

## (IMPORTANT) UPDATES IN IMAGIC COMMANDS

APRIL - SEPTEMBER 2014

### HEADER UPDATE:

>> New header index NUMFRAME / IDAT(74): Number of movie frames

### BUG FIXES:

>> EM2EM

Some bug fixes

>> DISPLAY

Option READ\_COORDINATES corrected

Option SAVE corrected

>> HEADERS

PRINTOUT of EM values: focal distance and spherical aberration exchanged

>> IMAGIC\_TO\_FREALIGN

Problems with output MRC file corrected

>> PICK-PARTICLES

Tale over EM and defocus values

### UPDATES:

>> ALIGN-IMAGE

Command ALIGN-DIRECT-IMAGE renamed to ALIGN-IMAGE

>> ALIGN-MOVIE-FRAMES

Many updates

>> ALIGN-IMAGE

Alignment can be started with and without input reference file

MPI parallelisation added

Many other updates

>> BINNING-IMAGES

New command. Same as COARSEN-IMAGE

>> CENTER-IMAGE

Help updated

>> CREATE-IMAGE

Some updates and corrections

- >> CREATE-PRETREATED-AMPLITUDES  
The pre-treated amplitudes can be resized/coarsened
- >> CTF-FIND  
User interaction changed
- >> CTF-FLIP  
MPI parallelisation added  
Does not use classes any more. These values can easily be taken over from class averages to their members (command HEADERS)
- >> DISPLAY  
If the display image is filled with images DISPLAY asks how to continue.  
New options added: PREVIOUS, NEXT etc.
- >> EQUIVALENT-MOVE and EQUIVALENT-SHIFT  
New commands, which are the same as EQUIVALENT-ROTATION
- >> EQUIVALENT-MOVE  
Take over of input header values updated  
If images in input file and images in file with “equivalent” parameters have different sizes ask if the parameters should be corrected accordingly or not
- >> EM2EM / IMPORT-EXPORT-IMAGES  
New format PROTOMO added  
“FEI” is an allowed import format. User is subsequently asked for additional details  
User interaction for TIFF updated
- >> EXCLUDE-IMAGE  
New command (using the EXCLUDE option EXCLUSIVE-COPY)
- >> EXTRACT-IMAGE  
New command (using the EXTRACT option EXCLUSIVE-COPY)
- >> FSC-GUI  
New command. Call the FSC GUI program (much nicer than the command command COMPARE-IMAGE) – Only if the GUI program is available.
- >> HEADERS  
Some options added in HISTOGRAM  
PRINTOUT of EM values: focal distance and spherical aberration exchanged
- >> IMAGIC\_TO\_FREALIGN  
File names of output MRC and Frealign parameter file can be different  
Problems with output MRC file corrected
- >> MSA-CLASSIFY  
Moving elements convergence criterion made less strict
- >> MSA-EXTRACT  
A fraction of bad class members can be ignored

- >> MSA-SUM  
Take over EM parameters to class averages
- >> PICK-PARTICLES  
User interaction changed (parameters in image space)  
Take over EM and defocus values
- >> PLT-EQUIVALENT-MOVE  
Add two movements stored in two input PLT file and dump the "equivalent" move parameters into the output PLT file
- >> THREEED-RECONSTRUCTION  
An additional normalized 3-D volume can be created

#### USER INTERACTION HAS CHANGED

(Please correct your script files):

- >> ALIGN-IMAGE
- >> ALIGN-MOVIE-FRAME
- >> CTF-FIND
- >> CTF-FLIP
- >> CREATE-PRETREATED-AMPLITUDES
- >> DISPLAY
- >> EM2EM / IMPORT-EXPORT-IMAGES
- >> MSA-EXTRACT
- >> PICK-PARTICLES
- >> SUM-IMAGES
- >> SURVEY-IMAGES

#### MARCH - APRIL 2014

#### BUG FIXES:

- >> THREEED-AUTO-MASK / AUTOMATIC-MASKING  
Masking was incorrect (March version)

#### UPDATES:

- >> ALIGN-MOVIE-FRAMES  
New command to align movie frames (from a EM camera, for example)
- >> ALIGN-DIRECT-TO-REFERENCE  
New command to align images to a reference (the old ALIGN-DIRECT)
- >> ALIGN-DIRECT  
Command doing both, ALIGN-DIRECT-TO-REFERENCE and ALIGN-MOVIE-FRAMES
- >> New/renamed automatic masking commands  
THREEED-AUTOMATIC-MASKING: masking 3D volumes

AUTOMATIC-MASK-IMAGES: masking 2D images  
MASK-AUTOMATICALLY: masking both, 2D images and 3D volumes

USER INTERACTION HAS CHANGED

(Please correct your script files):

- >> ALIGN-DIRECT
- >> THREEED-AUTOMATIC-MASKING
- >> THREEED-FILTER
- >> AUTO-MASK

MARCH 2014

BUG FIXES:

- >> EM2EM
  - > Error in converting internal data formats (float, byte...) corrected
  - > Import of stacked MRC files did not work any more
  - > SPIDER: Decode of header text corrected
- >> ANGULAR-RECONSTITUTION
  - Option: REFINE\_EULER\_ANGLES: Wrong error exit corrected

UPDATES:

- >> ALIGNMENT commands
  - Reference(s) can be band-pass filtered
- >> ALIGN-DIRECT
  - New: MPI parallel mode
  - New option to refine reference iteratively (intermediate new references, which can be created in various ways)

USER INTERACTION HAS CHANGED

(Please correct your script files):

- >> ALIGN-DIRECT

## JANUARY-FEBRUARY 2014

### HEADER UPDATE:

- >> New header values added to keep track of the single particles:
  - > LOCMICRO: Location number in the micrograph file, where the particle was picked
  - > IXMICRO: X coordinate in the micrograph, where the particle was picked
  - > IYMICRO: Y coordinate in the micrograph, where the particle was picked
  - > LOCORIG: Location number of the particle in the "original" file (usually this is the file created by PICK-PARTICLE or CUT-IMAGE/APERIODIC)

### BUG FIXES:

- >> EULER
  - Option NEW\_IMAGE did not create correct sonograms any more
- >> EM2EM
  - > Exporting to a stack of single image files did not work correctly (converting a set of FEI\_MRC files to MRC files, for example)
  - > CCP4/MRC: Pixel size (resolution) was not set correctly
  - > SPIDER: Import of stacked image files corrected
  - > SPIDER: Export to Spider corrected
  - > SHF format corrected

### UPDATES:

- >> Many commands
  - Error handling updated / corrected
- >> All commands using Fourier transforms (FT, filter, ...)
  - Images with odd dimensions are allowed now
- >> HEADERS
  - New WRITE option ORIGINAL\_LOCATION to (re)set the header index LOCORIG
- >> EM2EM
  - Digital Micrograph: Import of dm2, dm3 and dm4 images added
  - Resolution: In case of difference between header and user value: take user's value
- >> EXCLUSIVE-COPY
  - New EXTRACT option ORIGINAL\_IMAGES to extract only the original images, which are found in the indices LOCORIG of a header file with processed images
- >> ALIGN-DIRECT:
  - One can now iterate the alignment using intermediate sums as new references (similar to command ALIGN-NOISY but with more options)

## DECEMBER 2013

### BUG FIXES:

- >> ALIGNMENT commands  
Incorrect error message complaining about odd image sizes removed
- >> CENTER-IMAGE  
Bug fix (MPI parallel version)
- >> EM2EM
  - > SPIDER export corrected
  - > Incorrect MRC format LONG removed
  - > Input a set of images using <root\_name> plus <number>: the number "0" can be used now
  - > Input a set of images using <root\_name> plus <number>: the default extension was not used in the previous version
- >> EXCLUSIVE-COPY  
Option RADIAL\_SHIFT corrected
- >> MSA-RUN  
Bug fix (MPI parallel version)
- >> THREED-AUTOMATIC-MASK  
(Important) Header values are taken over from input to output file
- >> THREED-RECONSTRUCTION  
Bug fix (MPI parallel version)

## MAY - DECEMBER 2013

### GENERAL IMAGIC UPDATE:

- >> There are two versions now: 32-bit and 64-bit (internal precision)  
64-bit is needed when working with very large 3D volumes
- >> The IMAGIC header can be extended to store additional header values (currently used in MSA classification to store image coordinates in case the number of eigenimages is > 69). See IMAGIC header index IDAT1(4) = NBLOCKS to check if the header is extended
- >> Internal IMAGIC format LONG (integer\*8) added
- >> MPI parallel mode: correct handling if the number of processes is larger than the number of images
- >> Help and error messages updated

### BUG FIXES:

- >> Check IMAGIC version: re-enabled

- >> Alignment programs: HF cut value corrected
- >> ANGULAR-RECONSTITUTION
  - Option EACH\_TO\_BEST: Average AR ERROR corrected (in parallel mode)
- >> DISPLAY:
  - Option NAME / INDEX did not crash any more in next call of DISPLAY
  - New options list (including new option PREVIOUS) in case there is no more space on screen to display next image(s)
- >> EM2EM:
  - CCP4 option corrected (could not be chosen)
  - 3D options re-enabled

#### UPDATES:

- >> New command CREATE-MICROGRAPH
  - Same MODEL-MICROGRAPH
- >> CREATE-VOLUME
  - Same as THREED-TEST-IMAGE
- >> CTF-FIND:
  - Grey scale measurement between the two half images modified
- >> EM2EM:
  - See em2em update file
- >> HEADERS:
  - New option CLASS\_SUM\_INDEX to take over any header value from a class average into the headers of the classified (original) images
- >> IMAGE-MENU
  - Option to get the phases added
- >> MSA classification:
  - MSA classification can handle more than 69 eigenimages
- >> MOVE-IMAGE / ROTATE-IMAGE / SHIFT-IMAGE:
  - Use the header values to move/rotate/shift images
- >> PICK-PARTICLES:
  - CCF\_MATCHING: If the reference was rotated the rotation angle is stored header file of the extracted (boxed) particles
- >> MOVE, ROTATE and SHIFT:
  - New option HEADER to get parameter from headers
- >> SUM-IMAGE
  - Option to create odd/even sum added
- >> THREED-CREATE-VOLUME
  - Same as THREED-TEST-IMAGE

>> THREED-SCALE-DENSITIES:  
New command

USER INTERACTION HAS CHANGED  
(Please correct your script files):

>> ANGULAR-RECONSTITUTION  
>> EM2EM  
>> HEADERS  
>> IMAGE-MENU  
>> MSA-CLASSIFY  
>> MSA-SUM  
>> THREED-MODEL-MOLECULE  
>> THREED-RECONSTRUCTION

SEPTEMBER 2012 – APRIL 2013

BUG FIXES:

>> IMAGIC  
Wrong writings, help text etc. corrected

>> ABOUT-IMAGIC / LICENSE-INFORMATION  
Printout of IMAGIC version number corrected

>> ARITHMETIC-WITH-IMAGE  
Option ROOT corrected

>> IMAGIC-TO-FREALIGN  
Wrong writings of par file corrected (film number)

>> HEADERS  
Option TAKEOVER / CLASS-SUM\_DEFOCUS\_EM did not work

>> MSA-SUM  
Printout error corrected

>> PLOT  
Option STYLE / HISTOGRAM corrected

>> THREED-ADD, THREED-SUBTRACT, THREED-MULTIPLY, THREED-DIVIDE  
Commands did not start

## UPDATES:

- >> IMAGIC:  
New header value: ACTIVE – image is active or not  
(currently only used as an option in EXCLUSIVE-COPY)
- >> IMAGIC:  
Now also running on MS Windows 8
- >> IMAGIC:  
MS Windows: Parallel versions are now using OpenMPI
- >> IMAGIC:  
More detailed error messages in case of a program crash
- >> ABOUT-IMAGIC / LICENSE-INFORMATION  
Updated, printout of IMAGIC version number corrected
- >> ALIGN-EXTRACT-IMAGES:  
New program organisation to speed up the command  
Option EXCLUDE added  
Output file can be sorted or not (if output is a single file)
- >> AUTOMATIC.MASKING / THREED-AUTOMATIC.MASKING  
User interaction block updated. Ask if input is a 2D image or a 3D volume  
Printout modified
- >> CTF-FIND:  
Re-organisation of the related program (Downhill simplex algorithm removed, partial coherence search added and more)  
All input parameters are asked in Angstrom now, now Scherzer values any more  
There is a lot of printout for the first image to check if the iterations converge, or if the program should be stopped and restarted with other parameters.
- >> CTFFIND3:  
New parameter dAst added (needed in the new version of CTFFIND3)
- >> COARSE-IMAGE:  
New command added
- >> CREATE-IMAGE / TEST-IMAGE-CREATION:  
Option CHECKERS: No restrictions in image size
- >> DISPLAY:  
Pseudo buttons "Next" and "Stop" added in the SELECT option
- >> EM2EM / IMPORT-EXPORT:  
New user-interaction block  
New format JPEG  
TIFF format updated  
Type of MRC file (created by FEI, IMOD...) automatically detected  
Export to IMAGIC: also write a number of header values if wanted
- >> HEADERS:  
New READ/WRITE options added:

- ACTIVE, ELECTRON\_MICROSCOPY, EM\_AND\_DEFOCUS etc.
- >> MOVE-PLT-COORDINATES:  
The user has to specify the type of the PLT file (contour or coordinates).  
The options depend on this choice.
  - >> IMAGE-MENU, ARITHMETIC-WITH-IMAGE, ADD-NOISE, related commands:  
Input and output file can be the same
  - >> MSA-CLASSIFY:  
Printout updated
  - >> MSA-EXTRACT-IMAGES:  
New program organisation to speed up the command  
Output file can be sorted or not (if output is a single file)
  - >> PICK-PARTICLES:  
Old command PICK-ALL-PARTICLES removed
  - >> PICK-PARTICLES:  
Extracting particles now also possible in the parallel version
  - >> RESIZE-IMAGE:  
New command  
Options are BLOW-UP/DOWN, COARSE and RESIZE\_IN\_FS
  - >> SUM-IMAGES:  
New option to sum members of a checkerboard subdivision

#### USER INTERACTION HAS CHANGED

(Please correct your script files):

- >> ALIGN-EXTRACT-IMAGES
- >> AUTOMATIC.MASKING
- >> CTF-FIND
- >> EM2EM / IMPORT-EXPORT
- >> HEADERS
- >> MOVE-PLT-COORDINATES
- >> MSA-EXTRACT-IMAGES
- >> PICK-PARTICLES
- >> THREED-AUTOMATIC.MASKING

## JUNE - SEPTEMBER 2012

### BUG FIXES:

- >> ADD-NOISE, IMAGE-MENU/ADD-NOISE and THREED-MENU/ARITHM/NOISE  
The random number seed was set incorrectly
- >> CTF-FLIP  
The "use classes" option corrected
- >> CREATE-CURVE  
New command. Same as TEST-CURVE-CREATION
- >> CROSS-CORRELATION and MUTUAL-CORRELATION  
The location number of the reference was not used and the program crashed
- >> EM2EM  
The resolution value specified by the user was not used for all formats
- >> IMAGE-MENU (and many related commands)  
The MPI parallel version was not running correctly for all options
- >> MODEL-MICROGRAPH  
The FREE option did not work correctly
- >> PRETREAT-IMAGE  
User interaction did not ask for the type of the mask
- >> SUM-CURVE / CURVE\_SUM  
The command did only read one image
- >> THREED-MASK  
Option SOFT\_MASK corrected

### UPDATES:

- >> ALL COMMANDS  
TECLA added in Linux/Unix/Mac OS X: Within the user interaction block use arrows up and down recall previously entered answers and use TAB to complete or show file names etc.
- >> ARITHMETIC-WITH-IMAGE  
Option ROOT did not work any more
- >> CTF-FIND  
Refinement scheme for finding the correct CTF parameters changed.  
New convolution based PC CTF calculation  
Help and user interaction updated
- >> CTF-FLIP  
Program, help and user interaction updated
- >> DISPLAY-IMAGE  
Option WATCHDOG does not ask for a retention time any more

- >> EXCLUSIVE-COPY  
Copying (some) 2D sections out of a 3D volume did not work any more
- >> EM2EM  
TIA (Emispec) format added. TIA is the program used on FEI Tecnai and Titan microscopes for acquiring and displaying scanned images and spectra.
- >> HEADERS  
New option in WRITE/REF3D: NEW\_REF3D\_IF\_CHANGED  
Assign the next new 3D membership number to all images/headers for which IREF3D and IREF3D\_OLD are not the same (helpful in 3D/4D calculations).
- >> IMAGE-MENU  
Option COMPLEX\_MERGE added: merge amplitudes & phases  
or real and imaginary part
- >> IMPOSE-PLT-CONTOUR  
Updated
- >> MODEL-MICROGRAPH  
Random seed added  
Coordinates where to put the “particles” can be defined in an input PLT file
- >> MOVE-COORDINATES-PLT  
Program updated (runs much faster now)
- >> NEW COMMANDS related to MOVE-COORDINATES-PLT  
MANIPULATE-COORDINATES-PLT (same as MOVE-COORDINATES)  
COARSE-COORDINATES-PLT  
UNCOARSE-COORDINATES-PLT
- >> PREPARE-IMAGES  
Band-pass parameters are now stored in the image history
- >> SELECT-IMAGES  
New command calling the SELECT option of command EXCLUSIVE-COPY
- >> SELECT-IMAGES and SORT-IMAGES  
Get SORT/SELECT value from a) (own) HEADER, b) from a PLT\_FILE, or  
c) from ANOTHER\_FILE
- >> TEST-IMAGE-CREATION  
New option PLT\_INPUT added: Image(s) will contain points with grey values as  
specified in an input PLT file (each line contains the values: x,y,greyscale)
- >> THREEED-ADD-VOLUMES  
THREEED-SUBTRACT-VOLUMES  
THREEED-MULTIPLY-VOLUMES  
THREEED-DIVIDE-NY-VOLUME  
New commands calling the related option in the command  
THREEED-TWO-VOLUMES-OPERATIONS

## USER INTERACTION HAS CHANGED

(Please correct your script files):

- >> CTF-FIND
- >> CTF-FLIP
- >> DISPLAY option WATCHDOG
- >> EM2EM
- >> IMAGE-MENU
- >> IMPOSE-PLT-CONTOUR
- >> MODEL-MICROGRAPH
- >> MSA-EIGEN-FILTER
- >> SUM-CURVE / CURVE-SUM

## MAY - JUNE 2012

- >> IMAGIC  
New header value REF3DOLD (old 3D membership) in index 57
- >> ANGULAR-RECONSTITUTION  
Either use FISHER\_TRANSFORM, PEAK\_OVER\_STDV or NONE.  
**Attention: new UIB question!**
- >> DISPLAY  
Option SELECT: some time consuming questions while picking particles removed  
Option WATCHDOG: retention time added so that all new images are displayed
- >> HEADER  
BUG FIX: option WRITE / WIPE re-enabled  
PLT file input of defocus values added  
PLT file input of micrograph identification numbers added
- >> MOVE-IMAGE  
In PLT input the move parameters can come from a non-IMAGIC image processing program which uses "shift plus rotation". In such a case the parameters have to be converted to the IMAGIC standard, which is "rotation plus shift".  
**Attention: new UIB question added for PLT\_INPUT!**
- >> MSA-MASK  
BUG FIX: Option CONTOUR does not crash any more.  
Command is now calling program "inc2dmenu".  
**Attention: new UIB question!**

- >> MULTI-REF-ALIGN  
If the header of the original images contains rotate and/or shift parameters M-R-A stops with an error message. If these header parameters are not zero the images are not original and "equivalent rotation" always leads to silly results
- >> PRETREATED-AMPLITUDE  
New command to calculate pre-treated amplitudes (normally subsequently used in CTF-FIND)
- >> TWO-IMAGE-OPERATIONS  
BUG-FIX: ask for options did not work

## DECEMBER 2011 - APRIL 2012

- >> All ARITHMETRIC-WITH-IMAGE commands,  
all FOURIER-TRANSFORM commands,  
all INCORE-MENU commands  
all MASK-IMAGE commands  
and a number of standard image processing commands:  
The commands are now calling program "inc2dmenu":  
NOTE: inc2dmenu can run in parallel but not all options may be suitable for such a parallel processing. But it's the user's choice!  
NOTE: **The USER INTERACTION was CHANGED!**  
**Please check and update your script/batch job files!**
- >> INCORE- commands:  
Most of the commands renamed. **The prefix "INCORE" was removed.**
- >> ANGULAR-RECONSTITUTION:  
Option NEW / REMOVE corrected
- >> DISPLAY  
Option ZOOM modified (UIB)
- >> CTF-FIND, CTF-FLIP, CTF-OPERATIONS  
Rectangular object uncertainty implemented (carbon foil height)  
Some minor updates
- >> EM2EM / IMPORT-EXPORT  
MRC from FEI added
- >> EXCLUSIVE-COPY  
New option TWO\_INDICES to use two header indices for sorting
- >> HEADERS  
Options added to read 2D and 3D move (rot/shift) values
- >> INC-PREPARE renamed to PREPARE-IMAGES

- >> MASK-IMAGE:  
New masks added
- >> MSA-ALIGN:  
Output of un-classified images corrected
- >> PICK-PARTICLES  
Output modified
- >> TEST-IMAGE-CREATION  
New option (TEST\_CHART)  
Option PHANTOM updated
- >> THREED-MOVE  
Various options are available to get the input rotation/shift parameters  
Equivalent rotation/shift calculation added  
The rotation/shift parameters are stored in the output headers