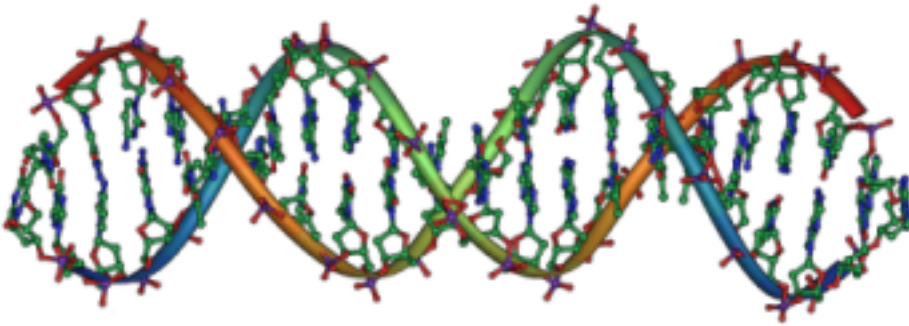
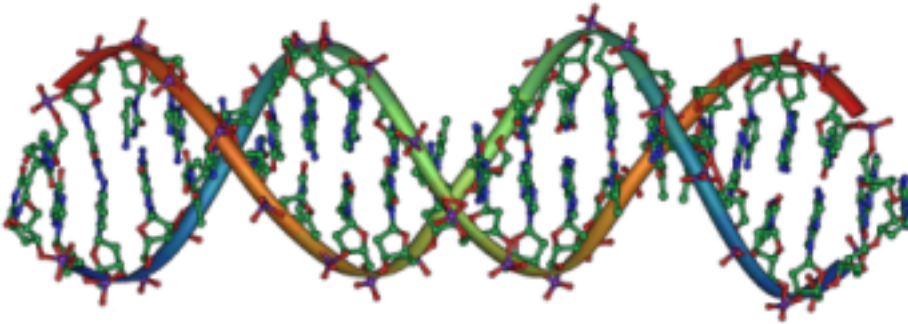


Bio Roll: Users Guide



Version 4.2.1 Edition

Bio Roll: Users Guide :



Version 4.2.1 Edition

Published Sep 2006

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Table of Contents

Preface	i
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	8
3.5. EMBOSS	9
3.6. Glimmer	9
3.7. Fasta.....	9
3.8. MrBayes	11
3.9. Phylip	12
3.10. T_Coffee.....	12
3.11. MPI-Blast	16
3.12. GROMACS	18
3.13. Bioperl.....	18
3.14. Biopython	19
A. Rocks Copyright	21
B. Third Party Copyrights and Licenses	22
B.1. Biopython	22
B.2. Clustal W	22
B.3. EMBOSS	22
B.4. FASTA	28
B.5. Glimmer.....	28
B.6. GROMACS.....	31
B.7. HMMER	37
B.8. mpiBlast.....	44
B.9. Mr.Bayes.....	45
B.10. NCBI.....	51
B.11. Perl Modules.....	51
B.12. Phylip.....	54
B.13. T_Coffee	54

List of Tables

1-1. Summary..... 1
1-2. Roll 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	4.2.1
Maintained By	Rocks Group
Architecture	i386, x86_64
Compatible with Rocks	4.2.1

Table 1-2. Roll Compatibility

Roll	Requires ^a	Optional ^b	Conflicts
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	
pbs		X	
sge		X	
viz		X	
web-server	X		

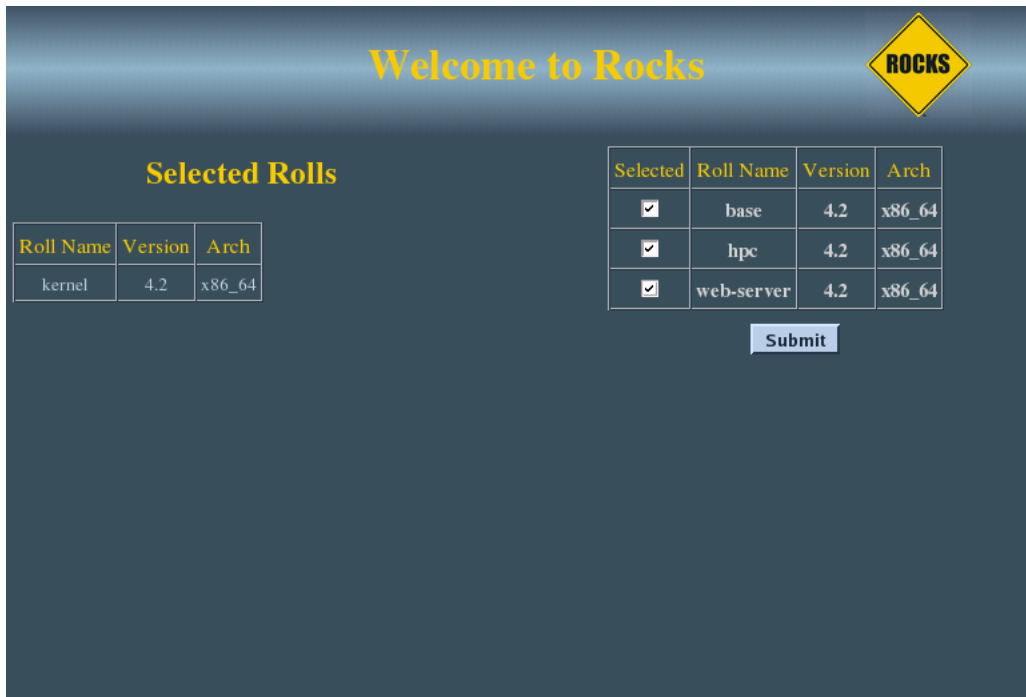
Notes:

- 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 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
# mount -o loop bio.iso /mnt/cdrom
# cd /home/install
# rocks-dist --install copyroll
# umount /mnt/cdrom
# 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](#)¹². 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](#)¹³. 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/`¹⁵. 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-3.00$ tar xzf patnt.tar.gz
```



This step is to be followed ONLY if you have downloaded 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.

```
-bash-3.00$ formatdb --help
```

gives you a list of all the available options to run `formatdb`. Make sure you choose the right set of options depending on whether you're running against a nucleotide database or a protein database.

- Create a test input file.

```
[nostramo@xxx ~]$ cat > test.txt
>Test
AGCTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAAGAGTGTCTGATAGCAGC
TTCTGAACTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGGTCACTAAATACTTTAACCAA
TATAGGCATAGCGCACAGACAGATAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTAAACGGTGCGGGCTGACGCGTACAGGAAACACAGAAAAAAG
CCCGCACCTGACAGTGCGGGCTTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTGAA
GTTCCGGCGGTACATCAGTGGCAAATGCAGAACGTTTTCTGCGTGTGCGGATATTCTGGAAAGCAATGCC
AGGCAGGGGCGAGTGGCCACCGTCTCTGCCCCGCCAAAATCACCAACCACCTGGTGGCGATGATTG
AAAAAACCATAGCGGCCAGGATGCTTTACCCAATATCAGCGATGCCGAACGTATTTTTGCCGAACTTTT
```

- Run the `blastall` program on the test input against the downloaded 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 patnt -p blastn -i test.txt -o result.txt
BLASTN 2.2.14 [May-07-2006]
```

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.

Database: Nucleotide sequences derived from the Patent division of GenBank

3,256,906 sequences; 1,981,990,296 total letters

Searching

Query= Test

(560 letters)

Sequences producing significant alignments:		Score	E
		(bits)	Value
emb CS104136.1	Sequence 1 from Patent WO2005049808	589	e-166
dbj DD171864.1	Method of producing amino acid by fermentation	589	e-166
dbj BD179435.1	Method and apparatus for recording sequential da...	589	e-166
dbj BD179434.1	Method and apparatus for recording sequential da...	589	e-166
dbj BD131253.1	Recording method and apparatus of sequence infor...	589	e-166
dbj BD131254.1	Recording method and apparatus of sequence infor...	589	e-166
dbj BD103218.1	Method and apparatus for recording information o...	589	e-166
dbj BD103217.1	Method and apparatus for recording information o...	589	e-166
dbj DD056878.1	Method and apparatus for recording information o...	589	e-166
dbj DD056877.1	Method and apparatus for recording information o...	589	e-166
gb AR384840.1	Sequence 1569 from patent US 6610836	262	1e-67
gb AR384989.1	Sequence 1718 from patent US 6610836	196	6e-48
dbj E38337.1	Process for producing L-methionine by fermentation	121	3e-25

The above example shows how to search for the test input in a patented 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 patnt -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/>¹⁶
- BLAST Help page on your cluster BLAST Help Page¹⁷
- BLAST Program selection Guide - http://www.ncbi.nlm.nih.gov/blast/BLAST_guide.pdf¹⁸

3.4. ClustalW

3.4.1. About

ClustalW is a multiple sequence alignment program. The version included with this distribution is v1.83.

3.4.2. Using ClustalW

ClustalW can be run at the command line as

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

```
*****  
***** CLUSTAL W (1.83) 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 here²⁰.

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 here²¹. 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

```
[nostramo@xxx ~]$ cat > test.txt
>Test
AGCTTTTTCATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAAAAAGAGTGTCTGATAGCAGC
TTCTGAACTGGTTACCTGCCGTGAGTAAATTTAAATTTTATTGACTTAGGTCACTAAATACCTTAACCAA
TATAGGCATAGCGCACAGACAGATAAAAAATTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTAACGGTGCGGGCTGACGCGTACAGGAAACACAGAAAAAAG
CCCGCACCTGACAGTGCAGGGCTTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTTGAA
GTTTCGGCGGTACATCAGTGGCAAATGCAGAACGTTTTTCTGCGTGTTGCCGATATTCTGGAAAGCAATGCC
AGGCAGGGGCGAGGTGGCCACCGTCTCTCTGCCCCGCCAAAATCACCAACCACCTGGTGGCGATGATTG
AAAAAACCATTAGCGGCCAGGATGCTTTACCCAATATCAGCGATGCCGAACGTATTTTTTGCCGAACTTTT
```

- 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/`.

```
[nostramo@xxx ~]$ fasta34
# fasta34
FASTA searches a protein or DNA sequence data bank
  version 3.4t25 Sept 2, 2005
Please cite:
  W.R. Pearson & D.J. Lipman PNAS (1988) 85:2444-2448

test sequence file name: test.txt
library file name: /opt/Bio/fasta/gst.seq
ktup? (1 to 6) [6] 1
Query library test.txt vs /opt/Bio/fasta/gst.seq library
searching /opt/Bio/fasta/gst.seq library

1>>>Test - 560 nt
vs /opt/Bio/fasta/gst.seq library

1287 residues in      1 sequences
Altschul/Gish params: n0: 560 Lambda: 0.192 K: 0.177 H: 0.360

FASTA (3.47 Mar 2004) function [optimized, +5/-4 matrix (5:-4)] ktup: 1
join: 77, opt: 62, open/ext: -12/-4, width: 16
```

```

Scan time: 0.000
Enter filename for results []: res.txt
How many scores would you like to see? [20]
The best scores are:
                                opt bits E(1)
gi|193547|gb|J04632|MUSGLUTA Mouse glutathione (1287) [r] 68 21.5 0.22
gi|193547|gb|J04632|MUSGLUTA Mouse glutathione (1287) [f] 62 19.8 0.55
More scores? [0]
Display alignments also? (y/n) [n] y
number of alignments [20]?

```

```

560 residues in 1 query sequences
1287 residues in 1 library sequences
Scomplib [34t25]
start: Wed Mar 15 16:14:08 2006 done: Wed Mar 15 16:14:51 2006
Total Scan time: 0.000 Total Display time: 0.010

```

Function used was FASTA [version 3.4t25 Sept 2, 2005]

Looking into res.txt we can see the results of our search.

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 page²².

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.

3.8.2. Usage

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

```
[nostromo@rocks-168 mrbayes]$ mb
```


MrBayes v3.1.2

(Bayesian Analysis of Phylogeny)

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.

MrBayes >

3.8.3. Further Information

A wealth of information about MrBayes is available at the following source - MrBayes Home Page²³

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 v3.65.

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 v3.84

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@rocks-168 ~]$ t_coffee /opt/Bio/t_coffee/example/sample_aln2.fasta

PROGRAM: T-COFFEE (Version_3.84)
-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]      Mlalign_id_pair Mslow_pair
-seq           S      [1]      /opt/Bio/t_coffee/example/sample_aln2.fasta
-aln           S      [0]
-method        S      [0]
.....
-dpa_keep_tmpfile FL     [0]      0
-dpa_debug     D      [0]      0
-multi_thread  S      [0]
-lib_list      S      [0]

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

INPUT SEQUENCES: 6 SEQUENCES [PROTEIN]
      Input File /opt/Bio/t_coffee/example/sample_aln2.fasta Seq lcms Length
```

```

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

```

```

COMPUTE PAIRWISE SIMILARITY [dp_mode: idscore_pair_wise]
[distance_matrix_mode: idscore]

```

```

      1cms  1cms_1 identity= 19% score=190
      1cms  2apr  identity= 34% score=340
      1cms  3app  identity= 31% score=310
      1cms  4ape  identity= 29% score=290
.....
      3app  4pep  identity= 34% score=340
      4ape  4pep  identity= 31% score=310

```

```

READ/MAKE LIBRARIES:[3]

```

```

      lalign_id_pair [method]
                [Submit Job][TOT= 15][ 0 %][ELAPSED TIME: 0
sec.][REMAINING TIME: -1073750336 sec.] [Submit Job][TOT= 15][100
%][ELAPSED TIME: 0 sec.][REMAINING TIME: 0 sec.]
                [Retrieve Job][TOT= 15][ 0 %][ELAPSED TIME: 0
sec.][REMAINING TIME: 6722352 sec.] [Retrieve Job][TOT= 15][100
%][ELAPSED TIME: 0 sec.][REMAINING TIME: 0 sec.]
      slow_pair [method]

```

```

.....
      Library Total Size: [5142]

```

```

      #### File Type=      WEIGHT Format= tc_weight Name= no | NOT PRODUCED
[WARNING:T-COFFEE:Version_3.84]

```

```

WEIGHTED MODE:t_coffee

```

```

      1cms 0.61
      1cms_1 3.32
      2apr 0.59
      3app 0.49
      4ape 0.48
      4pep 0.51

```

```

MAKE NEIGHBOR JOINING DENDROGRAM
      [MODE=nj][DONE]

PROGRESSIVE_ALIGNMENT [Tree Based]

      Group   7: [Group   6 (  1 seq)] with [Group   1 (  1 seq)]-->[Score=
53][Len=  176]
      Group   8: [Group   2 (  1 seq)] with [Group   7 (  2 seq)]-->[Score=
8][Len=  196]

.....

CLUSTAL FORMAT for T-COFFEE Version_3.84, CPU=0.94 sec, SCORE=34, Nseq=6,
Len=204

1cms          ---gevasvpltnyl-dsqyfgkiylgtpqgeftv-----lfdtgss
4pep          ----igdepleny1-dteyfgtigigtpaqdfv-----ifdtgss
1cms_1        y-tgslhwvpvtv---qqyw-----qftvdsvtisgvvaceggcqaieldtgs
2apr          a---gvgtvpmtdygndieyygqvvtigtpgkkfnl-----dfdtgss
4ape          s-tgsatttpids-l-ddayitpvqigtpaqtlnl-----dfdtgss
3app          aasgvatntptan---deeyitpvtig--gttlnl-----nfdtgsa
              *           *           :.:           :***:

.....

```

OUTPUT RESULTS

```

#### File Type= GUIDE_TREE Format=      newick Name= sample_aln2.dnd
#### File Type=      MSA Format=      clustalw Name= sample_aln2.aln

```

TIP: Change the Width of your MSA with the environment variable
ALN_LINE_LENGTH (all formats)

```

Command Line: t_coffee /opt/Bio/t_coffee/example/sample_aln2.fasta
[PROGRAM:T-COFFEE]

```

T-COFFEE Memory Usage: Current= 4.233 Mb, Max= 6.807 Mb

```

T-COFFEE CPU Usage: 940 millisec
[nostromo@rocks-168 ~]$

```

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 v1.4.0-May2006.

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.

```
[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          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
AGCTTTTTATTCTGACTGCAACGGGCAATATGTCTCTGTGTGGATTAAGAGTGTCTGATAGCAGC
TTCTGAACTGGTTACCTGCCGTGAGTAAATTTTATTTGACTTAGGTCACTAAATACTTTAACC
TATAGGCATAGCGCACAGACAGATAAAATTTACAGAGTACACAACATCCATGAAACGCATTAGCACCACC
ATTACCACCACCATCACCATTACCACAGGTAACGGTGCAGGCTGACGCGTACAGGAAACACAGAAAAAG
CCCGCACCTGACAGTGCAGGCTTTTTTTTTTCGACCAAAGGTAACGAGGTAACAACCATGCGAGTGTGAA
GTTTCGGCGGTACATCAGTGGCAAATGCAGAACGTTTTCTGCGTGTGCGGATATTCTGGAAAGCAATGCC
AGGCAGGGGCGAGTGGCCACCCTCTCTGCCCCGCCAAAATCACCACCCACCTGGTGGCGATGATTG
AAAAAACCATTAGCGGCCAGGATGCTTTACCCAATATCAGCGATGCCGAACGTATTTTTGCGCAACTTTT

```

```

[nostrromo@xxx mpiblast]$ /opt/mpich/gnu/bin/mpirun -np 4 /opt/Bio/mpiblast/bin/mpiblast -d ecoli.n

```

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

$MPI_DIR/bin/mpirun -np $NSLOTS -machinefile $TMP/machines /opt/Bio/mpiblast/bin/mpiblast -d ecoli

```

- Run

```

[nostrromo@xxx ~]$ qsub -pe mpich 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. MPICH 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

3.13. 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 Docs³⁵.

3.13.3. Further Information

Further information about bioperl is available at the Bioperl home page³⁶

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 documentation³⁷.

3.14.3. 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://www.cbcb.umd.edu/software/glimmer/>
12. <http://hmmer.wustl.edu/>
13. <ftp://ftp.genetics.wustl.edu/pub/eddy/hmmer/CURRENT/Userguide.pdf>
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18. http://www.ncbi.nlm.nih.gov/blast/BLAST_guide.pdf
19. <http://emboss.sourceforge.net/>
20. <http://emboss.sourceforge.net/support/>
21. <http://www.cbcb.umd.edu/software/glimmer/glim302notes.pdf>
22. <http://fasta.bioch.virginia.edu/>
23. <http://mrbayes.csit.fsu.edu/index.php>
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/>
32. <http://www.gromacs.org/gromacs/documentation/documentation.html>
33. [/gromacs/online.html](http://www.gromacs.org/gromacs/online.html)
34. [/gromacs/gmxfaq.html](http://www.gromacs.org/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
www.rocksclusters.org
version 4.2.1 (Cydonia)

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```

```
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Notes

1. <http://cvs.rocksclusters.org>