

MORPHOMATICA – Programme Description

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The programme MORPHOMATICA was initially designed and implemented by one of us (W. B.), with the mathematical framework provided by Prof. Linhart (Department of Mathematics, University of Salzburg). The functionality was strongly dependent of the requirements and suggestions of two other colleagues, Dr. Dan L. Danielopol and Dr. Angel Baltanás (UAM, Madrid) always with the biological requirements and the desired output in mind.

MORPHOMATICA, version 1.5, written by W. B. and version 1.6, expanded by W. N., uses the B-splines algorithm adapted to ostracod outlines by Johann Linhart. The mathematical background of the B-splines for an approximate description of ostracod outlines is presented in Bayer et al. (2002), Baltanás et al. (2003) and Neubauer (2007).

The program is a software application running under Microsoft Windows 98, NT 4.0, 2000, XP, which enables the user to apply the above described method to digitised ostracod outlines. The design of the program is based on experiences made during a bachelor project at the University of Salzburg (Bayer et al., 2002). The software package with the same name (cf. Linhart et al. 2006) is available at <http://palstrat.uni-graz.at>.

Working with MORPHOMATICA

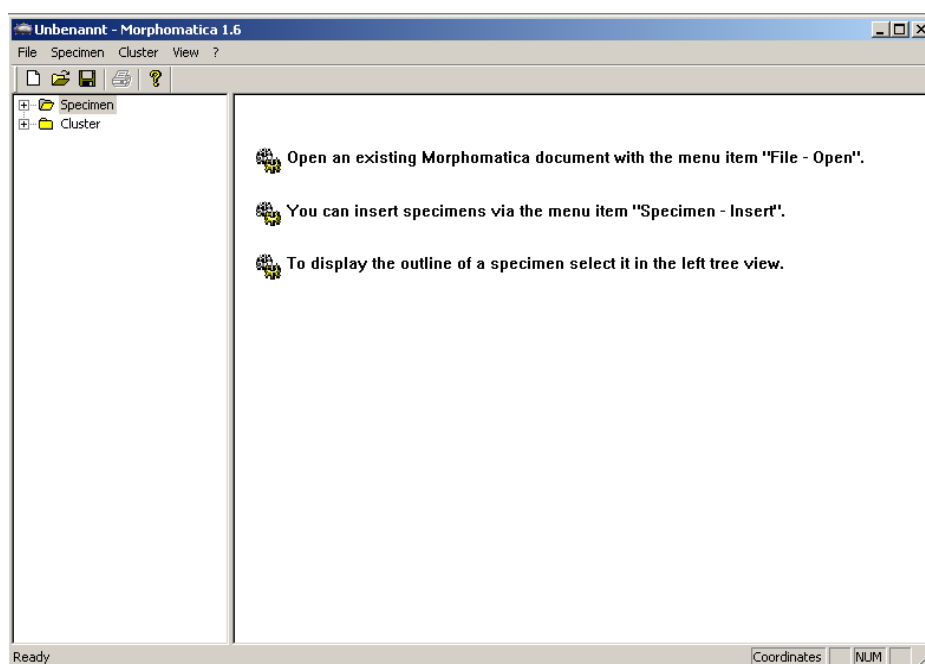
The following topics will be introduced:

- Create a new MORPHOMATICA document
- Insert a specimen from a file and how to work with it
- Calculate the approximation for the outline of a specimen
- Combine several specimen to a cluster, calculate the cluster mean and corresponding delta vectors

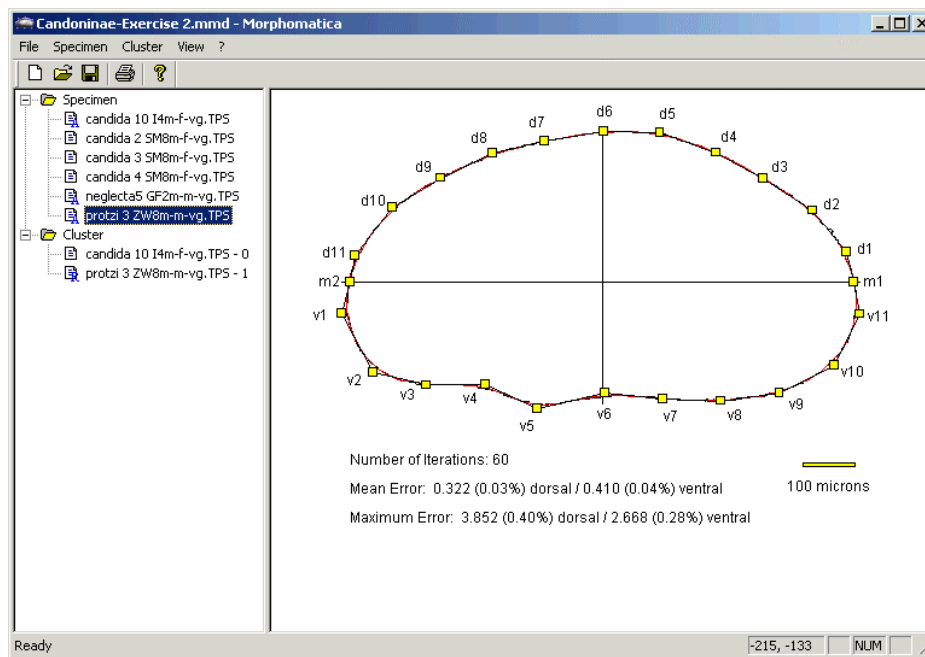
- Export specimen and cluster data for import into other applications
- Print specimen outlines and computational data
- Save a MORPHOMATICA document

The User Interface of MORPHOMATICA

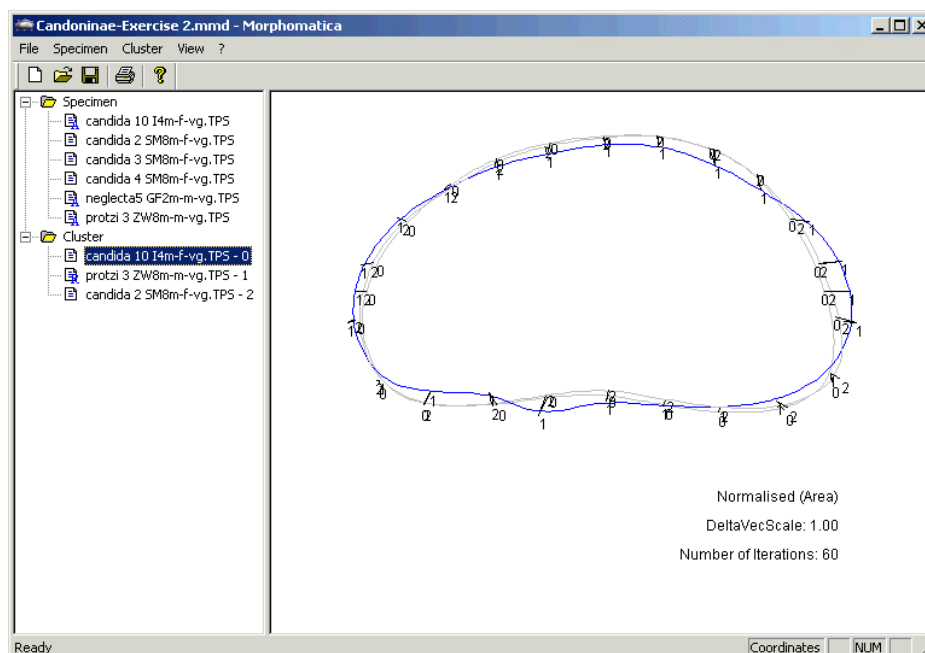
The user interface consists of a main application window, which is partitioned into two adjoining areas, and several dialog objects, which are displayed when additional input is required or parameters are to be manipulated. In the left part of the main window, the file names of the imported ostracod outlines and the associated approximations and clusters are displayed in the style of a directory tree. In this tree view, the user can select the file he intends to work on.



The contents of the right part of the window depend on the selected entry in the tree view. If an imported ostracod outline in the specimen directory of the tree view is selected, the right pane - the specimen view - displays its outline and if an approximation was calculated for the specimen, the according B-spline is drawn.



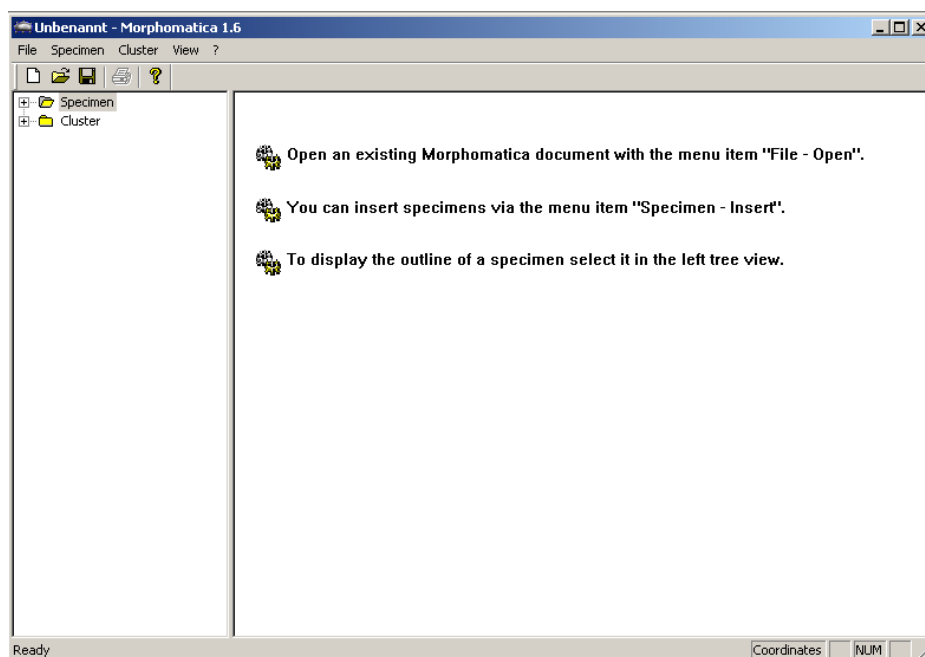
If alternatively an entry in the cluster directory of the tree view is selected, then the approximations of all specimens contained in the cluster, the associated delta vectors, and the optional mean specimen outline are displayed in the cluster view in the right pane.



Create a new MORPHOMATICA document

A new document is created every time MORPHOMATICA is executed. This means, that the document does not contain any specimen or corresponding approximation, and that all program parameters are initialised with certain predefined reasonable values. Alternatively, the user can create a new document with the menu item *File - New* at any time. If there is already an existing document being worked with, the user will be asked if he intends to save it. Without saving the contents of the previous document are discarded.

After the creation of a new document, the main program window looks as following:



As mentioned before, no specimens are contained in a new document. Now, you have to import specimens from an appropriate file format into the document.

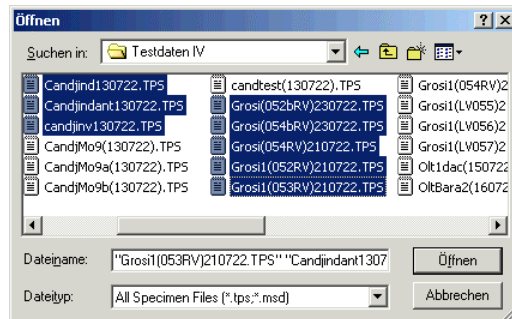
Working with a specimen

Insert a specimen into the document

To insert one or more specimens from a file into the document, use the menu item *Specimen - Insert*. MORPHOMATICA supports the file formats

- *.tps, a file format used by DigiTPS.
- *.msd, files created with the program Morphosys - in case that the file extension is different at your system, enter the appropriate extension in the "Filename" field.

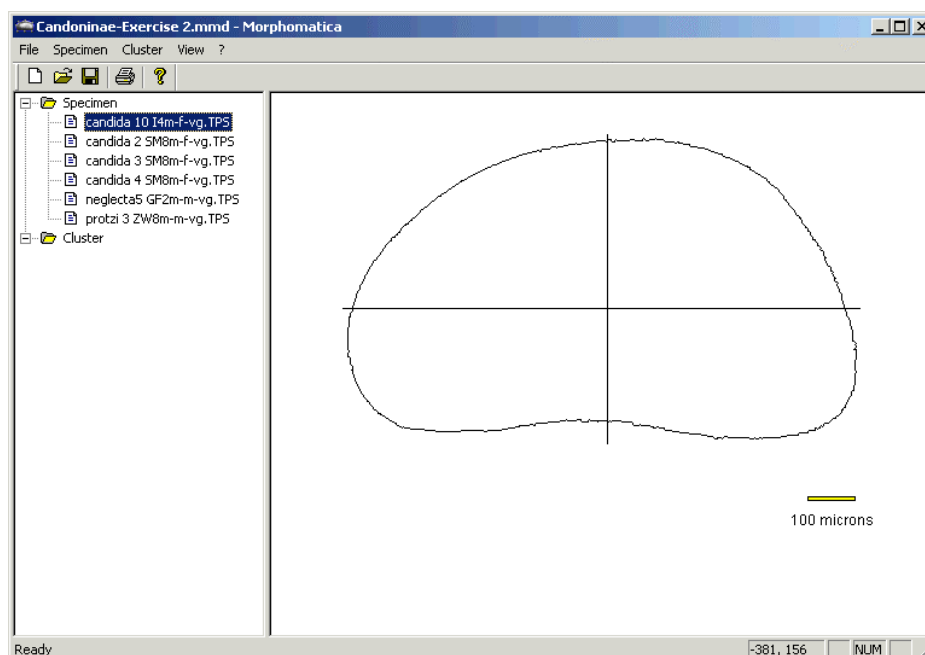
In the next step, an open dialog will be displayed in which you select the file(s) with the ostracod(s) you intend to import. The open dialog allows you to select one or more files at the same time:



After confirming the dialog with “open”, the specimens contained in the selected files are inserted into the document. Those specimens will be added to the specimen directory in the tree view with their related file names. If more than one specimen is stored in the imported file, the entries in the tree view are extended with an enumeration.

Display the outline of a specimen

To display the outline of an imported specimen you just have to select its name in the tree view on the left. The currently selected specimen is marked in the tree view with a blue background. The outline is displayed in the specimen view with additional information like the corresponding scaling of the outline or the coordinate axes.



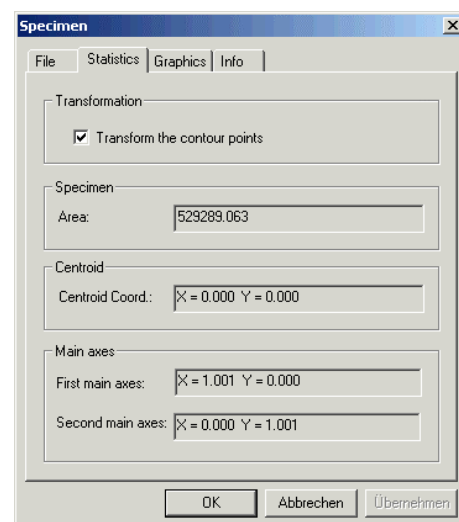
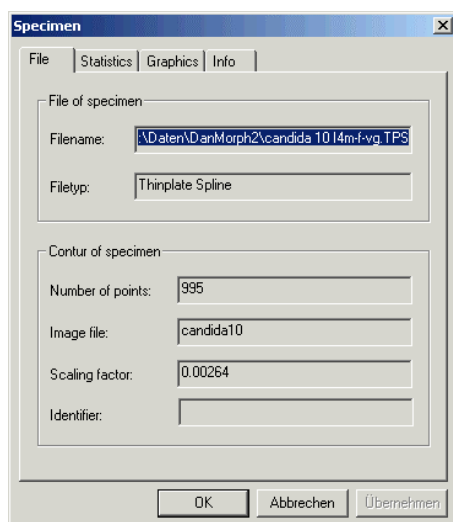
Remark: If a scale is stored for a specimen in the imported file, the scale labelled “100 micro meters” is shown, otherwise a scale labelled “100 pixel” is displayed.

Remark: Basically, a rotation and translation is automatically applied to every imported specimen such that the centroid of the specimen is located in the origin of the coordinate system and that the main axes of inertia are parallel to the coordinate axes.

Display file information for imported specimen

The file properties of a specimen can be shown with the menu entry *Specimen - Properties* and are located within the first property page *File* (see below, left).

The path of the file where the specimen was imported from is displayed at the top of the dialog, immediately followed by the file type. Additional information of the outline is displayed as well.

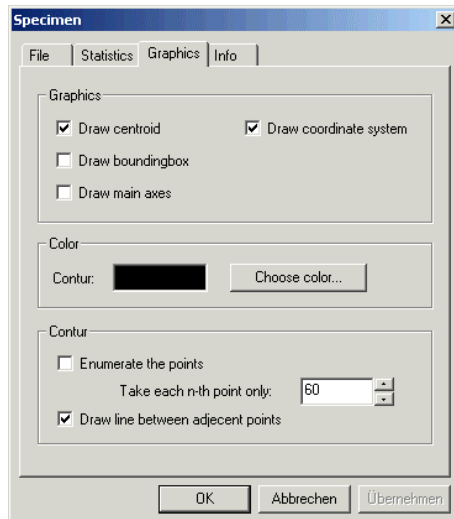


Display statistical data for specimen

Mathematical parameters, which are calculated from the outline defined in the specimen data file, are displayed within the property page *Statistics* (see above, right). As already mentioned, an imported specimen is transformed to meet certain conditions. The mathematical parameters for the transformation are listed below. If you do not want the outline to be transformed you can deselect the check box at the top of the dialog. In that case, the outline is displayed using the coordinates as defined in the data file.

Settings for the graphical representation

There are several options for the representation of the outline of a specimen. To set the options for a specific specimen, select its name in the tree view and choose the menu item *Specimen - Properties*. After opening the property page called *Graphics* the following options are shown:



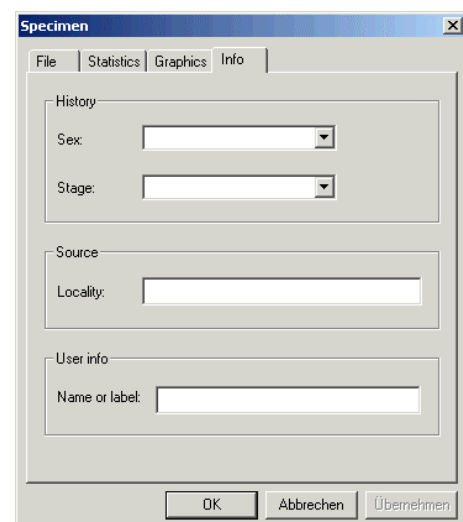
It is possible to change the following options:

- *Draw centroid*: If the check box is activated, the centroid of the specimen is marked.
- *Draw bounding box*: The bounding box enclosing all points of the outline of the specimen, as well as the coordinates of the corner points of this rectangle are displayed.
- *Draw main axes*: Selects, whether the main axes of inertia are drawn or not. This option is useful if the outline is not transformed to normal position.
- *Draw coordinate system*: Option to draw the axes of the coordinate system.
- *Colour*: To choose the colour for the specimen.
- *Enumerate the points (of contour)*: If the option is activated, then the points of the outline will be enumerated (only the number of each n-th point will be printed).
- *Draw line between adjacent points*: Given that the distance between the points of the outline is too large to form a continuous outline, selecting this option will connect the points with straight line segments.

Additional morphological data

Not only the imported outline of a specimen can be saved in a MORPHOMATICA document, it's also possible to specify additional morphological data.

For this, choose the menu item *Specimen - Properties* and in that dialog the page *Info*.



Remove a specimen from a MORPHOMATICA document

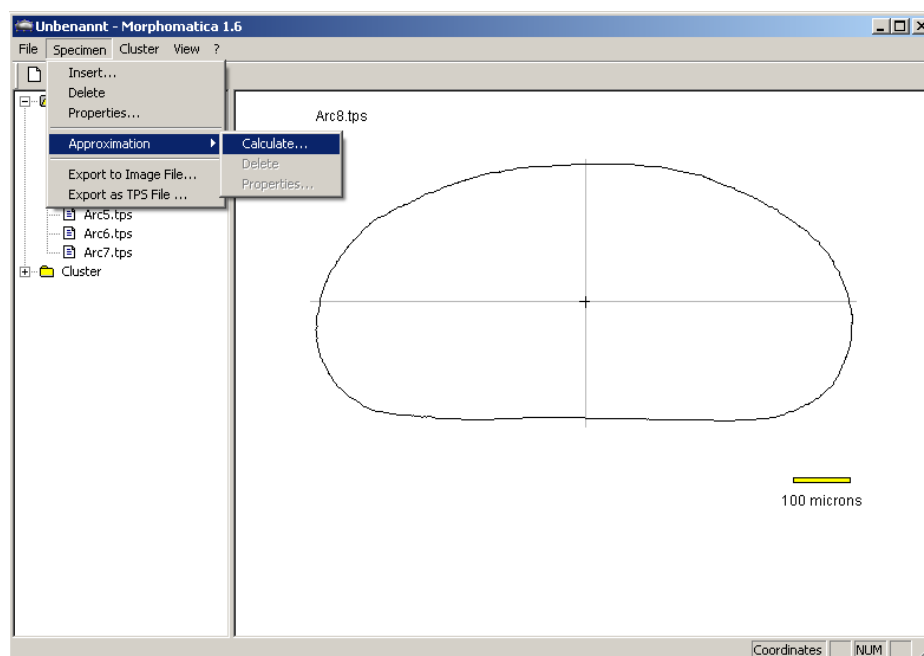
A specimen can be removed from the document at any time by selecting its name in the tree view and selecting the menu item *Specimen - Delete*. Alternatively, pressing the „Del“ - Key deletes the selected specimen.

Approximate a specimen

The outline of each specimen can be approximated with the B-spline method described in the Mathematical background section. The calculated approximation is drawn together with the outline in the specimen view.

Calculation of the approximation

To calculate the approximation from a selected specimen select the menu item *Specimen - Approximation - Calculate*.

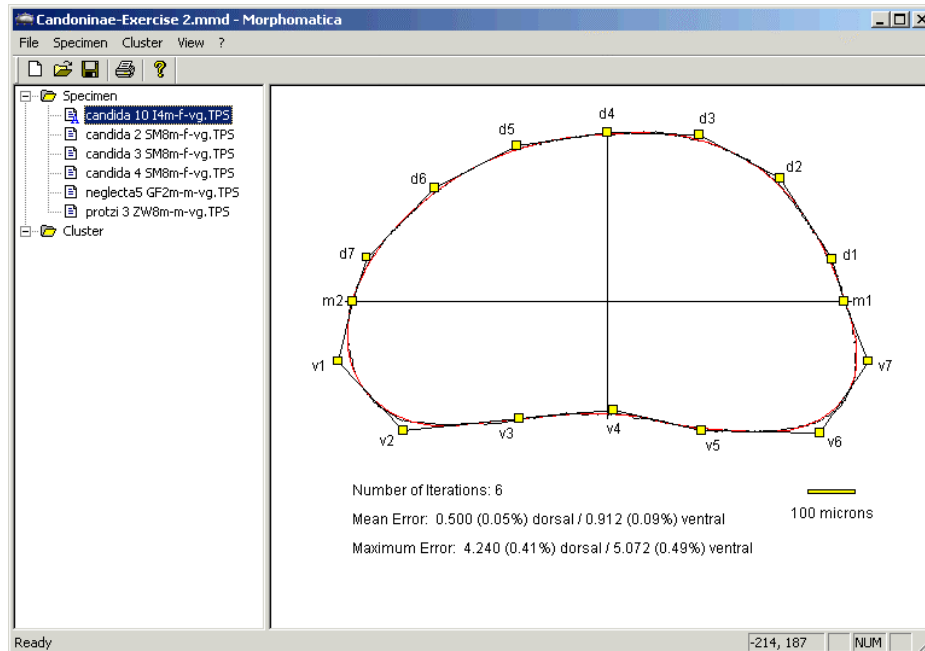
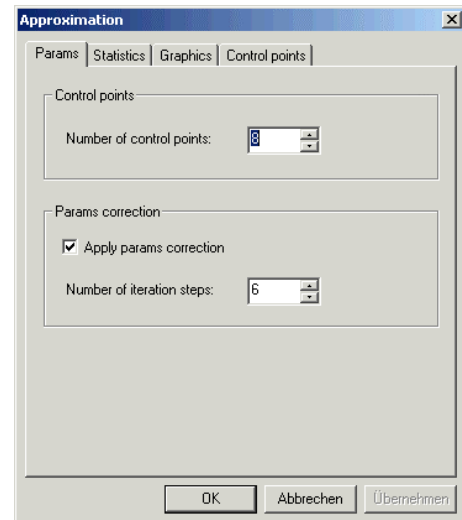


Parameters for the approximation

In the up-coming dialog, several parameters for the approximation can be varied.

It is possible to specify the number of control points to be calculated and the number of iterations for the parameter correction to be applied.

Next, the approximating B-splines are drawn over the outline of the specimen. Additionally, the control points of the upper and lower half of the B-splines are displayed and enumerated, as well as the corresponding control polygon. The calculated values for the approximation (such as the number of iterations, mean and maximum approximation error of the upper and lower half) are shown in the lower left corner of the specimen view.

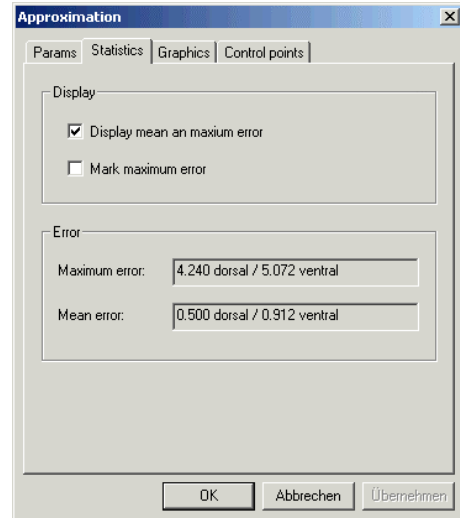


Remark: A specimen for which an approximation is fitted, is marked with a blue "A" next to its file name in the tree view.

Statistical data of the approximation

The calculated approximation values are listed in the property page *Statistics* too.

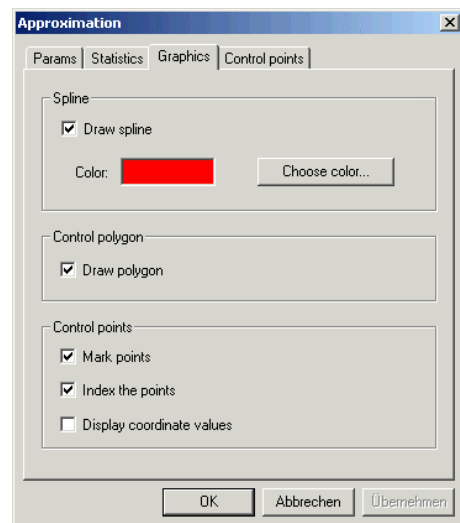
There it is also possible to select, whether the error values are to be displayed in the specimen view or not.



Settings for the graphical representation of the B-splines

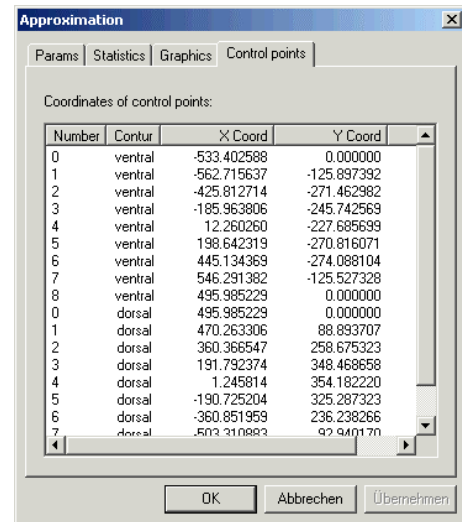
As with the representation of the outline of a specimen, there are several options for the representation of the approximating B-splines, which are accessible under the menu *Specimen - Approximation - Properties*. After selecting this menu item the following options are displayed in the property page *Graphics*. It is possible to vary the following options:

- *Draw spline*: If this check box is activated, the control points are drawn over the outline of the specimen. It is also possible to change the colour of the B-spline there.
- *Draw polygon*: By selecting this entry, the control polygon is drawn.
- *Mark points*: The control points are marked with yellow-filled rectangles. If the cursor is over any of those rectangles, the coordinates of the corresponding control point are displayed.
- *Index the points*: Each control point is enumerated.
- *Display coordinate values*: The coordinates of each control point are written next to it.



Display the calculated control points coordinates

The calculated control points can also be requested via the menu item *Specimen - Approximation - Calculate*.



Number	Contur	X Coord	Y Coord
0	ventral	-533.402588	0.000000
1	ventral	-562.715637	-125.897392
2	ventral	-425.812714	-271.462982
3	ventral	-185.963806	-245.742569
4	ventral	12.260260	-227.685699
5	ventral	198.642319	-270.816071
6	ventral	445.134369	-274.088104
7	ventral	546.291382	-125.527328
8	ventral	495.985229	0.000000
0	dorsal	495.985229	0.000000
1	dorsal	470.263306	88.893707
2	dorsal	360.366547	258.675323
3	dorsal	191.792374	348.468658
4	dorsal	1.245814	354.182220
5	dorsal	-190.725204	325.287323
6	dorsal	-360.851959	236.238266
7	dorsal	-503.310893	92.940170

Changing the approximation parameters

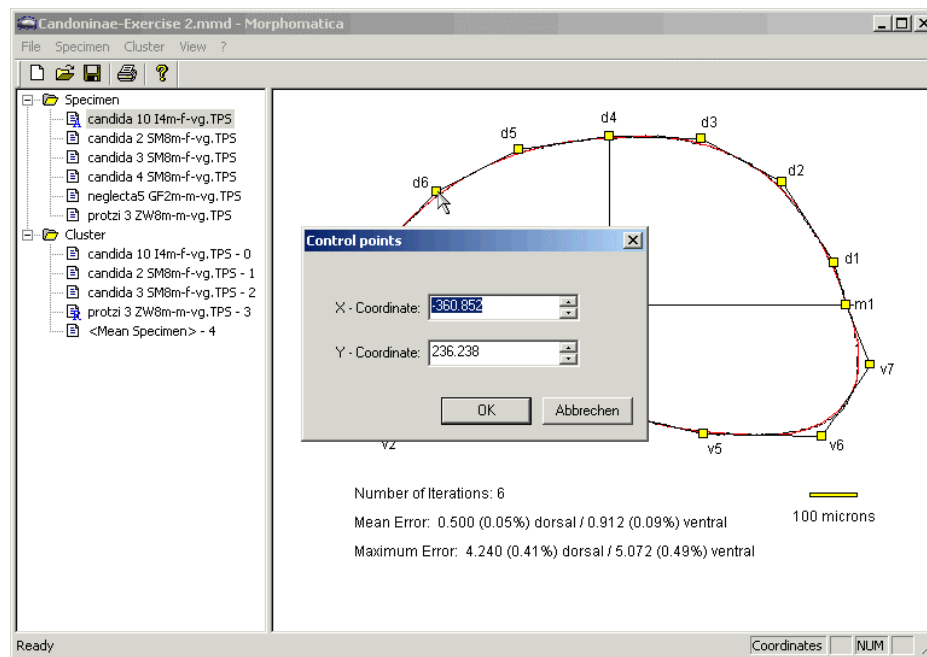
The parameters of an existing approximation can be changed with the menu item *Specimen - Approximation - Properties* at any time. In the general case a parameter change forces a recalculation of the approximation.

Delete the approximation of a specimen

An approximation of a specimen can be deleted with the menu item *Specimen - Approximation - Delete*.

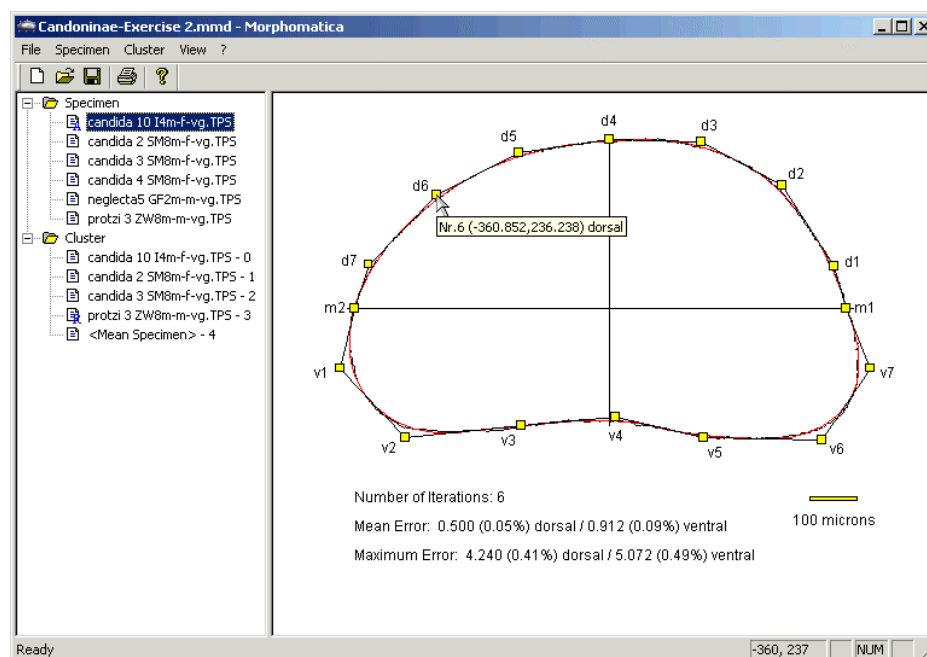
Change a control point interactively

The user can change the calculated control points interactively. To do this click on the yellow rectangle representing the control point you want the coordinates to change. The fields of the upcoming dialog are initialised with the actual position. You can now change the position by entering the new coordinates directly or by pressing the up and down cursor buttons next to the fields.



After closing the dialog with Ok, the B-spline is recalculated and the new approximation is drawn.

Remark: Place the mouse cursor over the yellow rectangle representing a control point if you want to know its coordinate values.



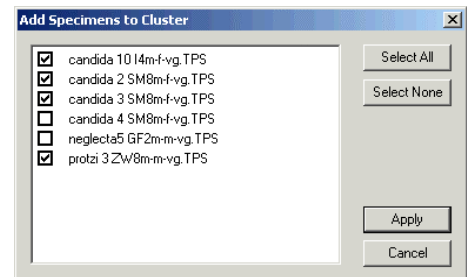
Cluster view of specimens

In the cluster view the approximating B-splines of all specimens in the cluster are simultaneously drawn over each other. This allows an easier comparison between several specimens in interest.

Add a specimen to the cluster

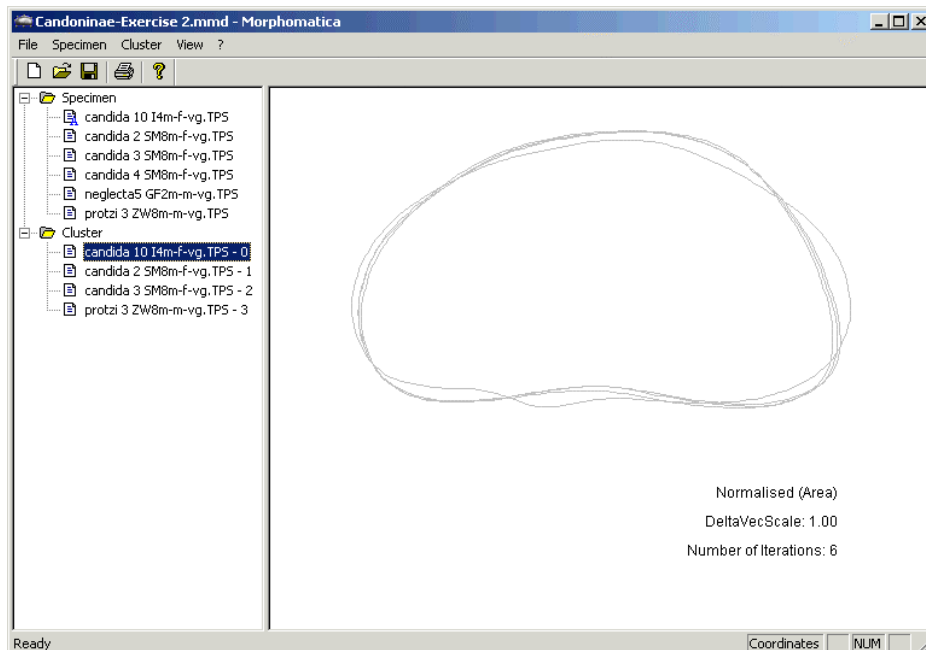
To insert a specimen from the specimen list into the cluster, mark its name in specimen directory of the tree view. Next insert the specimen with the menu item *Cluster - Insert*.

The filename of the specimen is appended in the cluster directory of the tree view.



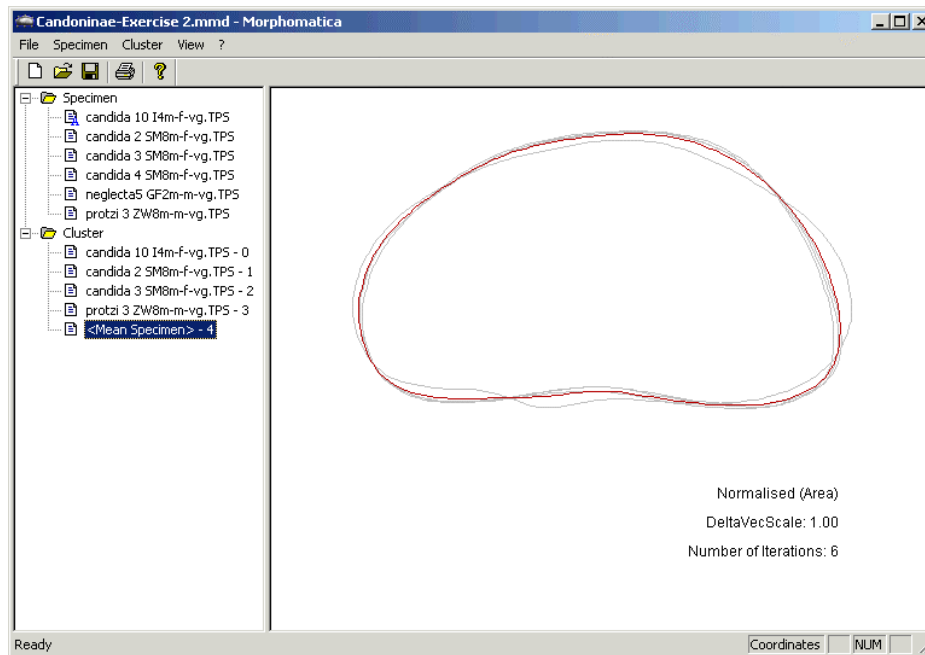
Alternatively, a specimen can be inserted to the cluster with a typical drag and drop operation within the tree view from the specimen directory into the cluster directory. If more specimens are to be inserted into the cluster, a convenient way is via the menu item *Cluster - Select*.

At the same time you add a specimen to the cluster the corresponding cluster approximation is calculated. Containing several specimens, the cluster view looks like the following:



Calculation of the cluster mean

As soon as one or more specimens are added to the cluster, the mean specimen of these can be calculated with the menu item *Cluster - Calculate mean specimen*. The outline of this mean specimen is drawn in the cluster view too, using a different colour. An entry named “<Mean Specimen>” is added in the cluster directory of the tree view representing this mean specimen.



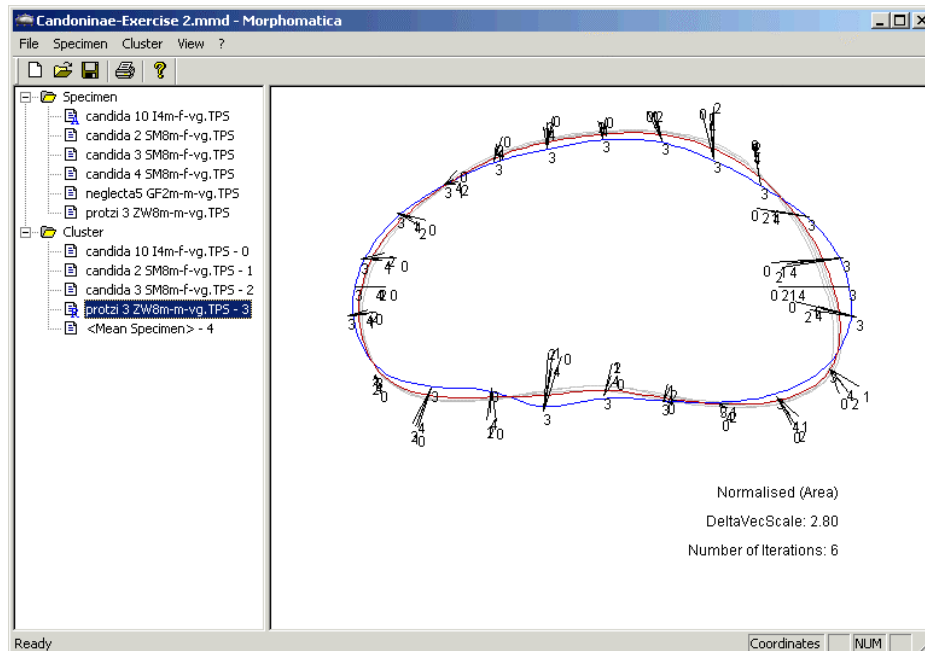
Remark: The mean specimen is not recalculated if new specimens are added to the cluster or specimens are removed from it. This behaviour is deliberate, such that multiple ways of comparison with the mean specimen are possible.

Selecting a specimen as reference

After two or more specimens are present in the cluster, one of these can be defined as the cluster reference. To define a specimen in the cluster as reference, select its name in the cluster directory of the tree view and use the menu item *Cluster - Mark as reference*.

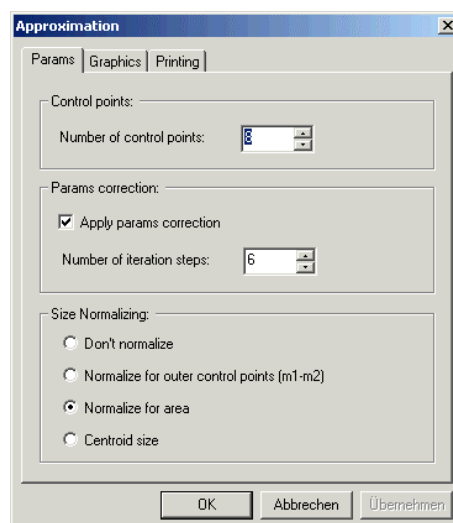
Automatically with the selection of a specimen as cluster reference, the delta vectors between this cluster reference specimen and all other specimens in the cluster are calculated and displayed. The name in the cluster directory of the reference specimen is further marked with a blue “R” next to it, to identify it as reference.

Remark: If the cluster reference specimen is changed, the delta vectors are automatically recalculated and actualised in the cluster view.



Settings for the cluster approximation parameters

If you need to change the parameters of the cluster, select the menu item *Cluster - Properties*. You can set the parameters for the approximation (of all specimens in the cluster) in the upcoming dialog (like before in the approximation for a single specimen).

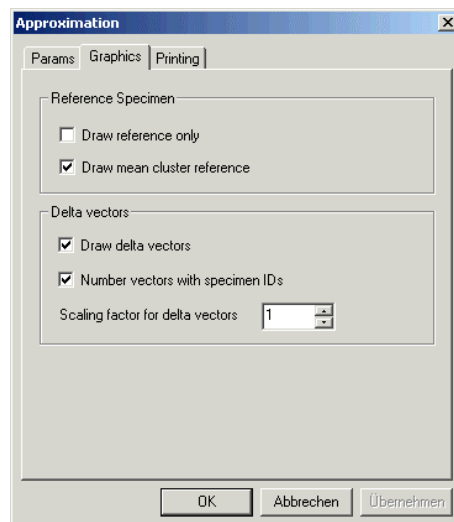


The options are as follows:

- Number of control points for upper and lower B-spline
- Number of steps in the parameter correction (the mathematical method used to improve the calculation of the approximation)
- Apply various normalisation operations. This allows for a size independent comparison of specimens.
 - *Normalize for outer control points:* The specimen approximations (i.e. the two B-splines) are transformed, such that the cluster points m1 on the left side and m2 on the right side of all specimens fit together.
 - *Normalize for area:* The specimen approximations are transformed, such that all have equal area (1000).
 - *Normalize for centroid size:* The specimen approximations are transformed, such that all have equal values for the centroid size of the outlines (the square root of the sum of squared Euclidean distances from each contour point to the centroid divided by the number of contour points k).

Settings for the cluster representation

It is possible to change the graphical representation with the menu item *Cluster - Properties*. The following options are shown in the property page *Graphics* of the property sheet.

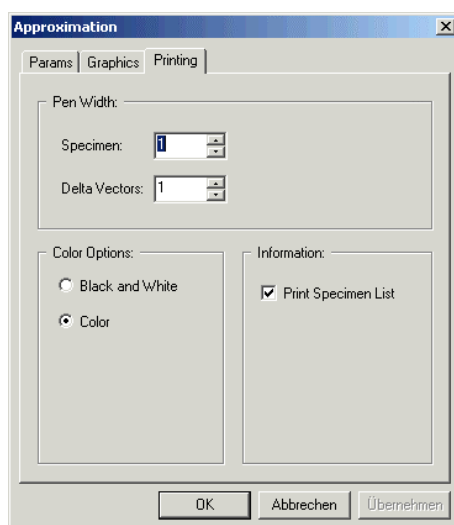


The following options can be set:

- *Draw reference only*: If this option is selected, only the reference specimen (but together with all the delta vectors) is drawn.
- *Draw mean cluster reference*: If the check box is activated, the mean specimen is drawn.
- *Draw delta vectors*: Whether the delta vectors should be displayed or not.
- *Number vectors with specimen Ids*: The endings of the delta vectors can be marked with the number of the specimen in the cluster view corresponding to the number in the cluster directory of the tree view.
- *Scaling factor for delta vectors*: Use this to scale the delta vectors appropriately. If two specimens are hardly different, this option can be used for a better comparison.

Settings for the print parameters

It is possible to change the printing settings in the property page *Printing* from the menu item *Cluster - Properties*.



The following settings can be applied:

- *Pen Width Specimen*: Specifies the pen width for the specimen in the printout.
- *Pen Width Delta Vectors*: Specifies the pen width for the delta vectors in the printout.
- *Colour Options*: Whether colour (e.g. for a overhead beamer presentation) or only black/white (e.g. for a paper) should be used.
- *Print Specimen List*: Should a separate list with the names of the specimens in the cluster be printed?

Listening the calculated cluster data

The calculated cluster data can be displayed with the menu item *Cluster - Display coordinates*. This replaces the cluster view in the right pane of the main application window with a spread sheet view, which lists all the relevant data of the cluster (such as the names of specimens, all calculated control points and the delta vectors to the reference specimen).

The meanings of the column headers are as follows:

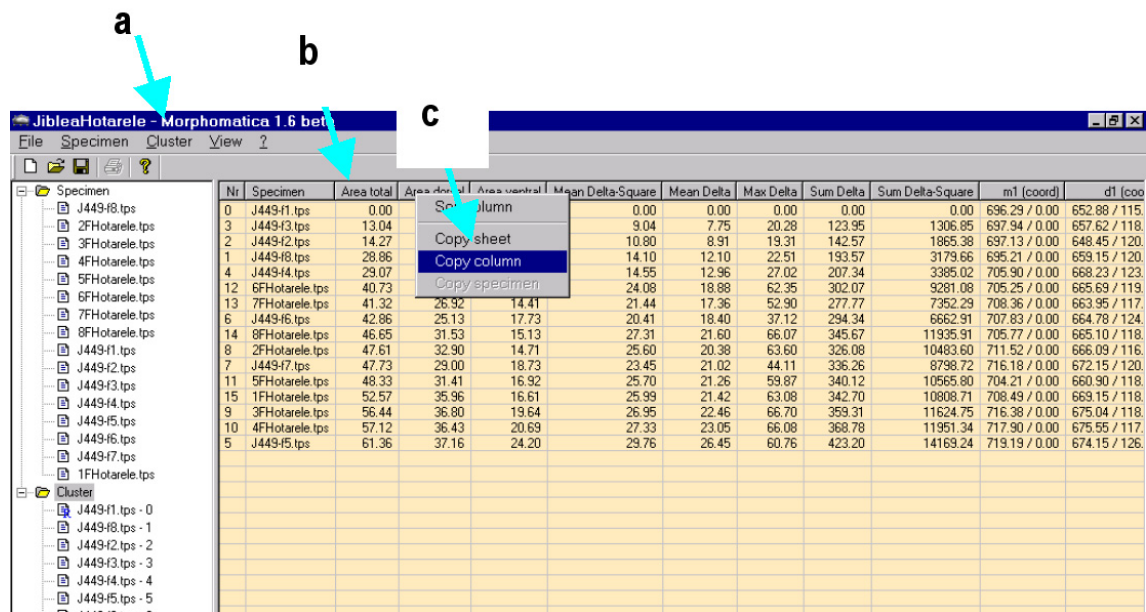
- *Nr*: Number of specimen according to its number in tree view.
- *Specimen*: Shorted file name of the specimen (including its position inside the file if necessary).
- *Area total*: Is the area deviation between the given specimen and the reference specimen.
- *Area dorsal*: Area total applied to the dorsal region only.
- *Area ventral*: Area total applied to the ventral region only.
- *Sum Delta*: Is the sum of all Euclidian distances between control points for the given specimen and those of the reference specimen.
- *Mean Delta*: Is the sum of the delta lengths divided by the number of control points.
- *Max Delta*: Is the maximum value in the set of Euclidian distances (delta length) between control points for the given specimen and those of the reference specimen.

- *Sum Delta-Quad*: Is the sum of all squared Delta Lengths (i.e. the Euclidian distances between the control points of a specimen and the corresponding homologous of the reference outline).
- *Mean Delta-Quad*: Is the square root of the Sum Delta-Quad divided by the number of control points.
- *Remaining columns*: Coordinates of the calculated control points (d...dorsal, v...ventral).

The specimen selected in the tree view, is marked in the cluster data view with a grey background.

The rows of the table can be sorted depending on the values in a column by clicking on this column header.

It is possible to copy either the whole sheet of displayed data or selected columns. For this action for instance select *Cluster - Display coordinates*, click on a column (Fig. below, see b), press the right key-mouse, move arrow to *Copy column* (Fig. below, see c). Open in Excel a new file and click *Insert*.

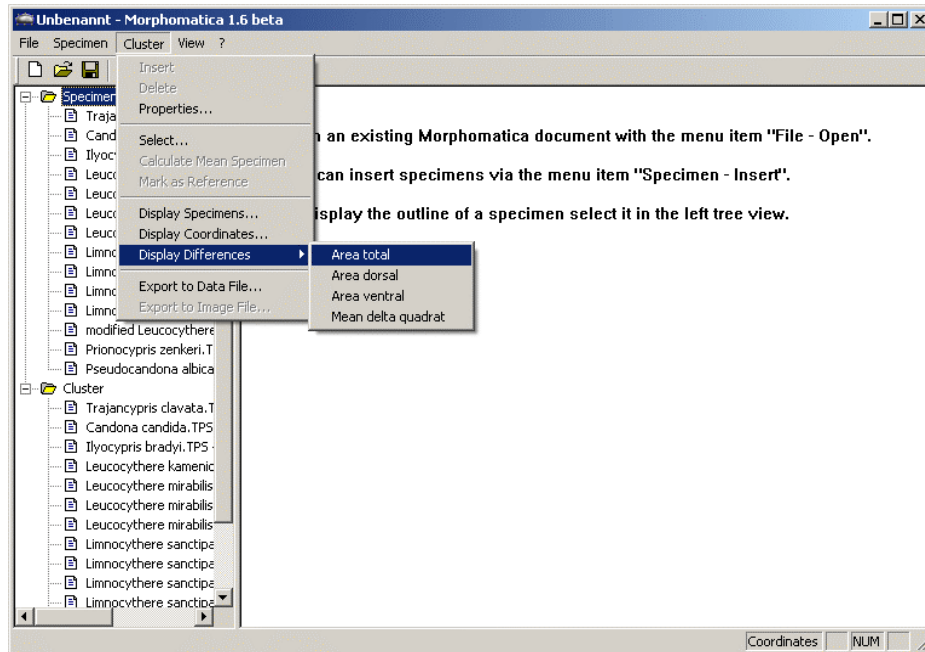


Evaluating of pairwise differences

The menu *Cluster – Display differences* shows a comparison of each two approximating B-splines of all specimens. The method of calculation can be chosen before. The result relies on the selected size normalization. The following methods are available:

- *Area total*: Evaluates the area between two approximating B-splines.
- *Area dorsal*: Area total applied to the dorsal region only.
- *Area ventral*: Area total applied to the ventral region only.
- *Mean delta square*: Is the square root of the sum of all Euclidian distances between the control points of two B-splines divided by the number of control points.

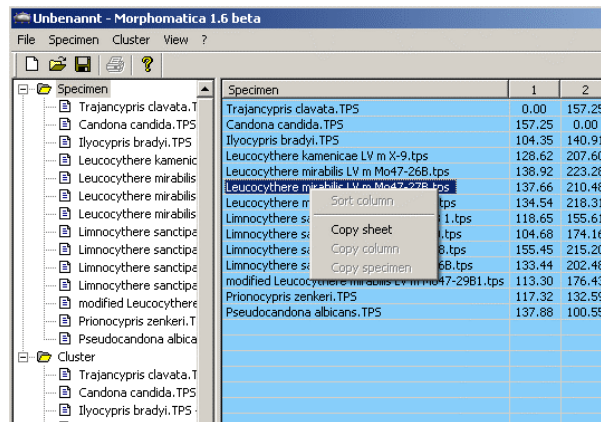
The possible methods of calculating and evaluating differences appear after choosing the menu item.



After selecting the method a matrix with the calculated values is printed out.

Specimen	1	2	3	4	5	6	7
Trajancypis clavata.TPS	0.00	157.25	104.35	128.62	138.92	137.66	134.54
Candona candida.TPS	157.25	0.00	140.91	207.60	223.28	210.48	218.31
Ilyocypris bradyi.TPS	104.35	140.91	0.00	110.93	114.40	79.55	95.42
Leucocythere kamenic	128.62	207.60	110.93	0.00	28.51	52.28	36.43
Leucocythere mirabilis LV m Mo47-268.tps	138.92	223.28	114.40	28.51	0.00	47.41	31.06
Leucocythere mirabilis LV m Mo47-278.tps	137.66	210.48	79.55	52.28	47.41	0.00	23.26
Leucocythere mirabilis LV m Mo47-2981.tps	134.54	218.31	95.42	36.43	31.06	23.26	0.00
Limnocythere sanctipatrii LV f Mo41-28 1.tps	118.65	155.61	47.30	81.29	79.88	68.57	78.00
Limnocythere sanctipatrii LV f Mo41-30.tps	104.68	174.16	67.11	62.29	60.90	59.42	61.20
Limnocythere sanctipatrii LV m Mo41-28.tps	155.45	215.20	138.65	71.22	92.73	100.61	99.37
Limnocythere sanctipatrii LV m Mo47-268.tps	133.44	202.48	122.17	47.85	70.36	81.32	77.11
modified Leucocythere mirabilis LV m Mo47-2981.tps	113.30	176.43	51.20	72.43	75.35	43.03	53.04
Prionocypris zenkeri.TPS	117.32	132.59	94.66	186.11	186.71	152.83	167.31
Pseudocandona albicans.TPS	137.88	100.55	116.68	175.74	196.41	183.34	191.41

By clicking the right mouse button into the matrix a menu, including options for processing appears.



Choosing the menu item *Copy sheet* will copy the matrix into the clipboard where the data are available for further work in other applications (e.g. MS Excel, Primer).

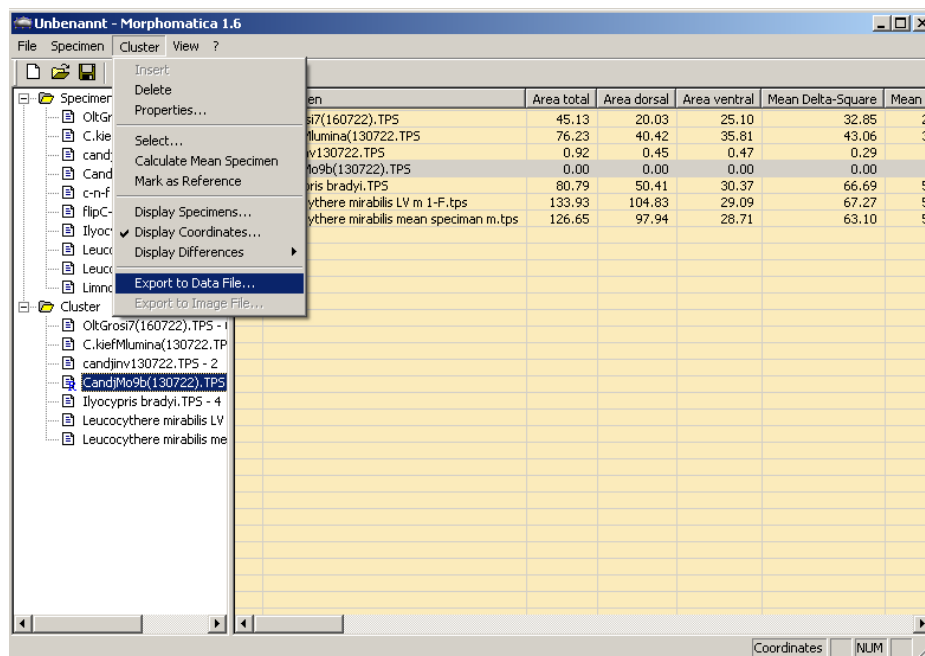
Example of an exported sheet opened with MS Excel:

	A	B	C	D	E	F	G	H	I
1	Trajancypis clavata.TPS	0	157.25	104.35	128.62	138.92	137.66	134.54	118.65
2	Candona candida.TPS	157.25	0	140.91	207.6	223.28	210.48	218.31	155.61
3	Ilyocypris bradyi.TPS	104.35	140.91	0	110.93	114.4	79.55	95.42	47.3
4	Leucocythere kamenicae LV m X-9.tps	128.62	207.6	110.93	0	28.51	52.28	36.43	81.29
5	Leucocythere mirabilis LV m Mo47-26B.tps	138.92	223.28	114.4	28.51	0	47.41	31.06	79.88
6	Leucocythere mirabilis LV m Mo47-27B.tps	137.66	210.48	79.55	52.28	47.41	0	23.26	68.57
7	Leucocythere mirabilis LV m Mo47-29B1.tps	134.54	218.31	95.42	36.43	31.06	23.26	0	78
8	Limnocythere sanctipatricii LV f Mo41-28 1.tps	118.65	155.61	47.3	81.29	79.88	68.57	78	0
9	Limnocythere sanctipatricii LV f Mo41-30.tps	104.68	174.16	67.11	62.29	60.9	59.42	61.2	29.08
10	Limnocythere sanctipatricii LV m Mo41-28.tps	155.45	215.2	138.65	71.22	92.73	100.61	99.37	108.29
11	Limnocythere sanctipatricii LV m Mo47-26B.tps	133.44	202.48	122.17	47.85	70.36	81.32	77.11	89.39
12	modified Leucocythere mirabilis LV m Mo47-29B1.tps	113.3	176.43	51.2	72.43	75.35	43.03	53.04	45.42
13	Prionocypris zenkeri.TPS	117.32	132.59	94.66	186.11	186.71	152.83	167.32	130.26
14	Pseudocandona albicans.TPS	137.88	100.55	116.68	175.74	196.41	183.34	191.4	137.45
15									
16									
17									
18									
19									
20									
21									
22									
23									

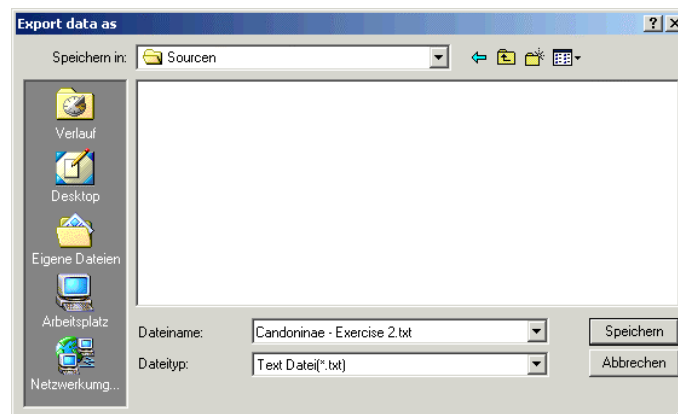
Remark: Due to the structure of the algorithm for computing the area deviation of shapes where the approximating B-spline changes direction cannot be calculated. In this case an error message comes up and you get the entry "n.c." for "not calculable" into the concerning cell. As a rule, such shapes occur only in faulty datasets.

Export specimen and cluster data

The calculated data of the cluster can be exported as a text file by using the menu item *Cluster - Export data*. The contents to export depend on the selected entry in the tree view.



In the upcoming dialog, you have to specify a file name for the export file.



After saving, this text file can be opened and further worked with (e.g. with MS Excel or other statistical programs).

Example of an exported text file opened with MS Excel:

Microsoft Excel - Candoninae - Exercise 2 - Export Cluster.txt

File Edit View Insert Format Tools Data Window Help

Arial 10 B I U

A1 = Specimen Info:

Specimen Name	Image File	Locality	Sex	Stage	Identifier
candida 10 l4m-fvg	candida10				
candida 2 SM8m-fvg	candida				
candida 3 SM8m-fvg	candida				
protzi 3 ZW8m-m-vg	protzi				
<Mean Specimen>					

Cluster Info:

Specimen Name	Mean Delta	Max Delta	Sum Delta	Sum Delta Qu	Mean Delta Quadrat
candida 10 l4m-fvg	39.561	79.406	949.462	46.714.844	44.119
candida 2 SM8m-fvg	32.866	67.451	788.779	32.621.813	36.868
candida 3 SM8m-fvg	35.620	68.589	854.889	37.803.234	39.688
protzi 3 ZW8m-m-vg	0.000	0.000	0.000	0.000	0.000
<Mean Specimen>	26.721	52.725	641.311	21.345.439	29.823

Cluster Approximation for Specimen: candida 10 l4m-fvg.TPS

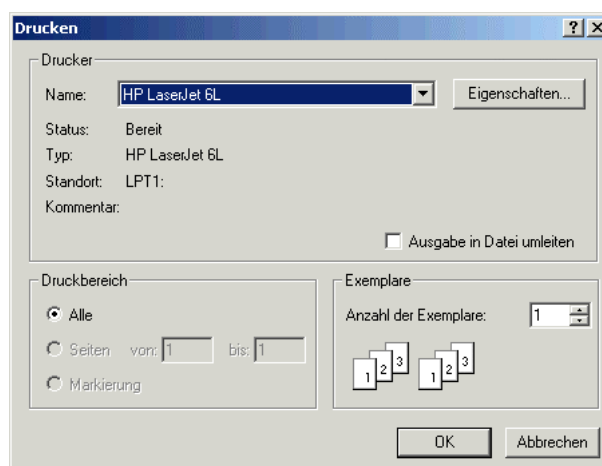
Index	Control Point	Delta Vector	Delta Length
	x y	x y	
m1	682.153 0.000	-79.230 0.000	79.230
d1	661.217 85.193	-79.207 -5.618	79.406
d2	577.713 227.285	-57.830 9.168	58.552
d3	477.239 363.250	-9.704 48.649	49.608
d4	327.898 448.340	-13.562 53.795	55.479
d5	164.820 485.552	-15.182 32.556	35.922
d6	3.639 483.057	3.188 24.977	25.179

Candoninae - Exercise 2 - Export

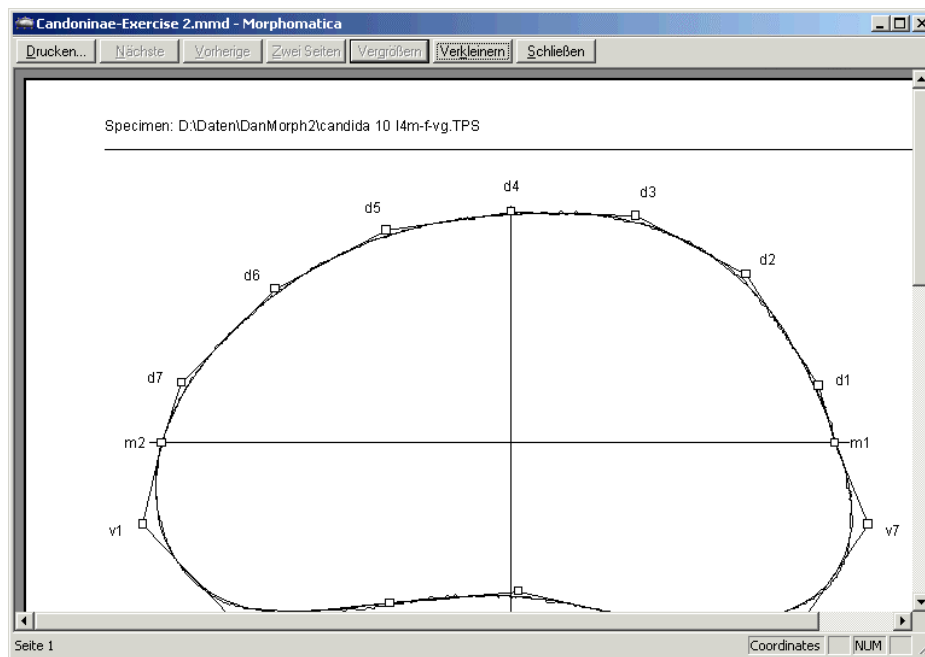
Ready NUM

Print a MORPHOMATICA document

The contents of a MORPHOMATICA document can be printed with the menu item *File - Print*. The contents to be printed depend on the selected entry in the tree view.



You can check the output before printing with the menu item *File - Print Preview*.

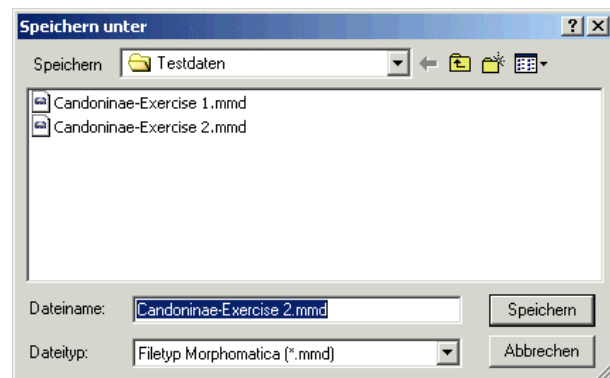


The printer settings (portrait, landscape, A4 or A3 format, etc.) can be done with the menu item *File - Print Setup*.

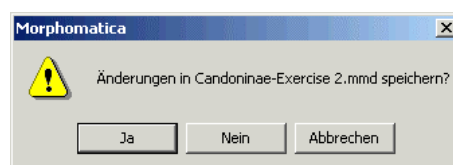
Save a MORPHOMATICA document

A MORPHOMATICA document can be save with the menu item *File - Save*.

You have to specify the desired path and file name (the file is saved in a XML file format).



If MORPHOMATICA will be closed and the current document is changed but not saved, the user is informed and the document can be saved immediately.



The complete contents of the MORPHOMATICA document are saved in a XML file. The files from which the specimens were imported are therefore no longer necessary. So, it's e.g. possible to send the XML file (with the extension *.mmd) alone per email to another user of MORPHOMATICA.

Remark: It is also possible to extract the specimens again in the TPS file format (Menu: Specimen -Export as TPS file).

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ZOBODAT - www.zobodat.at

Zoologisch-Botanische Datenbank/Zoological-Botanical Database

Digitale Literatur/Digital Literature

Zeitschrift/Journal: [Berichte des Institutes für Geologie und Paläontologie der Karl-Franzens-Universität Graz](#)

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