36     59     48:====*====
  38     90     79:====*====
```

```

40 110 110:=====*
42 133 135:=====*
44 147 149:=====*
46 151 151:=====*
48 129 145:===== *
50 131 132:=====*
52 102 116:===== *
54 92 99:===== *
56 80 83:=====*
58 68 68:=====*
60 43 55:===== *
62 44 44:=====*
64 42 35:=====*=
66 30 28:=====*
68 25 22:=====*=
70 20 17:=====*=
72 18 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:=====*

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)
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 2.8
gi|7290880|gb|AE003443.1|AE003443 Drosophila m (302357) [f] 157 34.3 3.3

```

```

gi|10727731|gb|AE003838.2|AE003838 Drosophila (263411) [r] 149 33.3 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
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 32.8 8.9
gi|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
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 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 page²³.

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
```

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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 Page](#)²⁴ and at the [MrBayes Wiki](#)²⁵

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

Further information about Phylip is available at the Phylip home page²⁶.

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 v8.14

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_8.14)
-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]
-template_mode S      [0]
-remove_template_file D      [0]      0
-profile_template_file S      [0]
-in            S      [0]
-seq           S      [1]      /opt/bio/tcoffee/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]
-relax_lib D [0] 1
-filter_lib D [0] 0
-shrink_lib D [0] 0
-out_lib W_F [0] no
-out_lib_mode S [0] primary
-lib_only D [0] 0
-outseqweight W_F [0] no
-dpa FL [0] 0
-seq_source S [0] ANY
-cosmetic_penalty D [0] 0
-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] aln 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] linked_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]
-outorder S [0] input
-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
-method_evaluate_mode S      [0]    default
-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        [0]    0
-prot_max_sim      D        [90]   90
-prot_min_cov      D        [0]    0
-pdb_min_sim       D        [35]   35
-pdb_max_sim       D        [100]  100
-pdb_min_cov       D        [50]   50
-pdb_blast_server  W_F     [0]    EBI
-blast             W_F     [0]
-blast_server      W_F     [0]    EBI
-pdb_db            W_F     [0]    pdb
-protein_db        W_F     [0]    uniprot
-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]
-subset2all        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_core        S        [0]    templates_jobs_relax_msa
-n_core           D        [0]    0
-lib_list          S        [0]
-prune_lib_mode    S        [0]    5
-tip              S        [0]    one
-rna_lib           S        [0]
-no_warning        D        [0]    0
-run_local_script  D        [0]    0
-plugins           S        [0]    default

```

```

-proxy          S          [0]      unset
-email          S          [0]
-clean_overaln D          [0]      0
-overaln_param S          [0]
-overaln_mode   S          [0]
-overaln_model  S          [0]
-overaln_threshold D      [0]      0
-overaln_target D          [0]      0
-overaln_P1     D          [0]      0
-overaln_P2     D          [0]      0
-overaln_P3     D          [0]      0
-overaln_P4     D          [0]      0
-exon_boundaries S        [0]

```

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

```

COMPUTE PAIRWISE SIMILARITY [dp_mode:] [distance_matrix_mode: ktup][Similarity Measure: idmat_si

```

Seq: 1cms
Seq: 1cms_1
Seq: 2apr
Seq: 3app
Seq: 4ape
Seq: 4pep

```

READ/MAKE LIBRARIES:[2]

```

proba_pair [method]

```

```

Multi Core Mode: 2 processors [subset]

```

```

[Submit Job][TOT= 8][100 %][ELAPSED TIME: 0 sec.]

```

```

MANUAL PENALTIES: gapopen=0 gapext=0

```

```

Library Total Size: [6175]

```

```

Library Relaxation: Multi_proc [2]

```

```

[Submit Job][TOT= 3087][100 %][ELAPSED TIME: 0 sec.]

```

```

Total Relaxation: [6175]--->[5092] Entries

```

```

#### File Type= WEIGHT Format= tc_weight Name= no | NOT PRODUCED [WARNING:T-COFFEE:V

```

```

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]
```

```

Group 8: [Group 5 ( 1 seq)] with [Group 4 ( 1 seq)]-->[Score= 83] [Len= 179]
Group 7: [Group 6 ( 1 seq)] with [Group 1 ( 1 seq)]-->[Score= 92] [Len= 176]
Group 9: [Group 8 ( 2 seq)] with [Group 3 ( 1 seq)]-->[Score= 74] [Len= 186]
Group 10: [Group 9 ( 3 seq)] with [Group 7 ( 2 seq)]-->[Score= 77] [Len= 186]
Group 11: [Group 2 ( 1 seq)] with [Group 10 ( 5 seq)]-->[Score= 24] [Len= 209]

```

```
CLUSTAL FORMAT for T-COFFEE Version_8.14 [http://www.tcoffee.org] [MODE: ], CPU=0.15 sec, SCORE=
```

```

1cms      GE---VASVPLTNY-----LDSQYFGKIYLGTPPQEFTVLFDTGSSDFWVPSIYCKSNA
4pep      -----IGDEPLENY-----LDTEYFGTIGIGTPAQDFTVIFDTGSSNLWVPSVYCSSLA
4ape      S-TGSATTPID-S-----LDDAYITPVQIGTPAQTLNLDFTGSSDLWVFSSETTASE
3app      AASGVATNPTA-----NDEEYITPVTIGG--TTLNLFDTGSADLWVFSSTELPASQ
2apr      AG---VGTVPMTDY-----GNDIEYYGQVTIGTPGKKFNLDFTGSSDLWIASTLCTN-C
1cms_1    Y-TGSLHWVPVTVQQYWQFTVDSVTISGVVVACEG-GCQAILDTGTSKLVGPSSD-----
                *           *           :  :           :*****: *

```

```

1cms      CKNHQRFDPKSSSTFQ-NLGKPLSIHYGTGS-MQGILGYDTVIVSNIVDIQQTVGLSTQE
4pep      CSDHNQFNPDDSSSTFE-ATSQELSIYGTGS-MTGILGYDTVQVGGISDTNQIFGLSETE
4ape      VDGQTIYTPSKSTTAKLLSGATWSISYGDGSSSSGDVYTDTVSVGGLTVTGQAVESAKKV
3app      QSGHSVYNPSATG-KE-LSGYTWSISYGDGSSASGNVFTDSVTVGGVTAHQAVQAAQQI
2apr      GSGQTKYDPNQSSTYQ-ADGRTWSISYGDGSSASGILAKDNVNLGGLLIKQTIELAKRE
1cms_1    -----ILNIQQAIGATQNQ
                : * . :

```

```

1cms      PGDVFTYAEFD-----GILGMAYPSLASEY-----SIPVFDNM-MNRHLVA----
4pep      PGSFLYYAPFD-----GILGLAYPSISASG-----ATPVFDNL-WDQGLVS----
4ape      SSSFTEDSTID-----GLLGLAFSTLNTVSPTQ----QKTFFDNA---KASLD----
3app      SAQFQDNTNND-----GLLGLAFSSINTVQPQS----QTTFDFTV---KSSLA----
2apr      AASFAS-GPND-----GLLGLGFDTITTVRG-----VKTPMDNL-ISQGLIS----
1cms_1    YGEFDIDCDNLSYMPVTVFEINGKMYPLTPSAYTSQDQGFCTSGFQSENHSQKWILGDVF
                ...           : * :           : . : :           : :

```

```

1cms      -QDLFSVYMDRN-G-QESMLTLGAIDPSY
4pep      -QDLFSVYLSSN-DDSGSVVLLGGIDSSY
4ape      -SPVFTADLGY---HAPGTYNFGFIDTTA
3app      -QPLFAVALKH---QQPGVYDFGFIDSSK
2apr      -RPIFGVYLGKAKNGGGGEYIFGGYDSTK
1cms_1    IREYYSVFDR-----ANNLVGLAKAI
                : .           :           :

```

```
OUTPUT RESULTS
```

```
#### File Type= GUIDE_TREE Format= newick Name= sample_aln2.dnd
```

```
#### File Type=          MSA Format=          aln Name= sample_aln2.aln
#### File Type=          MSA Format=          html Name= sample_aln2.html

# TIP :See The Full Documentation on www.tcoffee.org
# TIP 1: Get the most accurate protein alignments with: t_coffee <yourseq> -special_mode accurate
# TIP 4: -special_mode=expresso to fetch your structures automatically

# Command Line: t_coffee /opt/bio/tcoffee/example/sample_aln2.fasta [PROGRAM:T-COFFEE]
# T-COFFEE Memory Usage: Current= 11.819 Mb, Max= 13.181 Mb
# T-COFFEE CPU Usage: 160 millisec
# Results Produced with T-COFFEE (Version_8.14)
# 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 page²⁷
- On your cluster head node at `/opt/bio/tcoffee/doc/`
- T-Coffee Documentation²⁸

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 page²⁹

3.12. MPI-Blast

3.12.1. About

MPI-Blast is a program from LANL³⁰ 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 ~]$ cd $BLASTDB
[nostromo@xxx ~]$ 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.

```
[nostromo@xxx ~]$ gunzip ecoli.nt.gz
[nostromo@xxx ~]$ ls
ecoli.nt
[nostromo@xxx ~]$ 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 /home/nostromo/bio/ncbi/db/ecoli.nt -o T
Removed /tmp/reorderncq8B1
Created 4 fragments.
[nostromo@xxx ~]$ 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 create a test sequence file and run mpiblast on the sequence against the formatted database.

```
[nostromo@xxx ~]$ cat > test.txt
```

```
>Test
```

```
AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAGAGTGTCTGATAGCAGC
TTCTGAACTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGGTCACTAAATACTTAACC
TATAGGCATAGCGCACAGACAGATAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTAACGGTGCGGGCTGACGCGTACAGGAAACACAGAAAAAAG
CCCGCACCTGACAGTGC GGCTTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTGAA
GTTCCGGCGGTACATCAGTGGCAAATGCAGAACGTTTTCTGCGTGTGCGGATATTCTGGAAAGCAATGCC
AGGCAGGGGCAGGTGGCCACCGTCTCTGCCCCGCCAAAATCACCAACCACCTGGTGGCGATGATTG
AAAAAACCATTAGCGGCCAGGATGCTTTACCCAATATCAGCGATGCCGAACGTATTTTTGCGGAACTTTT
```

```
[nostromo@xxx mpiblast]$ /opt/openmpi/bin/mpirun -np 4 /opt/bio/mpiblast/bin/mpiblast -d ecoli.
```

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

```
#!/bin/bash

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

export MPI_DIR=/opt/openmpi/
export BLASTDB=$HOME/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.

3.12.4. Further Information

Further information about using mpiblast can be found at the MPI-Blast home page³¹.

For support, please join the mpiblast mailing list³²

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 4.0.5. 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 v1.3.3 is used as the MPI library.

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

- GROMACS Home Page³³
- GROMACS Documentation³⁴
- GROMACS Online Reference Manual³⁵
- GROMACS FAQ³⁶
- 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 Docs³⁷.

3.14.3. Further Information

Further information about bioperl is available at the Bioperl home page³⁸

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 documentation³⁹.

3.15.3. Further Information

Further information about biopython is available at the Biopython home page⁴⁰

Notes

1. <http://hmmer.janelia.org/>
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.tcoffee.org/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.janelia.org/#download>
12. <ftp://selab.janelia.org/pub/software/hmmer/CURRENT/Userguide.pdf>
13. <ftp://ftp.ncbi.nlm.nih.gov/blast/db/>
14. <ftp://ftp.ncbi.nlm.nih.gov/blast/db/>
15. <ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/>
16. <ftp://ftp.ncbi.nlm.nih.gov/blast/db/FASTA/>
17. <http://www.ncbi.nlm.nih.gov/BLAST/>
18. </blast/docs/>

19. http://www.ncbi.nlm.nih.gov/blast/BLAST_guide.pdf
20. <http://emboss.sourceforge.net/>
21. <http://emboss.sourceforge.net/support/>
22. <http://www.cbcb.umd.edu/software/glimmer/glim302notes.pdf>
23. <http://fasta.bioch.virginia.edu/>
24. <http://mrbayes.csit.fsu.edu/index.php>
25. <http://mrbayes.scs.fsu.edu/wiki/index.php/Manual>
26. <http://evolution.genetics.washington.edu/phylip.html>
27. http://www.tcoffee.org/Projects_home_page/t_coffee_home_page.html
28. http://www.tcoffee.org/Documentation/t_coffee/t_coffee_technical.htm
29. <http://www.jcvi.org/cms/publications/listing/abstract/article/tigr-assembler-a-new-tool-for-assembling-large-shotgun-sequencing-projects/>
30. <http://www.lanl.gov/>
31. <http://mpiblast.lanl.gov/>
32. <http://mpiblast.lanl.gov/Support.Lists.html>
33. <http://www.gromacs.org/>
34. <http://www.gromacs.org/gromacs/documentation/documentation.html>
35. <http://www.gromacs.org/gromacs/online.html>
36. <http://www.gromacs.org/gromacs/gmxfaq.html>
37. <http://doc.bioperl.org/>
38. <http://www.bioperl.org/>
39. <http://biopython.org/DIST/docs/tutorial/Tutorial.html>
40. <http://www.biopython.org/>

Appendix A. Rocks® Copyright

Rocks(r)
www.rocksclusters.org
version 5.6 (Emerald Boa)
version 6.1 (Emerald Boa)

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```

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```

```
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```

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```

```
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Ty Coon, President of Vice
```

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BLAST - open source parallel BLAST

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