Perl for Crystallographers – FoFc example code

This **Perl** program will reformat FoFc structure factor data from a very complex *condensed* paginated tabulated format[4] into a fully formatted XTAL3.2 input file[5], with the hkl input lines formatted appropriately for SHELX76.

The program makes use of **Perl**'s file manipulation features as well as powerful string and array control capabilities.

Program Listing

```
#!/usr/bin/perl

$name=$ARGV[0];
($code,$alt)=split(/\//,$name);
$line=`grep $code ../REFINE.CODES`;
($code,$name,$user)=split(/\t/,$line);
$code2=$code; $code2=~tr/[A-Z]/[a-z]/;

print "TITLE  $code - \"$name\" by $user\n";
print "compid $code2\n";
print "master yes\n\n";
print "ADDREF\nreduce ftof2\nhklin hkl frel sigf\nsetid hkl\n";

$h="0"; $k="0"; $l="0"; $page=1; $line=1;
do{
 while(pop(@page)){}
 while(<>){
   next if(length($_) < 10);
   next if(/^#/);
   next if(! /\w/);
   if(/Page(| )([0-9]+)/) {last if(int($2) > $page);}
   next if($_=~/[A-Z]/);
   push(@page,$_);
 }
 $n=1;
 while($n < 5) {
  print STDERR "Page $page column $n\n";
  foreach $_ (@page) {
    $i=i+20*$n;
    $HKL=substr($_,$i,18);
    next if(length($HKL) < 8);
    if($HKL=~/l/) {
      ($h,$k,$l)=split(/,/,$HKL);
      $h=~s/\s//g;
      $k=~s/\s//g;
      $l=~s/\s//g;
      if($l ne "l") {print "Error:($h,$k,$l) \$l ne \"l\"\t\t\"$HKL\"\n";}
      next;
    }
    $HKL=~s/^\s*//;
    $HKL=~s/ +/,/g;
    ($l,$fo,$fc,$sf)=split(/,/,$HKL);
    $hkl=sprintf("%4s%4s%4s%10.2f%8.2f",$h,$k,$l,$fo/10.0,$sf/100.0);
    print "$hkl\n";
  }
  $n++;
 }
 $page=$2;
}while(!eof());
print "setid\n\nFINISH\n";
```

[1] http://www.iucr.ac.uk/iucr-top/welcome.html
[2] int.index.html
[3] int.perl.html
[4] int.perl.hkl.code.html#table
[5] int.perl.hkl.code.html#output

Selection of Example Input FoFc Tables[6]

```
DPPM-H OXO ANION                                                    Page 1
    Columns are  10Fo   10Fc   100Sig, * for Insignificant
  l  kFo   Fc  Sig    l  kFo   Fc  Sig    l  kFo   Fc  Sig    l  kFo   Fc  Sig
   -11,  0, l        10   58  506 3311*   5   68  274 2408*  12  163   94  328
  2  194  192  320   11   57  506 3415*   6  362  304  200   13  110   94 1457*
  4  275  289  234     -11,  5, l         7  196  149  336   14   57   94 2294*
  6  176  177  336    1  125  506 1312*   8   68  149 3105*    -10,  5, l
  8   62  177 2600*   2   61  506 3167*   9  480  494  186    1   99   94 2037*
 10  370  377  171    3  169  153  359   10   71  494  857*   2  360  361  229
   -11,  1, l         4  132  153 2006*  11  531  539  160    3  102  361 1798*
  1  273  294  237    5   62  153 3013*  12   64  539  845*   4  600  588  171
  2   99  294  585*   6  437  481  192   13  365  394  186    5  193   92  373
  3  315  328  229    7   66  481 2827*  14   59  394 2489*   6  508  564  200
  4  157  328  404*   8  475  534  178     -10,  2, l         7  127  564 1831*
  5  162  174  374    9   59  534 3385*   1   71  394 2890*   8  501  559  193
  6   64  174  951*  10  338  391  210    2  320  282  225    9  427  432  198
  7   63  174 3407*    -11,  6, l         3   68  282 3309*  10  229  263  301
  8  128  174  468*   1   59  391 3382*   4  122  282  561*  11  363  305  196

 .... rest cut off for brevity
```

Note that the flow of incremental hkl values goes down each column of an page in turn before starting on the next page, so the script needs to read in one page at a time and then read each column in turn before proceeding to the next page, all the time keeping track of the current **h** and **k** values.

Selection of Example Output XTAL Format[7]

```
TITLE  XXX012 - "sharp7" by P.R.Sharp
compid xxx012
master yes

ADDREF
reduce ftof2
hklin hkl frel sigf
setid hkl
   0   0  10      5.80   33.11
   0   0  11      5.70   34.15
 -11   5   1     12.50   13.12
 -11   5   2      6.10   31.67
 -11   5   3     16.90    3.59

 .... lines cut here for brevity

  11   4   1     14.60    3.73
  11   4   2      5.70   23.88
  11   5   0      5.90   24.64
  11   5   1      5.80   32.65
  11   6   0     31.50    2.22
setid

FINISH
```

[Index[8]] [FoFc example[9]] [Registration Form[10]] [WDC9 Form[11]] – 10th Sept. 1996 – © B. Craig Taverner[12] **– Not to be copied or reproduced without permission –** Author's current manuscript[13]

6 int.perl.hkl.table.html
7 int.perl.hkl.output.html
8 int.index.html
9 int.perl.hkl.code.html
10 http://www.gh.wits.ac.za/indaba/reg-indaba.html
11 http://occam.gh.wits.ac.za/iucr/docs/wdc9t.html
12 http://www.gh.wits.ac.za/craig/
13 http://www.gh.wits.ac.za/~craig/aiucr/int.perl.code.html