IUCrJ

Volume 10 (2023)

Supporting information for article:

MRC2020: improvements to Ximdisp and the MRC image-processing programs

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TABLE I: Updated brief description of MRC programs

Densitometry

1. NIKSCN ** Digitization using NIKON densitometer.

2. JLSCAN ** Digitization using JOYCE-LOEBL densitometer.

General processing

1. HEADER Print out information in header records.

2. IMCON ** Convert raw densitometer output into MAPFORMAT.

3. LABEL Image handling of various kinds.

4. FFTRANS Fast Fourier transform.

5. TRNOUT Output amplitudes and phases to printer.

6. TRMASK Mask transform for filtering.

7. INTERPO General 2D reinterpolation program.

8. INTERPO3D 3D version of INTERPO.

9. SWAPXY Swap XY axes of a 3D or 2D image or stack or images.

10. BOXIM Standard boxing program for selection of an area.

11. BOXIMAGE Similar to above, but leave boxed area in original position.

12. IMEDIT General editing program for image headers.

13. MEDIAN ** Median filtering for smoothing images.

14. ENHANCE ** Apply various radial filter functions to transforms.

15. IMEXCHANGE ** Convert MAPFORMAT into ASCII for editing/exchange.

16. REMORIG Remove origin with taper for crude high-pass filtering.17. TAPEREDGEK Taper edge of an image to remove spikes in transform.

18. TWOFILE Linear combination, or multiply/divide data in two files.

19. TIF2MRC Convert TIFF format files to MAPFORMAT.

20. MRC2TIF Convert MRC format files to TIFF.

21. SPIDERTOMRC ** Convert SPIDER format files to MAPFORMAT.

22. JOINSTK V1 00 Joins multiple image stacks.

23. BANDPASS High/low bandpass image filtration with selection of smooth function cutoffs.

24. IMAGE CONVERT converts old style (pre-2000) maps to new post 2000 format

25. BYTE SWAP MAP Byte swaps map data to change map enddianness.

26. CTFCALCK Calculate and plot CTF curves.

27. CTFFIND2 Predecessor of Grigorieff CTFFIND3 and CTFFIND4

28. CTFFINDA Predecessor of CTFFIND2

29. PADBOX Pads an image or map with zeroes.

30. PADCORCUT Pads an image, applies CTF then cuts to original box size.

31. SMOOTH Smoothing by 3x3 local averaging.

Two-dimensional crystals

1. EMTILT Calculate tilt angles from lattice parameters.

2. MASKTRANA Mask transform for filtering, like TRMASK.

3. AUTOCORRL Autocorrelation calc + expansion 2 use with QUADSERCH.

4. QUADSERCHK Correlation peak search on lattice, with profile fit.

5. CCUNBENDK Unbend image using list of peaks from QUADSERCH.

6. MMBOXA Read amplitudes and phases from transform and display surrounding box.

7. MMLATREF Lattice parameter refinement based on MMBOX.

8. TTBOXK Correct for tilted transfer function, gives amplitudes and phases.

9. TTMASK Combined MASKTRAN and TTBOX, masking + TTF corr on tilted images.

10. TTREFINE Refine defocus, astigmatism, tilt params on tilted images.

11. TTBOXREF ** Lattice parameter refinement on images with TTF correction.

12. CTFSEARCH Refine or search for correct defocus, astigmatism, on untilted images.

13. CTFAPPLYK Apply CTF to data from MMBOX, with graphical output.

14. ORIGTILTK Combine data from different images using crystal symmetry.

15. LLFILT ** Lattice line fitting for smooth curves and structure factors.

16. LATLINEK Agard's least squares latline fit of amplitudes and phases.

17. ALLSPACEA Determine space group, origin, beamtilt for single image.

18. AVRGPHASES ** Overall averaging of projection data from ORIGTILT.

19. AVRGAMPHS Overall averaging of amplitude and phase projection data.

20. MAKETRAN Create reference transform from MTZ file with given defocus.

21. SCALIMAMP3D Scales image amplitudes to selected reference data.

22. LATLINPRESCAL Corrects image amplitudes for CTF.

23 MMTOMKLCF Creates MKLCF file from MMBOX or CTFAPPLY.

24. PICKPROFK Spot integration, using least-squares profile-fitting.

25. PLTILTK Plot tilt geometry distribution.

26. PLTSYNCP3 Plot output from SYNCFITP3.

27. PREPMKLCF Prepare latline output for MKLCF.

28. TWOLATTK Plots two lattices to see if there is overlap.

29. DIVIDEQ Divides merged list of amps and phases into two equal halves.

30. HALFSTAT Calculates phase difference between two halves of data.

Electron diffraction patterns

1. BACKAUTOK Calculate radial background and find centre of pattern.

2. AUTOINDEXK Find two simplest lattice vectors automatically.

3. PICKAUTOK Integrate and background correct electron diffraction spots.

4. MERGEDIFF Merge e.d. data and do a host of corrections.

5. AVRGFDELF Average multiple measurements of delta-F from MERGEDIFF.

6. SYNCFITP3 Fit lattice line curves to output from MERGEDIFF.

7. F2MTZ ** Convert formatted data (A,P) to MTZ format (CCP4 Suite).

8. AVRGINTENS Overall averaging of electron diffraction intensities in projection.

Helical structures

1. HLXSEARCH Determine tilt and origin.

2. HLXDUMP Dump layer line data from transform.

3. HLXFIT Orientations and origins of different particles.

4. HLXFITT Updated version of HLXFIT.

5. HLXAVG Average data from different particles.

6. HLXFOUR Fourier program

7. HLXPROJ 2D filtered image from layer line data.

8. EM2FOLD Impose twofold normal to axis.

9. HLXSEPDAT Feeder for HLXSEPR.

10. HLXSEPR Separate overlapping Bessel functions.

11. HLXLLOUT Graph standard layer line data.

12. HLXSIMUL Simulate image of helix.

13. HCUT Removes layer lines outside defined resolution range.

14. LLGRAPH Plots layer line data.

Icosahedral viruses

1. REFINE ** Find orientations and origins by self-common lines.

2. X60CORR ** Cross common lines between two particles of known orientation to find rela-

tive hand and scaling.

3. RACMAT ** Extract data from transforms needed for solving for big G's.

4. RACBG ** Solve for big G's.

5. RACLG ** Convert big G's to little g's.

6. RACFB ** Fourier summation from little g's to make 3D map.

7. MAPCONV ** Convert 3D Fourier map to MRC format.

8. PROJGEN ** Compute general projection of 3D map.

9. X60REF ** Find orientations and origins by cross-common lines between unknown parti-

cle and projections of current best model.

10. SHELLS ** Section map on spherical shells for display

Rotational averaging and filtering

1. RFILTIM Rotational filtering.

ROTAV Rotational averaging of 2D images or 3D maps about z axis.
IMROTRAN Rotate/translate 2D image—search to maximize correlation.

Calculating and contouring maps (from CCP4 suite)

1. FFT Crystallographic Fourier program.

2. EXTEND Extend maps/images to multiple unit cells.

3. PLUTO General contouring, atomic model plotting program.

General display

LASERTONE General program for conversion of image to postscript file.
LASERPLOT General program for conversion of plot file to postscript file.
LASERTEXT General program for conversion of text to postscript file.

4. HISTOK Make histogram of densities in an image.

5. CURVY2K Product graph on line printer.

6. Ximdisp LMB raster graphics display for X-terminals.

7. THREED Display 2D array as simulated 3D contoured surface.
8. SURF, LIGHT Produce shaded surface representations of 3-D maps.

^{**} These programs are now obsolete or not included in the current distribution via CCP-EM. They may still be available from the authors of Crowther et al (1996).