

MorphCol Supplement 2 (14.7.2005)

3.3. Polar fourier analysis of outlines

Polar fourier analysis is a method of analyzing shapes of a curve, in our case closed, plane curves. The shape of foraminiferal tests is estimated by expansion of the periphery as a function of angle θ about the test's centroid (center of gravity) by a Fourier series. The radius R at angle θ (polar coordinates) is then given by the formula (Davis, 1973)

$$R(\theta) = R_0 + \sum_{k=1}^{\infty} [A_k \cos(k\theta) + B_k \sin(k\theta)]$$

where θ denotes the polar angle from an arbitrary reference line, R_0 is the average radius of a circle, which best fits the outline, k is the harmonic number, and the A_k 's and B_k 's are the amplitudes of the trigonometric terms of the harmonic function with the number k (the harmonic function is the sum between the angular brackets).

Given N radii R_j at equiangular distances about the test's center of gravity, the amplitudes of each harmonic function can be determined by

$$R_0 = (1/N) \sum_{j=1}^N R_j \quad \text{and}$$

$$A_k = (2/N) \sum_{j=1}^N R_j \cos(k\theta_j) \quad \text{and} \quad B_k = (2/N) \sum_{j=1}^N R_j \sin(k\theta_j)$$

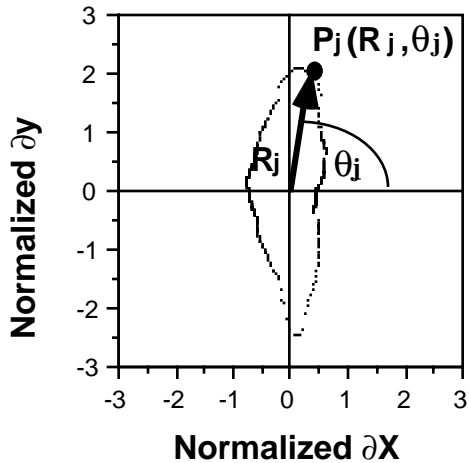


Figure 12.

(Figure 12) Polar coordinates of point P_j of an normalized outline (mean radius normalization method).

Prior to harmonic analysis the original outline must transformed with respect to the gravity center, the distances between points must be at equal angular distances, and the outline should be normalized using the method of mean radius normalization.

These steps are identical to the first steps with Trace_33.batch.out and Sprep53.out described in sections 3.1 through 3.2.2 above.

New steps in Fourier analysis are described in the following:

In order to avoid rotational bias when comparing phases of power spectra between different curves, all outlines need to be in homologous position and should therefore have identical starting points and identical directional sense of the outline extraction. While the directional sense is already given in program Trace_33.batch out, the starting point is kept constant by manually placing the apex of the foraminiferal shell constantly to the horizontal line at 240 pixels on the imaging frame (e.g. placement of the apex to the middle of the image).

Maximum homologous position between a series of outlines is achieved with program Homolo31.out (in batch mode), which rotates a given outline around the center of gravity against a predefined reference outline until maximum correlation is attained. The homologized outlines can then either be averaged to a single curve (using program Averou3.out) or directly fed to program Harman2.out (which runs in batch mode), and which then calculates the coefficients of harmonic functions for each outline. If desired, the outline can be reconstructed from its fourier coefficients by inverse Fourier transformation using program Recon1.out (see flow scheme illustrated in Figure 13a).

Flow-scheme for harmonic analysis

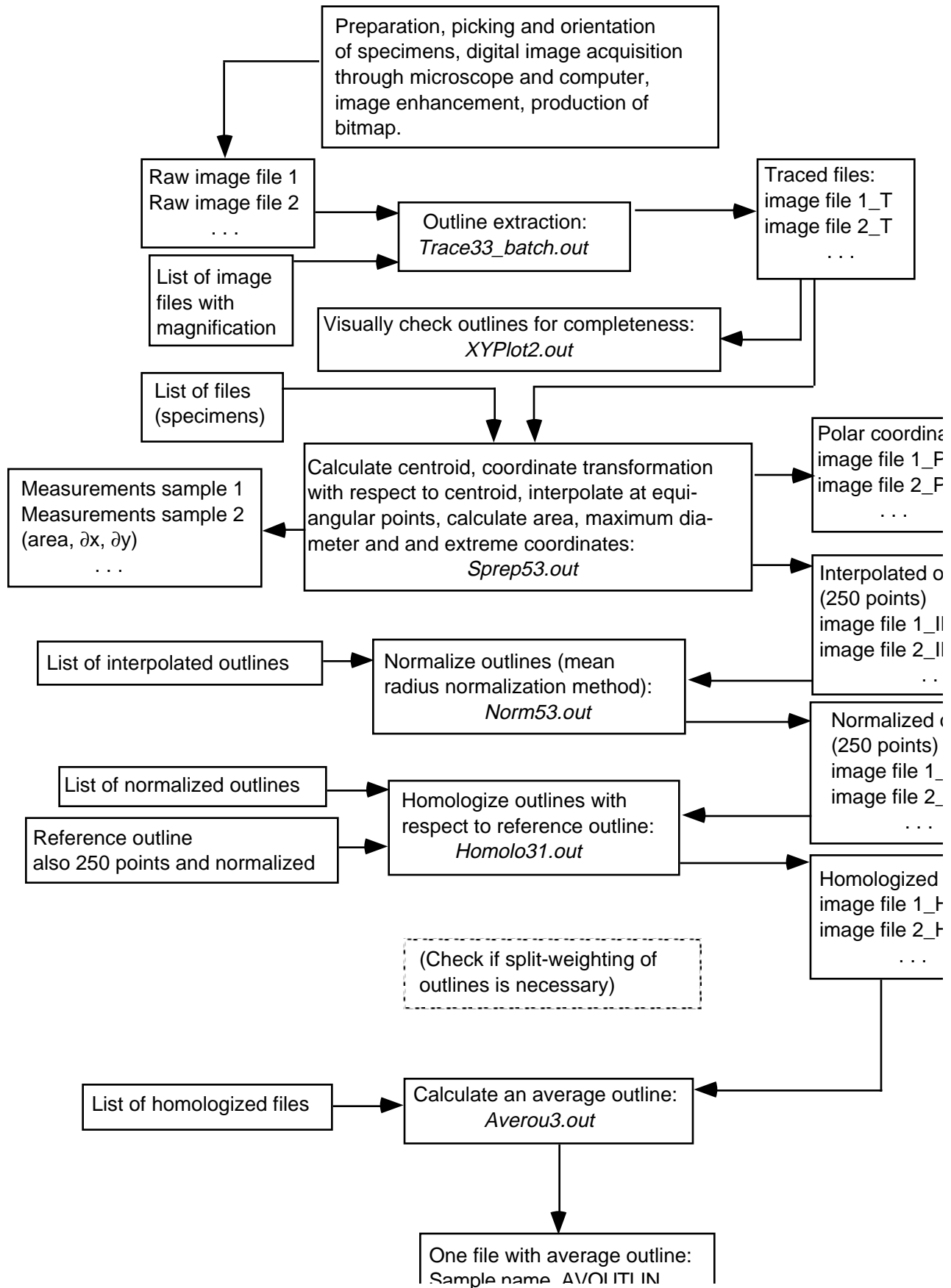


Figure 13a. Flow diagram for Fourier shape analysis on averaged outlines.

3.3.1. Preparation for harmonic analysis - rotation of outlines into homologous positions: Program Homolo31.out

Given a series of normalized outlines with (usually 250) points at equiangular distances, the program Homolo31.out compares each outline with a reference outline (also normalized and with identical number of points) and then rotates the specimen outline about its centroid (=origin) until it matches best with the reference outline. For each increment of rotation the best fit is estimated by finding the maximum linear correlation coefficients between corresponding points of the specimen outline and the reference outline. Because the program compares the radii at similar angular arguments it is important, that the senses of direction and the starting point during outline extraction of the reference curve and the specimen outlines were identical. If the rotation angle exceeds 30° in clock or anticlockwise directions without finding a best fit position the program is interrupted and the curves need to be visually checked. The program was written for usage in batch mode.

Input files:

There are two input files:

1.) A file called Ref_char_nchamber_coil, which contains cartesian coordinates of the normalized reference outline. The reference outline must have the same number of points as the specimen outlines. If the number of points are not identical or if a particular file is missing, a message is written to the error report. The name of the file containing the reference outline can be up to 21 characters long.

A collection of reference outlines is given in the directory Reference outlines. The naming of reference outlines follows the following standard: The first three characters are Ref in order to indicate reference outlines. An abbreviation of the species name is given from position 5 to 11 in the name, a K, U or S indicates Keel, Umbilical or Spiral position of the reference specimen, the last character indicates the coiling direction (s for sinistral, d for dextral coiling. Example: Ref_GPERTEN_K_6Ch_s (see index for the encoding of species names and the corresponding sample, where the reference outline was taken from).

2.) The second input file is a list with name FILE_LIST containing the names of all files with the individual specimen outlines (INPUT). FILE_LIST is a character variable of length 20.

Output files:

For each specimen outline there are two output files written to disk, one ending with suffix _HOM, and the other ending with suffix _CORR. The first contains the cartesian x,y coordinates of the rotated and homologized specimens in position of the maximum correlation with respect to the reference specimen. The names of the _CORR files are composed from the corresponding INPUT file. The files ending with _CORR contain the linear correlation coefficients between rotated outlines of the specimen and the reference specimen as a function of the rotation angle. Given are the direction of the last rotational operation, the total angle of rotation (in degrees) and the correlation coefficients of the rotated specimen with respect

to the reference outline for every position. The names of these files are also composed from the corresponding INPUT file. One file called "Errors_during_Homolo" is written to disk containing runtime error reports.

Operation:

After launching the program, the operator is prompted for the name of the reference outline (a name with 21 characters in maximum). Thereafter the names of the interpolated and normalized outlines (file_list) must be entered. The program calculates the the rotated outlines and the angular steps with the corresponding correlation coefficients.

Known problems:

Not known.

Note, that decimals in the input file must be separated by a point (not by a comma).

3.3.2. Preparation for harmonic analysis - calculate an average outline: Program Averou3.out (in batch mode)

At this level of preparation the analyst may decide whether to calculate harmonic functions from an average outline of all homologized curves, or whether to determine the harmonic functions from each individual homologized curve and then to calculate average harmonic functions. For the first case program Averou3.out was written, which calculates an average outline from the previously homologized curves. This is performed by calculating the mean radial length ρ at their corresponding angular values θ from the homologized curves. As was necessary for program Homolo31.out the number of points, directional sense and the starting point during outline extraction of the homologized curves must all be identical.

Input files:

There are two kinds of input files: One file (=FILE_LIST) containing a list of the file names (=INPUT) with the cartesian X and Y coordinates of the individual homologized outlines, from which the average outline is calculated. FILE_LIST is a character variable of 20 characters lengths. The other input files are the individual files with the X,Y (cartesian) coordinates of the homologized outlines. The names of these files are interpreted through the character variable INPUT. The expression of INPUT is used to compose the name of the output file (suffix _AVOUTLIN).

Output files:

Output is a single file with the suffix _AVOULIN containing the cartesian X,Y coordinates of the desired mean outline.

Operation:

After starting Averou3.out the program first asks whether all outlines are in homologous position. Enter y for yes or n for no. If no was the answer the program stops. If yes was the answer the program continues and inquires for two options: Option 1 (=simple averages) is the case if no split-weighting needs to be applied (e.g. if samples have comparable specimen numbers in

the input file during option 1 are simply the names of the outline files (19 characters long). The program prompts for the name of the list containing all homologized outlines.

If split-weighting needs to be applied (=option 2), a split factor and a size fraction must be provided, and input files are slightly different: The file `file_list` contains - in that sequence - the split factor (20 characters), the size fraction (10 characters), and the name of the homologized outline (19 characters long). The program prompts for the name of that modified file list. The other files are again the homologized outlines.

After entry of the file list the outlines are read and averaged with the respective method. In case 1 one file `name_AVOUTLIN` is written to disk containing the cartesian coordinates of the averaged outline. In case 2 two files are written to disk: `name_AVOUTLIN` (averaged outline) and `FILE_LIST_spw`, which is a list of the homologized outline file names with each name listed by a factor indicated by "split factor".

Known difficulties:

No problems were encountered so far.

Note, that decimals in the input file must be separated by a point (not by a comma).

3.3.3.1. Harmonic decomposition of a single outline: Program HARMAN.out (single mode only)

Given a single closed plane curve consisting of N discrete points the program `HARMAN.out` calculates the Fourier coefficients A_k and B_k of the first k harmonic functions, the corresponding radial coefficients ρ_k and phase angle Φ_k of the polar form of the fourier series, and the power $POWER(k)$ of the discrete spectrum of the curve as a function of k (see Figure 14a-c).

Input files:

Input is a single file (name maximum 10 characters long) containing the cartesian x,y coordinates in normalized form (mean diameter normalization method).

Output files:

One single output file "HARMONICS" is written to disk, containing in that sequence the harmonic number k , α_k , β_k , ρ_k , Φ_k , and $Power(k)$.

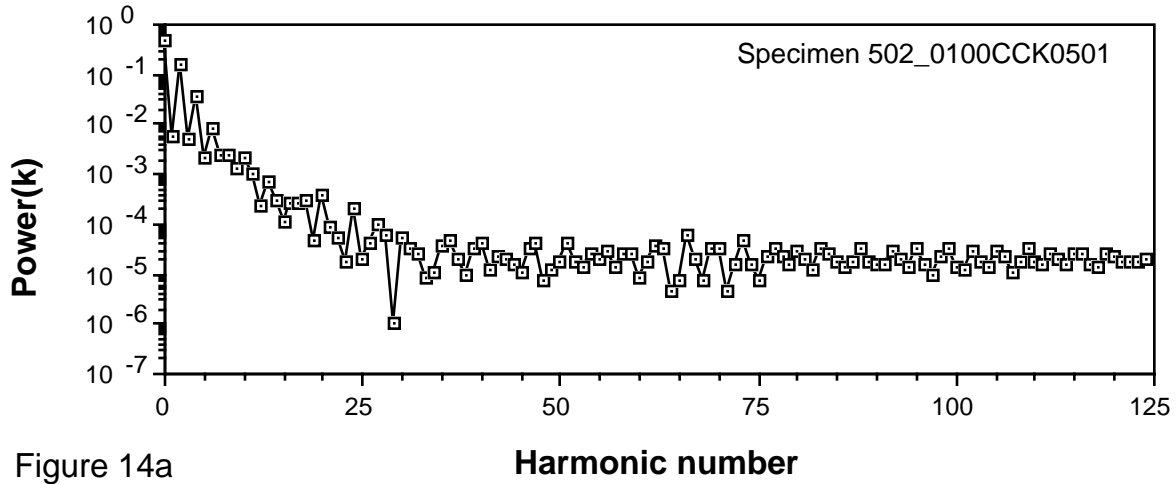


Figure 14a

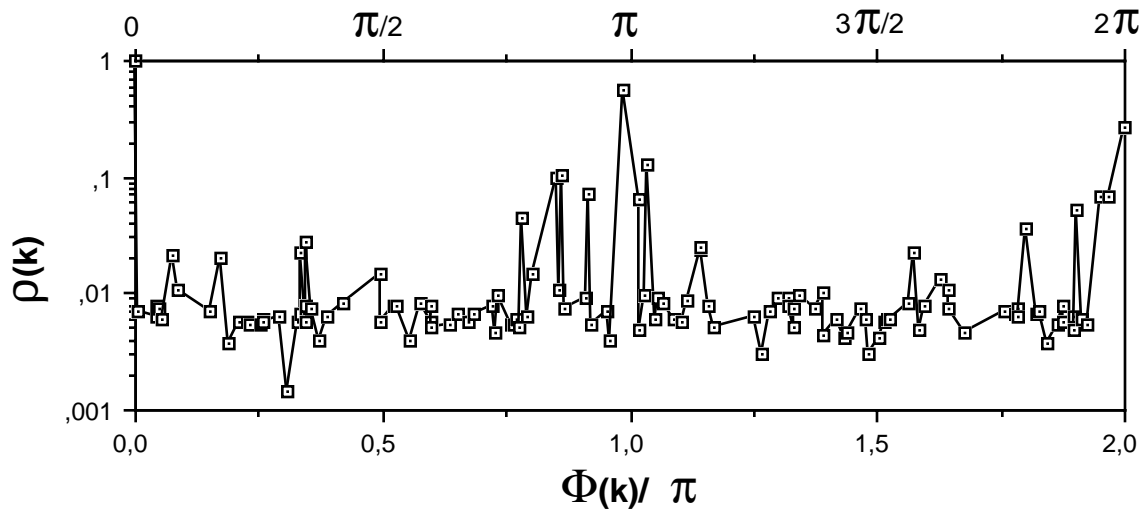


Figure 14b

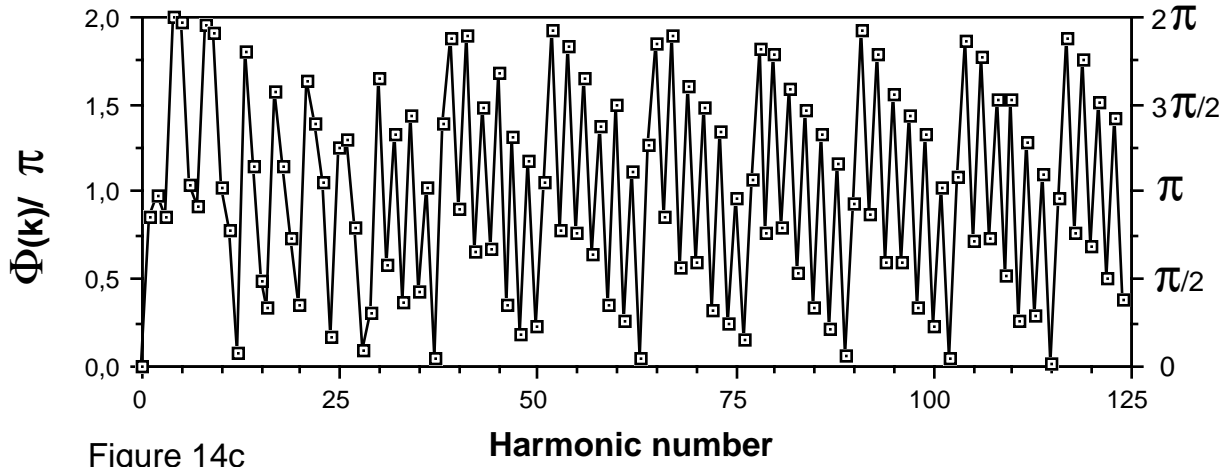


Figure 14.
(Figure 14) Power-spectra (logarithmic scale) in normal (Figure 14a) and polar (Figure 14b) form, and phase relationships (Figure 14c) of normalized outline of specimen 502_0100CCK0501 in keel view (all from same specimen shown in Figures 2 through 4, 6, 7 and 10). The normalized outline consists of 250 points, the maximum number of harmonic functions is therefore 125 (k=0 through 124).

Operation:

After launching the program prompts for the name of the file with the outline, and then writes the file HARMONICS to disk.

Problems:

None.

Note, that decimals in the input file must be separated by a point (not by a comma).

3.3.3.2. Harmonic decomposition of a number of outlines:

Program HARMAN2.out (in batch mode)

Program Harman2.out was directly adapted from Harman.out (single mode) by implementing a batch mode of operation. It runs on a suite of normalized and/or homologized outlines and generates the same results for each outline (e.g. the coefficients α_k , β_k , ρ_k , Φ_k , and Power(k)).

Input files:

Input are

- a single file called FILE_LIST containing a list of all names of files (filename), that have the cartesian coordinates of the interpolated and normalized and/or homologized outlines. FILE_LIST is a character variable and can bear any name of 20 characters length.

- all files, that contain the X,Y coordinates of the outlines, that have

all files ending with suffix `_NORM` or `_HOM`). The names of these files are interpreted through the character variable `INPUT`. The expression of `INPUT` is used to compose the name of the corresponding output file (suffix `_HARM`), which contains the harmonics coefficients, phase angles and the power of the spectra.

Output files:

For each outline a single file `specimen_HARM` (a string 20 characters long) is written to disk, containing in that sequence the harmonic number k , α_k , β_k , ρ_k , Φ_k , and `Power(k)`, with k running from 0 to 124 (e.g. 125 rows for 250 points in the outline). Note that there is no header in these output files.

Operation:

After launching the program prompts for the list containing the Names of interpolated and normalized outlines (maximum 20 character long, for example `LIST_NORM_FILES`). Enter that list and the program generates the files containing the harmonics matrix for every outline.

Problems:

None.

Note, that decimals in the input file must be separated by a point (not by a comma).

3.3.3.3. Alternative method of analysis of harmonic data using programs `Harm_Filter2.out` and `Harm_Stats.out`

In section 3.3 and in Figure 13a analysis of harmonic functions is discussed by first calculation of an averaged outline from a series of individual outline curves (using program `Averou3.out`) and then performing harmonic decomposition of the average outline curve (using program `Harman.out`).

In the following section an alternative way of analysis is discussed and illustrated (see Figure 13b): Given a series of interpolated and normalized and/or homologized

Flow-scheme for alternative way of harmonic analysis

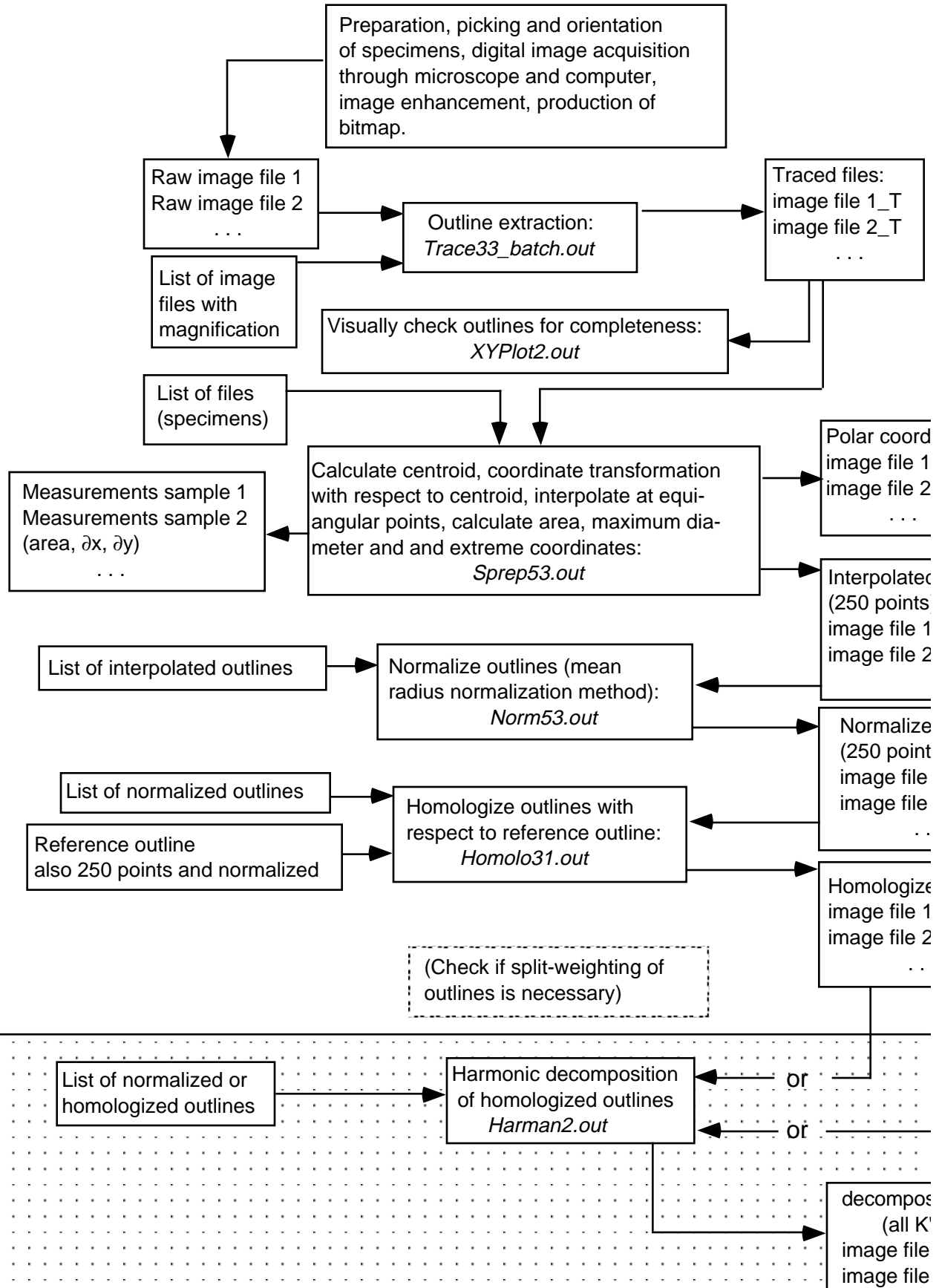


Figure 13b: Flow-scheme of alternative harmonic analysis by performing statistics of fourier coefficients in the K-space.

outlines, harmonic decomposition into the fourier spectra is performed for every single outline. This is done with program Harman2.out, which allows batch processing (see section above).

In a second step each matrix of harmonic coefficients is filtered in the K-space, e.g. for every outline the harmonic coefficients are selected out for a given value of K, and the values assembled into a single files per value of K, each bearing the K'th harmonic coefficients of all individual outlines of that particular sample. This is done with program Harm_Filter2.out.

In a third step the K-filtered and assembled values for α_k , β_k , ρ_k , Φ_k , and Power(k) are statistically analyzed by calculating the means and 95 confidence intervals for α_k , β_k , ρ_k , Φ_k , and Power(k) per K.

In the last step outlines can be back-transformed from K-space into real space by reconstruction of the "statistical" or "mean" per sample obtained from the means of the fourier components. This is then done by using program Recon2.out (program only available in single sample mode).

3.3.3.4. Program Harm_Filter2.out (in batch mode)

Given is a suite of files, each containing the coefficients α_k , β_k , the amplitude ρ_k , the phase angle Φ_k , and the Power(k) for 125 polar harmonic functions from individual closed plane outlines of microfossils. K is the harmonic number. For each specimen in a particular sample there is one such file, which were calculated with program Harman2.out. The data in each input file is arranged in the following order (There are no header lines):

$K, \alpha_k, \beta_k, \rho_k, \Phi_k, \text{Power}(k)$
 $0, \alpha_0, \beta_0, \rho_0, \Phi_0, \text{Power}(0)$
 $1, \alpha_1, \beta_1, \rho_1, \Phi_1, \text{Power}(1)$
...
 $124, \alpha_{124}, \beta_{124}, \rho_{124}, \Phi_{124}, \text{Power}(124)$

For every specimen given in the file list LIST_HARM_FILES program Harm_Filter2.out reads these harmonic components throughout from a set of outlines and selects out the values for a range of K=0 to a predefined upper limit of K. The upper limit of K is prompted at the beginning of the program (*). The components of harmonic function of a particular order K are then assembled together from all specimen outlines and written to an external file with the corresponding name Comp_harmon_K=... . Example: For all specimens in sample 503A011080X and K being 50 the file 503A011080X_Filt_Harm_K=050 is generated holding only harmonic components of the order 50. These files can be loaded into program

Harm_Stats.out in order to calculate in K-space the means and confidence intervals for each harmonic component (see section further below).

(*) Note: There is a previous version of program Harm_Filter2.out called Harm_Filter.out, but which runs only in single mode, e.g. for a single value of K.

Input files:

There are two sorts of input files:

1.) A number of files specimen_HARM (20 chars long), each containing the full set of harmonic functions per specimen outline from K=0 to 124.

2.) A single file LIST_HARM_FILES containing a list of the above specimen_HARM files.

Output files:

For every value of K a single file is written to disk with the generalized name sample_Filt_Harm_K=. . ., each containing the components of harmonic functions of order K for every specimen.

Operation:

After launching Harm_Filter2.out the program prompts for the input of the upper limit of K, which should be entered as an integer number (≤ 124 in the current version). Usually, only the first few harmonic functions are necessary, e.g. enter a value < 20 or so.

Thereafter the program prompts for the input of the name of the file containing a list of all specimen_HARM files, that were generated previously with program Harman2.out. Enter the name of that list (maximum 20 characters in length).

Then press return and the program runs.

Problems:

No problems known so far.

3.3.3.5. Program Harm_Stats.out

This program determines the statistics (e.g. sample means and 95% confidence intervals per sample) in K-space for the values of α_k , β_k , ρ_k , Φ_k , Power(k) (e.g. for every individual value of K). The means and confidence intervals of α_k , β_k , ρ_k , Φ_k , Power(k) can then, for example be plotted against the age for every K in order to investigate outline shape changes in K-space.

Input files:

There are two sorts of input files:

- 1.) A number of files with the generalized name sample_Filt_Harm_K=. . ., each containing the set of harmonic functions for all specimen outlines in that sample for that particular value of K.
- 2.) A single file with the generalized name LIST_sample_Filt_Harm containing a list of the filenames with the K-filtered harmonic components, that were previously generated with program Harm_Filter2.out.

Output files:

A single file with the generalized name sample_HARM_STATS is written to disk containing the sample designation, the geological age (in Ma), the number of averaged outlines per harmonic number, and the means and 95% confidence intervals of α_k , β_k , ρ_k , Φ_k , Power(k) for each value of K.

Operation:

After launching Harm_Stats.out the program asks for the geological age of the sample. Enter a real number, 5 characters in length. The the program prompts for the list containing the names of the filtered harmonics files. Enter a name, for example LIST_sample_Filt_Harm, with 26 characters in maximum. Then the program runs through all files given in that list.

Problems:

No problems known so far.

MorphCol Supplement #2 - Program listings

6.12.1 Listing of program Harman2.f

```
PROGRAM HARMAN
C
C Version 2, October 13, 1997, by Michael Knappertsbusch
C Minor corrections added July 3, 2005.
C
C !!! Processing in batch mode !!!
C
C Harmonic analysis of a closed plane curve consisting of
C N discrete points. Points are given as cartesian coordinates
C U and V. The program converts U and V into polar coordinates
C R and Theta and then goes through a polar fourier analysis.
C The number of harmonics (K) to be calculated is determined by KMAX.
C Output are the coefficients ALPHAK and BETAK of the Fourier
C series as a function of K, the corresponding coefficients and
C phase angle AK and PHIK of the polar form of the fourier series,
C and the power POWERK of the discrete spectrum of the curve as
```

```
C      a function of K.
C
C      Parameters are calculated after Davis, 1986, pages 248 ff.
C
C      Input files are:
C      - File with name FILE_LIST containing a list of all
C        names of files (filename), that contain the cartesian
C        coordinates of the interpolated and normalized outlines.
C        FILE_LIST is a character variable and can bear any
C        name of 20 characters length.
C
C      - All files, that contain the X,Y coordinates of the
C        outlines, that have previously been interpolated and
C        normalized; i.e. all files ending with suffix _NORM).
C        The names of these files are interpreted through the
C        character variable INPUT. The expression of INPUT is
C        used to compose the name of the corresponding output
C        file (suffix _HARM), which contains the harmonics
C        coefficients, phase angles and the power of the spectra.
C
C      Output files are:
C      - One file per outline, that contains the harmonics
C        coefficients, phase angles and the power of the spectra.
C        The names of the output files are also composed through
C        the character variable INPUT by addition of the suffix
C        _HARM to the name of filename.
C
C      Note: All file handling for morphometric analyses follows a name
C      convention:
C
C      filename      = Name of sample, 15 characters long.
C      filename_T    = Input file for raw curves with cartesian coordinates, 17
C      characters long.
C      filename_POL  = Polar coordinates of filename,          19
C      characters long.
C      filename_INT  = Interpolated (cartesian) coordinates of filename,  19
C      characters long.
C      filename_NORM = Normalized curve,                        20 characters
C      long.
C      filename_HARM = Harmonic coefficients etc. of filename, 20
C      characters long.
C
C
C      INTEGER K,KMAX,N
C      DOUBLE PRECISION PI
C      DOUBLE PRECISION SUMR,SUMA,SUMB,RJ,THETAJ
C      DOUBLE PRECISION U,V,ALPHA,K,BETA0,BETAK,AK,PHIK
C      DOUBLE PRECISION POWERK
C      CHARACTER*20 FILE_LIST,OUTPUT
C      CHARACTER*20 INPUT
C
C      PARAMETER(PI=3.14159265)
C
C      WRITE(9,*) '*****'
C      WRITE(9,*) '*
C      WRITE(9,*) '*      Harmonic decomposition of interpolated *'
C      WRITE(9,*) '*      and normalized outlines          *'
```

```
WRITE(9,*) '*           Processing in batch mode           *'
WRITE(9,*) '*                               *'
WRITE(9,*) '*           Version 2.1, 3 July 2005           *'
WRITE(9,*) '*           By Michael Knappertsbusch         *'
WRITE(9,*) '*                               *'
WRITE(9,*) '* *****'
WRITE(9,*) ' '
C WRITE(9,*) 'Enter the number of harmonics to calculate (KMAX)'
C READ(9,*) KMAX

WRITE(9,*) ' . . .Names of interpolated
1and normalized outlines needed. . .'
WRITE(9,*) '           enter list containing names
2 of files (20 chars)'
READ(9,2) FILE_LIST
2 FORMAT(A20)
C
C OPEN(20,FILE=FILE_LIST,STATUS='OLD')
4 READ(20,6,END=999) INPUT
6 FORMAT(A20)
WRITE(9,3) INPUT
3 FORMAT(' . . .Reading new file ',A20,' . . .')
C
C Determination of actual filenames:
C
C OUTPUT=INPUT(1:15)//'_HARM'
C
C OPEN(18,FILE=INPUT,STATUS='OLD')
C OPEN(19,FILE=OUTPUT,STATUS='NEW')
C
C
C N=0
C SUMR=0.0
C
C ***** First calculation of zero harmonic (K=0):
C
C K=0
C
C 5 READ(18,*,END=10) U,V
C N=N+1
C
C Transform cartesian coordinates into polar coordinates RJ
C and THETAJ:
C
C CALL POLAR(U,V,RJ,THETAJ)
C
C SUMR=SUMR+RJ
C GOTO5
C
C Calculate last sum:
C
C 10 CALL POLAR(U,V,RJ,THETAJ)
C SUMR=SUMR+RJ
C N=N+1
C
C Determine necessary number of Kmax:
C
C -----
```

```
C
  ALPHAK=0.0
  BETA0=SUMR/N
  AK=BETA0
  PHIK=0.0
  POWERK=(AK**2)/2
C
  WRITE(19,*) K,',',ALPHAK,',',BETA0,',',AK,',',PHIK,',',POWERK
C
  REWIND(18)
C
C
C
C*****      Now calculation of all other harmonics:
C
  DO 15, K=1,KMAX
    SUMA=0.0
    SUMB=0.0
  20  READ(18,*,END=25) U,V
      CALL POLAR(U,V,RJ,THETAJ)
      SUMA=SUMA+RJ*COS(K*THETAJ)
      SUMB=SUMB+RJ*SIN(K*THETAJ)
      GOTO 20
C
C  Last sum:
C
  25  CALL POLAR(U,V,RJ,THETAJ)
      SUMA=SUMA+RJ*COS(K*THETAJ)
      SUMB=SUMB+RJ*SIN(K*THETAJ)
C
  ALPHAK=2*SUMA/N
  BETAK=2*SUMB/N
  AK=SQRT(ALPHAK**2+BETAK**2)
  PHIK=ARCTAN(ALPHAK,BETAK)
  POWERK=(AK**2)/2
C
  WRITE(19,*) K,',',ALPHAK,',',BETAK,',',AK,',',PHIK,',',POWERK
C
  REWIND (18)
  15  CONTINUE
C
  GOTO4
C
  999 WRITE(9,*) 'Analysis for all curves terminated'
C
  STOP
  END
```

```
C*****
*****
  SUBROUTINE POLAR(US,VS,RS,THETAS)
C*****
*****
```

C Converts cartesian coordinates US,VS into polar coordinates
C RS and THETA. Origin of local coordinate systems is at 0,0.
C The calling unit gives US and VS as input. RS and THETAS are
C returned to the calling unit. THETAS in Radians.
C

DOUBLE PRECISION US,VS,RS,THETAS
DOUBLE PRECISION ARG,PI

C
C PARAMETER(PI=3.14159265)

C
C RS=SQRT(US**2+VS**2)

C
C First special cases:
C

IF (US.GT.0.AND.VS.EQ.0) THEN
 THETAS=0
ELSE IF (US.EQ.0.AND.VS.GT.0) THEN
 THETAS=PI/2
ELSE IF (US.LT.0.AND.VS.EQ.0) THEN
 THETAS=PI
ELSE IF (US.EQ.0.AND.VS.LT.0) THEN
 THETAS=2*PI/3
END IF

C
C For all other cases:
C

IF (US.GT.0.AND.VS.GT.0) THEN
 ARG=ABS(VS/US)
 THETAS=ATAN(ARG)
ELSE IF (US.LT.0.AND.VS.GT.0) THEN
 ARG=ABS(US/VS)
 THETAS=ATAN(ARG)+PI/2
ELSE IF (US.LT.0.AND.VS.LT.0) THEN
 ARG=ABS(VS/US)
 THETAS=ATAN(ARG)+PI
ELSE IF (US.GT.0.AND.VS.LT.0) THEN
 ARG=ABS(US/VS)
 THETAS=ATAN(ARG)+3*PI/2
END IF

C
C RETURN
C END

C *****
C *****

DOUBLE PRECISION FUNCTION ARCTAN(US,VS)

C *****
C *****

C
C Calculates the arcus tangent as a function of the X-coordinate US
C and the Y-coordinate VS. All angular values are in Radians.
C ARCTAN is returned in Radians.
C

DOUBLE PRECISION US,VS

```
C
PARAMETER(PI=3.14159265)
C
IF (US.GT.0.AND.VS.EQ.0) THEN
  ARCTAN=0
ELSE IF (US.EQ.0.AND.VS.GT.0) THEN
  ARCTAN=PI/2
ELSE IF (US.LT.0.AND.VS.EQ.0) THEN
  ARCTAN=PI
ELSE IF (US.EQ.0.AND.VS.LT.0) THEN
  ARCTAN=2*PI/3
END IF
C
C For all other cases:
C
IF (US.GT.0.AND.VS.GT.0) THEN
  ARG=ABS(VS/US)
  ARCTAN=ATAN(ARG)
ELSE IF (US.LT.0.AND.VS.GT.0) THEN
  ARG=ABS(US/VS)
  ARCTAN=ATAN(ARG)+PI/2
ELSE IF (US.LT.0.AND.VS.LT.0) THEN
  ARG=ABS(VS/US)
  ARCTAN=ATAN(ARG)+PI
ELSE IF (US.GT.0.AND.VS.LT.0) THEN
  ARG=ABS(US/VS)
  ARCTAN=ATAN(ARG)+3*PI/2
END IF
C
RETURN
END
```

6.12.2 Listing of program Harm Filter.f

```
Program HARM_FILTER
C
C Version 1.0, 5 July 2005, by Michael Knappertsbusch
C
C Given is a suite of files, each containing K=125 polar harmonic
C functions of individual
C closed plane outlines of microfossils (e.g. one file per specimen).
C These harmonic
C functions were calculated with program Harman2.out.
C The harmonic functions include the coefficients AlphaK and BetaK,
C the amplitude AK,
C the phase angle PhiK, and the PowerK, with K being the number of
C the harmonic functions.
C The data in each input file is arranged in the following order (There
C are no header lines):
C
C K, AlphaK, BetaK, AK, PhiK, PowerK
```

```
C      1, Alpha1, Beta1, A1, Phi1, Power1
C      2, Alpha2, Beta2, A2, Phi2, Power2
C      . . . . .
C      . . . . .
C
C      Program HARM_FILTER reads the harmonic components throughout
C      from a set of outlines and
C      selects the values for a predefined value of K. The components of
C      harmonic function K are
C      then composed and written into an external file with the name
C      Comp_harmon_K=...
C      Example: For K=50 the file "Comp_harmon_050" is generated.
C
C      This file can then loaded into a statistics program in order to calculate
C      means, standard
C      deviations etc. for each component of number K.
C
C
C      Input:
C          There are two sorts of input files:
C          1.) A number of files specimen_HARM (20 chars long), each
C      containing the full set of
C          harmonic functions per specimen outline from K=0 to 124.
C          2.) A single file LIST_HARM_FILES containing the list of the
C      above specimen_HARM files.
C
C      Output:
C          One single output file Comp_harmon_K=... (name is 17 chars
C      long) is written, containing the
C          components of harmonic functions with number K.
C
C
C
C      Note: All file handling for morphometric analyses follows a name
C      convention:
C
C      filename      = Name of sample, 15 characters long.
C      filename_T    = Input file for raw curves with cartesian coordinates, 17
C      characters long.
C      filename_POL  = Polar coordinates of filename,          19
C      characters long.
C      filename_INT  = Interpolated (cartesian) coordinates of filename,    19
C      characters long.
C      filename_NORM = Normalized curve,                          20 characters
C      long.
C      filename_HARM = Fourier coefficients, phase angles and power of
C      curve 20 characters long.
C
C
C
C      Needs subroutine Int_Char_Conv
C
C
C      INTEGER K,KD          ! K is the running
C      harmonic number, KD is the desired harmonic number to be filtered from
C      the matrix
C      ...
C      DOUBLE PRECISION ALPHA K,BETA K          ! Harmonic
```

```
DOUBLE PRECISION AK,PHIK,POWERK           ! Amplitude AK,
phase angle PhiK, and the power POWERK
CHARACTER*27 OUTPUT                         ! Name of the output
file(s) [27 chars long]
CHARACTER*20 FILE_LIST,INPUT               ! INPUT contains
the harmonics of an outline
C                                           ! FILE_LIST ist the file
containing the names of the harmonic data files.
CHARACTER*3 APP                            ! Appendix to the
name of the output file in order to
CHARACTER*1 TAB                            ! indicate
which harmonic functions were calculated.
CHARACTER*11 SAMPLE                        ! Character string to
calculate output names.
C
TAB=CHAR(9)                                ! Tabulator; this is
Macintosh specific.
C
WRITE(9,*) '*****'
WRITE(9,*) '*                               *'
WRITE(9,*) '*           Program Harm_Filter           *'
WRITE(9,*) '* Filtering for selected harmonic functions *'
WRITE(9,*) '*                               *'
WRITE(9,*) '*           Version 1.0, by M. Knappertsbusch           *'
WRITE(9,*) '*                               *'
WRITE(9,*) '*****'
WRITE(9,*) ' '
WRITE(9,*) 'Attention: Harmonic files must
* be organized samplewise !'
WRITE(9,*) ' '
WRITE(9,*) 'Enter number of harmonic
1 function to be selected (max 124)'
WRITE(9,*) '(Example: 12)'
READ(9,*) KD
C
WRITE(9,*) ' . . .Enter list with names of
* harmonic files. . . '
WRITE(9,*) ' LIST_HARM_FILES or max. 20 chars long)'
READ(9,3) FILE_LIST
3
FORMAT(A20)
C
C
C Compose the name of the output file from the input file and file
numbering according to K:
C
OPEN(15,FILE=FILE_LIST,STATUS='OLD')
READ(15,2) SAMPLE
2
FORMAT(A11)
REWIND(15)
C
CALL INT_CHAR_CONV(KD,APP)
OUTPUT=SAMPLE//'_Filt_Harm_K= '//APP      ! Output: 27chars long
(=12chars+12chars+3chars)
C
OPEN(14,FILE=OUTPUT,STATUS='NEW')
C
C Writing header lines to the output file:
C
```

```
WRITE(14,*) '*'
WRITE(14,4) TAB,TAB,TAB,TAB,TAB,TAB
4  FORMAT('Specimen',A1,'K',A1,'Alpha(K)',
*      A1,'Beta(K)',A1,'A(K)',A1,'Phi(K)',
*      A1,'Power(K)')
C
5  READ(15,7,END=100) INPUT
7  FORMAT(A20)
C
OPEN(16,FILE=INPUT,STATUS='OLD')
C
DO 10, I=0,KD
  READ(16,*) K,ALPHAK,BETAK,AK,PHIK,POWERK
10 CONTINUE
C
WRITE(9,*) '. . .Calculating. . .'
C
C
C
C  Writing data to output file:
C
WRITE(14,15) INPUT,TAB,K,TAB,ALPHAK,
* TAB,BETAK,TAB,AK,TAB,PHIK,TAB,POWERK
15  FORMAT(A20,A1,I3,A1,4(F10.7,A1),F10.7)
CLOSE(16)
C
GOTO5                      ! Read next specimen
C
100 STOP
END
```

```
SUBROUTINE INT_CHAR_CONV(M,SUFFIX)
```

```
C
C  Subroutine to convert an integer number into the same expression,
but
C  as character. This is used for the composition of calculated file
C  names in the calling unit. The three chars long character variable
C  SUFFIX is returned to the calling unit.
C
```

```
INTEGER N(0:124),M
CHARACTER*3 STRING(0:124),SUFFIX
```

```
C
C  Reading strings from 0 through 124 (note: this can programmed
C  more elegantly by single character composition):
C
```

```
DATA (STRING(I),I=0,124) /'000',
* '001','002','003','004','005',
* '006','007','008','009','010',
* '011','012','013','014','015',
* '016','017','018','019','020',
* '021','022','023','024','025',
* '026','027','028','029','030',
* '031','032','033','034','035',
```

```
* '041','042','043','044','045',  
* '046','047','048','049','050',  
* '051','052','053','054','055',  
* '056','057','058','059','060',  
* '061','062','063','064','065',  
* '066','067','068','069','070',  
* '071','072','073','074','075',  
* '076','077','078','079','080',  
* '081','082','083','084','085',  
* '086','087','088','089','090',  
* '091','092','093','094','095',  
* '096','097','098','099','100',  
* '101','102','103','104','105',  
* '106','107','108','109','110',  
* '111','112','113','114','115',  
* '116','117','118','119','120',  
* '121','122','123','124'/
```

C
C
C
C

Program interruption if there are more than 125 harmonic functions:

```
IF (M.GT.124) THEN  
  WRITE(9,*) 'ERROR:'  
  WRITE(9,*) 'Number of harmonic  
* functions too big !'  
  WRITE(9,*) 'Adapt dimensions  
* in Subroutine INT_CHAR_CONV'  
  WRITE(9,*) 'The program stops now'  
  PAUSE 100  
100 CONTINUE  
  STOP  
END IF
```

C
C
C

Setting numeric N from 0 through 124:

```
DO 10, I=0,124  
  N(I)=I  
10 CONTINUE
```

C
C

```
DO 20, I=0,124  
  IF (M.EQ.N(I)) THEN  
    SUFFIX=STRING(I)  
  END IF
```

20
C

```
CONTINUE
```

```
RETURN  
END
```

6.12.3 Listing of program Harm Stats.f

PROGRAM HARM STATS

```
C
C   Version 1.0, by Michael Knappertsbusch, 12.7.2005
C
C   Taken and modified from program Stats.f, version 7.
C
C
C   Purpose:
C   Program Harm_Stats calculates simple univariate statistics of
harmonic coefficients
C   of the single order K from a series of files bearing the K'th harmonic
functions of a
C   foraminiferal outline.
C
C   The input data are matrices, in which the columns bear the specimen
name, harmonic
C   number K, the k'th harmonic coefficients AlphaK, BetaK, the
amplitude AK, the
C   phase angle PhiK, and the PowerK. Each row contains the values for
the K'th harmonic function
C   for a single specimen outline.
C   These input data matrices are generated with program Harm_Filter.f.
C
C
C   !!! Note: Batch processing mode !!!
C
C   Input files:
C   There are two types of input files:
C   1.) A file with variable FILE_LIST (max. 20 chars long) containing the
names of all
C   individual files Comp_harmon_K=nnK to be treated. The individual
C   Comp_harmon_K=nnK were composed with program Harm_Filter.out,
and these with program
C   Harman2.out.
C
C   2.) One or several files with the generalized name
Comp_harmon_K=..K
C   (in variable INPUT). The names of these Comp_harmon_K=nnK files
are
C   always 17 chars long. They contain the k'th harmonic coefficients
AlphaK, BetaK,
C   the amplitude AK, the phase angle PhiK, and the PowerK for each
outline.
C
C   Content of input files Comp_harmon_K=nnK:
C
C   Header information (the first 2 lines from the top)
C   Data body including (from left to right):
C   SPECIMEN:      Specimen
C   K:             Harmonic number
C   AlphaK:       First harmonic coefficient of order K (AlphaK)
C   BetaK:        Second harmonic coefficient of order K (BetaK)
C   AK:           Amplitude of order K
C   PhiK:         Pase angle Phi of order K
C   PowerK:       Power amplitude of order of K.
C   DEV:          Deviation of total keel residual area from the value
of AREA, in per cent
```



```
C
      TAB=CHAR(9)                ! Tabulator on a iMac (machine
dependent value)
C
C
C
      WRITE(9,*)
'*****'
      WRITE(9,*) '*'
      WRITE(9,*) '*          Program Harm_Stats 1.0          *'
      WRITE(9,*) '*      Calculates statistics of harmonic functions      *'
      WRITE(9,*) '*      (batch processing mode)          *'
      WRITE(9,*) '*'
      WRITE(9,*) '*      12.7.2005 by Michael Knappertsbusch      *'
      WRITE(9,*) '*'
      WRITE(9,*) '*'
      WRITE(9,*) '*      Usage in combination with programs      *'
      WRITE(9,*) '*      Harman.out and Harm_Filter.out          *'
      WRITE(9,*) '*'
      WRITE(9,*) '*'
'*****'
C
      WRITE(9,*) ' '
      WRITE(9,*) ' '
C
C
C
      WRITE(9,*) ' Enter the age of the sample'
      WRITE(9,*) ' (In Ma [5 chars] Example: 00.00)'
      READ(9,*) AGE
C
C
      Get the list with the specimen_HARM names and open it:
C
      WRITE(9,*) 'Now, enter the list containg
* the names of the filtered harmonics files'
      WRITE(9,*) '      (LIST_sample_
*Filt_Harm or [max 26 chars] )'
      READ(9,'(A26)') FILE_LIST
      OPEN(17,FILE=FILE_LIST,STATUS='OLD')
C
C
      Prepare the OUTPUT file:
C
      Calculate the name of the output file by taking the sample name (=first
11 characters)
C
      of the specimen names given in FILE_LIST. Then open the OUTPUT file.
C
      READ(17,9) SAMPLE                ! Determination of sample
name (11 chars)
      9  FORMAT(A11)
      REWIND(17)
C
      OUTPUT=SAMPLE//'_HARM_STATS'
      OPEN(16,FILE=OUTPUT,STATUS='NEW')
C
C
      Write header line to output file:
C
      WRITE(16,*) '*'
```

```
2   FORMAT('Sample_K',A1,'Age (Ma)',A1,'#of outlines',A1,
*   'AlphaK',A1,'±CI AlphaK',A1,
*   'BetaK',A1,'±CI BetaK',A1,
*   'AK',A1,'±CI AK',A1,
*   'PhiK',A1,'±CI PhiK',A1,
*   'PowerK',A1,'±CI PowerK')
C
C
C
C
C
C***** Main loop for samples starts here:
C
90  READ(17,'(A27)',END=2001) INPUT           ! Read new file (new
specimen) from FILE_LIST
    WRITE(9,3) INPUT
3   FORMAT('. . .Reading file ',A27,'. . .')
C
C   Open INPUT and determine the number of specimens (record lines) in
it:
C
    OPEN(15,FILE=INPUT,STATUS='OLD')      ! Input file
C
C
C   Determine number of records in the input file.
C   First, read header block again:
C
    DO 4 I=1,2
      READ(15,1) HEADER1
4   CONTINUE
C
    NMAX=0
5   READ(15,8,END=1000) SPECIMEN
8   FORMAT(A20)
    NMAX=NMAX+1
    GOTO5
1000 REWIND(15)
C
    ROOT=SQRT(REAL(NMAX))
C
C
C   Now proceed with statistical analysis:
C
C   Read first 2 lines of header block:
    DO 6 I=1,2
      READ(15,1) HEADER1
6   CONTINUE
1   FORMAT(A1)
C
C
C   Determine extrema:
C
C   Read first data line:
    READ(15,*) SPECIMEN,K,(X(I),I=1,5)
C
C
-
```

C Special case: Statistics if there is only one data record available
(NMAX=1):

C
IF (NMAX.EQ.1) THEN
DO 7 I=1,5
MINX(I)=X(I)
MAXX(I)=X(I)
MEANX(I)=X(I)
VARX(I)=0.0
STDIX(I)=0.0
CIX(I)=0.0
LCIX(I)=X(I)
UCIX(I)=X(I)
7 CONTINUE
GOTO 2000 ! Write results to output file and stop program.
END IF

C
C
C Now, proceed with calculation of extrema:

C
DO 10 I=1,5
MINX(I)=X(I)
MAXX(I)=X(I)
10 CONTINUE
C
C Read next data line:
15 READ(15,*,END=999) SPECIMEN,K,(X(I),I=1,5)

C
DO 20 I=1,5
IF (X(I).LE.MINX(I)) THEN
MINX(I)=X(I)
END IF

C
IF (X(I).GT.MAXX(I)) THEN
MAXX(I)=X(I)
END IF
20 CONTINUE
GOTO 15

C
999 REWIND(15)

C
C
C Calculate means:

C
C Read header block again:
DO 25 I=1,2
READ(15,1) HEADER1
25 CONTINUE

C
C Initialize SUMX(i):

C
DO 30 I=1,5
SUMX(I)=0.0
30 CONTINUE
C
35 READ(15,*,END=888) SPECIMEN,K,(X(I),I=1,5)

C

```
C
      DO 40 I=1,5
        SUMX(I)=SUMX(I)+X(I)
40    CONTINUE
      GOTO 35
C
888  DO 50 I=1,5
      MEANX(I)=SUMX(I)/NMAX
50   CONTINUE
C
      REWIND(15)
C
C
C
C
C   Determine the variances, standard deviations and the 95% confidence
intervals:
C
C   Again, read header block:
      DO 51 I=1,2
        READ(15,1) HEADER1
51   CONTINUE
C
C   Re-initialize SUMX(i):
C
      DO 60 I=1,5
        SUMX(I)=0.0
60   CONTINUE
C
C   Calculate sums of squares of differences from the means:
C
65   READ(15,*,END=777) SPECIMEN,K,(X(I),I=1,5)
C
      DO 70 I=1,5
        SUMX(I)=SUMX(I)+(X(I)-MEANX(I))**2
70   CONTINUE
      GOTO 65
C
777  DO 80 I=1,5
      VARX(I)=SUMX(I)/(NMAX-1)
      STDX(I)=SQRT(VARX(I))
      CIX(I)=1.96*STDX(I)/ROOT
      LCIX(I)=MEANX(I)-CIX(I)
      UCIX(I)=MEANX(I)+CIX(I)
80   CONTINUE
C
C
C
C   Output of results to file "sample_HARM_STATS":
C
2000 WRITE(16,85) INPUT,TAB,AGE,TAB,NMAX,TAB
      * ,MEANX(1),TAB,CIX(1),TAB
      * ,MEANX(2),TAB,CIX(2),TAB
      * ,MEANX(3),TAB,CIX(3),TAB
      * ,MEANX(4),TAB,CIX(4),TAB
      * ,MEANX(5),TAB,CIX(5)
85   FORMAT(A27,A1,F6.3,A1,I3,A1,9(F9.6,A1),F9.6)
```

C
C

CLOSE(15)
GOTO 90

! Read new file from FILE_LIST

C

2001 PAUSE 100
100 CONTINUE
STOP
END