PROGRAM NAME: maskedfastacoords.pl

LICENSE: GNU General Public License (GNU-GPL)

LAST UPDATE: September 25, 2001

DESCRIPTION: Retrieving positions for masked regions of masked sequences in

fasta format. Program can also output those coords in GFF format,

where you can define several fields from command-line.

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1 Introduction

1.1 Program description

Retrieving positions for masked regions of masked sequences in fasta format. Program can also output those coords in GFF format, where you can define several fields from command-line.

1.2 Input

The following example illustrates both, "classical" (using 'N') and soft (using lowercase letters), masking of fasta sequences as they can be obtained from a program such REPEATMASKER¹. Sequence is splitted into 50 chararacter-length lines.

The sequence 'Masked_fasta_sequence' is 325 nucleotides long. Masking is distributed in the following coords:

100	N-masking
188	soft-masking
200	N-masking
245	soft-masking
284	soft-masking
278	n-masking (soft)
	188 200 245 284

1.3 Output

The program can produce three different outputs returning the coords of the sequence masked segments: only "classical" masking ('N' or 'n'), only soft-masking ('[a-z]'), both. From the previous example we must obtain the following results:

Basic-masking			Soft-masking		Merged-masking			
51	100	N-masking	128	188	soft-masking	51	100	N-masking
189	200	N-masking	212	245	soft-masking	128	188	soft-masking
274	278	n-masking	269	284	soft-masking	189	200	N-masking
		C			C	212	245	soft-masking
						269	273	soft-masking
						274	278	n-masking (soft)
						279	284	soft-masking

1.4 To Do

- We can define mask checking as three different subroutines that will be called by reference, so that a variable name (called for instance \$test) will be set depending on command-line options.[Section 3.2, page 7]

¹http://www.genome.washington.edu/UWGC/analysistools/repeatmask.htm

2 Implementation

2.1 Program outline

TO DO

• This is a first draft of the maskedfastacoords.pl.

```
\langle maskedfastacoords 2a \rangle \equiv
2a
         ⟨PERL shebang 9a⟩
         #
         # MODULES
         #
         ⟨Use Modules 2f⟩
         # VARIABLES
         ⟨Global Vars 2g⟩
         # MAIN LOOP
         ⟨Main Loop 2h⟩
         # FUNCTIONS
         ⟨Functions 3b⟩
2b
       \langle Program Info 2b \rangle \equiv
         my $PROGRAM = 'getfastamasked.pl';
         my $VERSION = '0.1_alpha';
2c
       \langle Prog\ USAGE\ 2c \rangle \equiv
         #$PROGRAM [options] < fasta_file > coords_file
       \langle Prog\ DESC\ 2d \rangle \equiv
2d
         #Retrieving masked regions coords from fasta files.
       ⟨Program Description 2e⟩≡
2e
         #
              ⟨Prog USAGE 2c⟩
         #
              ⟨Prog DESC 2d⟩
         #
         #
2f
       \langle Use\ Modules\ 2f\rangle \equiv
         ⟨Use Modules - Benchmark 9c⟩
         ⟨Use Modules - Getopt 3e⟩
         ⟨Use Modules - Bio::Seq 3c⟩
       ⟨Global Vars 2g⟩≡
2g
         ⟨Boolean 9b⟩
         (Stderr subs vars 11b)
         my ($id,$seq) = (",");
```

```
\langle Main Loop 2h \rangle \equiv
2h
        &parse_cmdline(); # PROG-START
        &report('PROG-FINISH',&timing($T));
        exit(0);
3a
      \langle messages: program running 3a \rangle \equiv
         'PROG-START'
                          => "$line$s\n$s Running $PROGRAM\n$s".
                              "$s HOST: $host".
                              "$s USER: $USER".
                              "$s DATE: $DATE\n$s\n$line$s" ,
         'PROG-FINISH' => "$s\n$line$s\n$s $PROGRAM FINISHED\n$s".
                              "$s TOTAL TIME: \%s\n$line" ,
      \langle Functions 3b \rangle \equiv
3b
        (Parsing command line options 4a)
        (Main program function 6f)
        ⟨Common PERL subs - Benchmark 9e⟩
        ⟨Common PERL subs - STDERR 10f⟩
```

2.2 BIOPERL modules

Bio::Seq² is the BIOPERL³ main sequence object while Bio::SeqIO⁴ is the BIOPERL support for sequence input/output into files. BIOPERL is also available from CPAN⁵.

3 Program functions

3.1 Processing command-line options

```
3e     ⟨Use Modules - Getopt 3e⟩≡
          use Getopt::Long;
          Getopt::Long::Configure qw/ bundling /;

3f     ⟨perl requires - Getopt 3f⟩≡
          "Getopt::Long" - processing command-line options.
```

²http://bioperl.org/Core/POD/Bio/Seq.html

³http://bioperl.org/

⁴http://bioperl.org/Core/POD/Bio/SeqIO.html

⁵http://search.cpan.org/search?dist=bioperl

See 'man Getopt::Long' for further info about this package.

```
4a
     \langle Parsing\ command\ line\ options\ 4a \rangle \equiv
       sub parse_cmdline() {
            $SIG{__WARN__} = sub { &warn('UNKNOWN_CL_OPTION',$T,$_[0]) };
            GetOptions(
                         ⟨command-line options - masking 5c⟩
                         ⟨command-line options - fasta 6b⟩
                         ⟨command-line options - GFF 6d⟩
                         ⟨command-line options with exit 4c⟩
                         ) | (&warn('CMD_LINE_ERROR',$T), exit(1));
            $SIG{__WARN__} = 'DEFAULT';
            &report("PROG-START");
        } # parse_cmdline
4h
     ⟨warnings: command-line 4b⟩≡
        'UNKNOWN_CL_OPTION' =>
          $Warn."Error trapped while processing command-line:\n".(" "x16)."\%s\n",
        'CMD_LINE_ERROR' =>
          $spl.$spw." Please, check your command-line options!!!\n".$Error."\n".
          spw." ".("."x12)." Type \"maskedfastacoords.pl -h\" for help.\n".spl,
```

3.1.1 Defining help and auxiliary code chunks

The following command-line checkings look for those options exiting the program: 'help' and 'version'. Both need to output to screen without any other message/warning being displayed at the same time.

```
\langle command\text{-line options with exit } 4c \rangle \equiv
4c
         "version"
                        => \&prt_version,
         "h|help|?" => \&prt_help,
       \langle command-line\ help\ -\ help\ 4d \rangle \equiv
4d
         -h, -help
                                      Shows this help.
         -version
                                      Shows current version and exits.
4e
       \langle Parsing\ command\ line\ options\ 4a \rangle + \equiv
         sub prt_version() {
              &report('SHOW_VERSION', $PROGRAM, $VERSION);
               exit(1);
         } # prt_version
4f
       \langle messages - parsing command-line 4f \rangle \equiv
         'SHOW VERSION' => $sp."### \%s - \%s\n".$sp,
           Printing command-line help to STDERR:
       \langle Parsing\ command\ line\ options\ 4a \rangle + \equiv
4g
         sub prt_help() {
              print STDERR «"+++EndOfHelp+++";
         PROGRAM:
                                          $PROGRAM - $VERSION
               ⟨Prog DESC 2d⟩
         IISAGE:
                       ⟨Prog USAGE 2c⟩
         DESCRIPTION:
```

```
Retrieving positions for masked regions of masked sequences
      in fasta format. Program can also output those coords in GFF
      format, where you can define several fields from command-line.
 REQUIRES:
      (perl requires help 5a)
 COMMAND-LINE OPTIONS:
      ⟨command-line help 5b⟩
  BUGS:
            Report any problem to 'jabril\@imim.es'.
 AUTHOR:
            $PROGRAM is under GNU-GPL (C) 2000 - Josep F. Abril
  +++EndOfHelp+++
      exit(1);
  } # prt_help
\langle perl \ requires \ help \ 5a \rangle \equiv
  $PROGRAM needs the following Perl modules
  installed in your system, we used those available
  from the standard Perl distribution. Those that
 are not in the standard distribution are marked
 with an '(*)', in such cases make sure that you
 already have downloaded them from CPAN
  (http://www.perl.com/CPAN) and installed.
    ⟨perl requires - BioPerl 3d⟩
    ⟨perl requires - Getopt 3f⟩
    (perl requires - Benchmark 9f)
\langle command\text{-line help 5b} \rangle \equiv
 A double dash on itself "-" signals end of the options
  and start of file names (if present). After double dash,
 you can use a single dash "-" as STDIN placeholder.
 Available options and a short description are listed here:
  + General options:
    ⟨command-line help - help 4d⟩
    (command-line help - masking 6a)
    ⟨command-line help - fasta 6c⟩
  + GFF output:
    ⟨command-line help - GFF 6e⟩
3.1.2 Defining command-line options
\langle command\text{-line options} - masking 5c \rangle \equiv
  "s|soft-masked" => ,
  "m|merge-masked" => ,
```

5a

5b

5c

```
6a
      \langle command\text{-line help - masking 6a} \rangle \equiv
        -s, -soft-masked
                                 Default is looking for "N" masked sequence
                                   segments. This option distinguish between
                                   upper/lower-case and assumes lower-case to
                                   define masked regions too (so called soft-masking).
                                  Default is differentiating classical-masking
        -m, -merge-masked
                                   (with "N"s) from soft-masking. This option merges
                                   both as if they were the same masking type
                                   (it also enables soft-masking search so previous
                                   option is not required when passing this one).
      \langle command-line\ options\ -\ fasta\ 6b \rangle \equiv
        "l|large-fasta" => ,
      \langle command-line\ help\ -\ fasta\ 6c \rangle \equiv
6c
                                  For large genomic sequence you can enable
        -1, -large-fasta
                                   Bio::SeqIO to work with temporary files
                                   avoiding memory overload (though it makes
                                   the script to run slowly).
      \langle command-line\ options\ -\ GFF\ 6d\rangle \equiv
6d
        "g|gff"
                         => ,
        "seq-name=s"
                         =>
        "source=s"
                         => ,
        "f|feature=s"
                         => ,
        "strand=s"
                         => ,
        group=s"
                         => ,
6e
      \langle command-line\ help\ -\ GFF\ 6e \rangle \equiv
        -g, -gff
                                  Output in GFF format (default coords).
                                 Sets sequence GFF field (default "noname").
        -seq-name <string>
                                 Sets source GFF field (default "masked").
        -source <string>
        -f, -feature <string> Sets feature GFF field (default "masked").
                                 Sets strand GFF field (default ".").
        -strand <string>
        -group <string>
                                 Sets group GFF field (default none).
     3.2
           Main program function
6f
      \langle Main\ program\ function\ 6f \rangle \equiv
        sub main() {
            my $seqin = Bio::SeqIO->new(-format => 'FASTA', -fh => \*STDIN);
            while (my $sequence = $seqin->next_seq()) {
                 my ($sid,$len,$seq,@nuc,@coords,$masked_flg,$match,$msk_num);
                 @coords = ();
                 (Setting sequence variables from fasta record 6g)
                 (Finding masked regions coords 7a)
                 (Writing masked regions coords in GFF 7b)
             }; # while
        } # main
      \langle Setting \ sequence \ variables \ from \ fasta \ record \ 6g \rangle \equiv
6g
       print STDERR "### READING FASTA....\n";
        $sid = $sequence->display_id();
        $len = $sequence->length();
        $seq = $sequence->seq();
```

TO DO

• We can define mask checking as three different subroutines that will be called by reference, so that a variable name (called for instance \$test) will be set depending on command-line options.

```
\langle Finding\ masked\ regions\ coords\ 7a \rangle \equiv
7a
       print STDERR "###
                                    PARSING SEQUENCE: $sid ($len bp)\n";
       @nuc = split //og, $seq;
       (\$masked flg,\$match) = (\$F,\$F) ;
       for (my n = 0; n <= \mu c; n <= \mu c;
            match = ( nuc[n] = /[NnXx]/o ) ? T : F;
            ( !$masked_flg && $match ) && do {
                $masked_flg = $T ;
                # $n contains the last non-masked nucleotide
                push @coords, ($n + 1);
                next;
            };
            $masked_flg && do {
                $match && (next);
                $masked_flg = $F ;
                # $n contains the last masked nucleotide now
                push @coords, $n;
           };
       }; # for nuc in $seq
       # if last nucleotide is masked, previous loop not includes its coord.
       $masked_flg &&( push @coords, $len);
7b
     \langle Writing \ masked \ regions \ coords \ in \ GFF \ 7b \rangle \equiv
       $msk_num = scalar(@coords) / 2;
       print STDERR "###
                                   WRITING GFF COORDS: $msk_num masked regions found.\n";
       for (my n = 0; n <= \#coords; n+=2) {
           my GFFstring = ("\s\t" x 5).(".\t" x 3).".\n";
           printf STDOUT $GFFstring, $sid, "masked", "masked", @coords[$n..($n + 1)];
       }; # for coords in @coords
```

A empty appendix section

A.1 empty appendix subsection

B Common code blocks

B.1 PERL scripts

```
9a
      \langle PERL \ shebang \ 9a \rangle \equiv
        #!/usr/bin/perl -w
        # This is perl, version 5.005_03 built for i386-linux
        ⟨Program Description 2e⟩
        ⟨GNU License 12⟩
        (Version Control Id Tag 11f)
        use strict;
        # BEGIN {
             ⟨Program Info 2b⟩
             my $DATE = localtime;
             my $USER = defined($ENV{USER}) ? $ENV{USER} : 'Child Process';
             my $host = 'hostname';
             chomp($host);
        # } # BEGIN
9b
      \langle Boolean 9b \rangle \equiv
        my (\$T,\$F) = (1,0); \# for 'T'rue and 'F'alse
```

B.1.1 Timing our scripts

The 'Benchmark' module encapsulates a number of routines to help to figure out how long it takes to execute a piece of code and the whole script.

```
9c ⟨Use Modules - Benchmark 9c⟩≡
use Benchmark;
⟨Timer ON 9d⟩
```

See 'man Benchmark' for further info about this package. We set an array to keep record of timing for each section.

```
\langle Timer\ ON\ 9d \rangle \equiv
9d
        my @Timer = (new Benchmark);
      \langle Common\ PERL\ subs - Benchmark 9e \rangle \equiv
9e
        sub timing() {
             push @Timer, (new Benchmark);
             # partial time
              $_[0] ||
                   (return timestr(timediff($Timer[$\pi\timer],$Timer[($\pi\timer - 1)])));
             # total time
             return timestr(timediff($Timer[$#Timer],$Timer[0]));
         } # timing
9f
      \langle perl \ requires - Benchmark \ 9f \rangle \equiv
         "Benchmark" - checking and comparing running times of code.
```

B.1.2 Printing complex Data Structures

With 'Data:: Dumper' we are able to pretty print complex data structures for debugging them.

```
9g
       \langle Use\ Modules - Dumper\ 9g \rangle \equiv
         use Data::Dumper;
         local $Data::Dumper::Purity = 0;
         local $Data::Dumper::Deepcopy = 1;
      B.1.3
             Common functions
10a
       \langle Skip\ comments\ and\ empty\ records\ 10a \rangle \equiv
         next if /^{\#/0};
         next if /^\s*$/o;
         chomp;
10b
       \langle Common\ PERL\ subs - Min\ Max\ 10b \rangle \equiv
         sub max() {
             my $z = shift @_;
              foreach my $1 (@_) { $z = $1 if $1 > $z };
         } # max
         sub min() {
             my $z = shift @_;
              foreach my 1 (@) \{ z = 1 \text{ if } 1 < z \};
              return $z;
         } # min
10c
       \langle Common\ PERL\ subs - Text\ fill\ 10c \rangle \equiv
         sub fill_right() { [0].([2] x ([1] - length([0]))) }
                               (\$[2] \times (\$[1] - length(\$[0])).\$[0]
         sub fill_left()
         sub fill_mid()
             my $1 = length($_[0]);
             my $k = int(($_[1] - $1)/2);
              (\$_[2] \times \$k).\$_[0].(\$_[2] \times (\$_[1] - (\$1+\$k)));
         } # fill_mid
          These functions are used to report to STDERR a single char for each record processed (useful for reporting
      parsed records).
10d
       ⟨Common PERL subs - Counter 10d⟩≡
         sub counter { # $_[0]~current_pos++ $_[1]~char
              print STDERR "$_[1]";
              ((\$_[0] \$ 50) == 0) \& (print STDERR "[".&fill_left(\$_[0],6,"0")."]\n");
         } # counter
```

B.1.4 Common functions for reporting program processes

sub counter_end { # \$_[0]~current_pos

} # counter_end

 $\langle Global\ Vars - Counter\ 10e \rangle \equiv$

10e

Function 'report' requires that a hash variable '%Messages' has been set, such hash contains the strings for each report message we will need. The first parameter for 'report' is a key for that hash, in order to retrieve the message string, the other parameters passed are processed by the sprintf function on that string.

\$_[1]~char

 $((\$_{0}) \$ 50) != 0) \& (print STDERR "[".&fill_left(\$_{0}, 6, "0")."]\n");$

```
10f ⟨Common PERL subs - STDERR 10f⟩≡
sub report() { print STDERR sprintf($Messages{ shift @_ },@_) }
```

my (\$n,\$c); # counter and char (for &counter function)

The same happens to 'warn' function which also uses the hash variable '%Messages' containing the error messages.

```
11a
       \langle Common\ PERL\ subs - STDERR\ 10f \rangle + \equiv
         sub warn() { print STDERR sprintf($Messages{ shift @_ }, @_) }
          Those are accessory variables for the messages strings:
11b
       \langle Stderr subs vars 11b \rangle \equiv
         my $1ine = ('#' \times 80)."\n";
         my $s = '### ';
         my $Error = "\<\<\ ERROR \>\>\ ";
         my $Warn = "\<\< WARNING \>\> ";
         my $spl
                     = "\<\<\-\-\-\-\-\-\-\-\-\>\>\n";
                     = "\<\<\<
                                            \>\>\> ";
         my $spw
          And here the main messages hash:
11c
       \langle Stderr subs vars 11b \rangle + \equiv
         my %Messages = (
              # ERROR MESSAGES
              (warnings: command-line 4b)
              # WORKING MESSAGES
              (messages: program running 3a)
             ); # %Messages
```

B.2 BASH scripts

```
11d
       \langle BASH \ shebang \ 11d \rangle \equiv
        #!/usr/bin/bash
        # GNU bash, version 2.03.6(1)-release (i386-redhat-linux-gnu)
         (Version Control Id Tag 11f)
        SECONDS=0 # Reset Timing
        # Which script are we running...
        L="###############"
         { echo "$L$L$L$L";
           echo "### RUNNING [$0]";
           echo "### Current date: 'date'";
           echo "###"; } 1>&2;
11e
       \langle BASH \ script \ end \ 11e \rangle \equiv
         { echo "###"; echo "### Execution time for [$0] : $SECONDS secs";
           echo "$L$L$L$L";
           echo ""; } 1>&2;
         #
        exit 0
```

B.3 Version control tags

This document is under Revision Control System (RCS). The version you are currently reading is the following:

```
11f ⟨Version Control Id Tag 11f⟩≡
# $Id: maskedfastacoords.nw,v 1.2 2001/09/19 19:45:27 jabril Exp $
```

B.4 GNU General Public License

12 $\langle GNU \ License \ 12 \rangle \equiv$

```
# #-----#
                        maskedfastacoords
                                                               #
# #-----#
#
    Remember to put a short description of your script here...
#
     Copyright (C) 2001 - Josep Francesc ABRIL FERRANDO
# This program is free software; you can redistribute it and/or modify
# it under the terms of the GNU General Public License as published by
# the Free Software Foundation; either version 2 of the License, or
# (at your option) any later version.
# This program is distributed in the hope that it will be useful,
# but WITHOUT ANY WARRANTY; without even the implied warranty of
# MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
# GNU General Public License for more details.
# You should have received a copy of the GNU General Public License
# along with this program; if not, write to the Free Software
# Foundation, Inc., 675 Mass Ave, Cambridge, MA 02139, USA.
# #-----#
```

C Extracting code blocks from this document

From this file we can obtain both the code and the documentation. The following instructions are needed:

C.1 Extracts Script code chunks from the NOWEB file

Remember when tangling that '-L' option allows you to include program line-numbering relative to original NOWEB file. Then the first line of the executable files is a comment, not a shebang, and must be removed to make scripts runnable.

C.2 Extracting different Config Files

```
13c ⟨tangling 13a⟩+≡
notangle -R"root" $WORK/$nwfile.nw | \
cpif $DATA/root_config ;
```

C.3 Extracting documentation and LATEX'ing it

```
13d
      \langle tangling 13a \rangle + \equiv
        notangle -Rweaving $WORK/$nwfile.nw | cpif $WORK/nw2tex ;
        notangle -RLaTeXing $WORK/$nwfile.nw | cpif $WORK/ltx ;
        chmod a+x $WORK/nw2tex $WORK/ltx;
      \langle tangling\ complementary\ LaTeX\ files\ 13e \rangle \equiv
13e
        notangle -R"HIDE: LaTeX new definitions" $WORK/$nwfile.nw | cpif $DOCS/defs.tex;
        notangle -R"HIDE: TODO" $WORK/$nwfile.nw | cpif $DOCS/todo.tex ;
13f
      \langle weaving 13f \rangle \equiv
        ⟨BASH shebang 11d⟩
        # weaving and LaTeXing
        ⟨BASH Environment Variables 14b⟩
         ⟨tangling complementary LaTeX files 13e⟩
        noweave -v -t4 -delay -x -filter 'elide "HIDE: *"' \
                  $WORK/$nwfile.nw | cpif $DOCS/$nwfile.tex ;
        # noweave -t4 -delay -index $WORK/$nwfile.nw > $DOCS/$nwfile.tex
        pushd $DOCS/ ;
        latex $nwfile.tex ;
        dvips $nwfile.dvi -o $nwfile.ps -t a4;
        popd;
        (BASH script end 11e)
```

```
14a
      ⟨LaTeXing 14a⟩≡
        ⟨BASH shebang 11d⟩
        # only LaTeXing
        (BASH Environment Variables 14b)
       pushd $DOCS/;
       echo "### RUNNING LaTeX on $nwfile.tex" 1>&2;
        latex $nwfile.tex ;
       latex $nwfile.tex;
       latex $nwfile.tex ;
       dvips $nwfile.dvi -o $nwfile.ps -t a4;
        # pdflatex $nwfile.tex ;
       echo "### CONVERTING PS to PDF: $nwfile" 1>&2;
       ps2pdf $nwfile.ps $nwfile.pdf ;
       popd ;
        ⟨BASH script end 11e⟩
```

C.4 Defining working shell variables for the current project

```
14b
      ⟨BASH Environment Variables 14b⟩≡
        #
        # Setting Global Variables
        WORK="/home/ug/jabril/development/softjabril/maskedfastacoords" ;
        BIN="$WORK/bin";
        PARAM="$BIN/param" ;
        DOCS="$WORK/docs";
        DATA="$WORK/data" ;
        nwfile="maskedfastacoords" ;
        export WORK BIN PARAM DOCS DATA nwfile;
14c
      \langle tangling 13a \rangle + \equiv
        # BASH Environment Variables
        notangle -R'BASH Environment Variables' $WORK/$nwfile.nw | \
                  cpif $WORK/.bash_VARS ;
        source $WORK/.bash_VARS ;
```