MRC Software
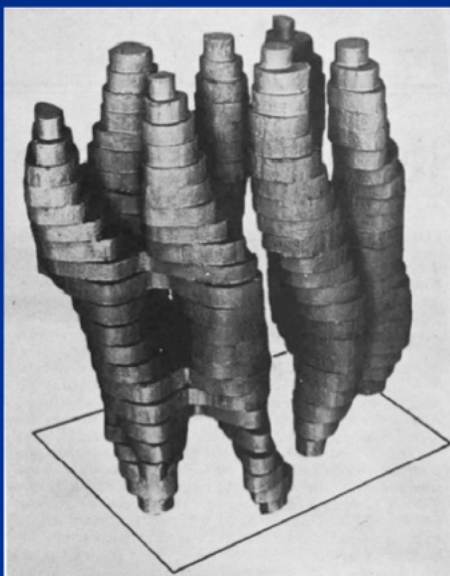
Henning Stahlberg,
Biozentrum, Uni Basel, Switzerland
c-cina.org

2dx Workshop
Basel, August 23–26, 2016
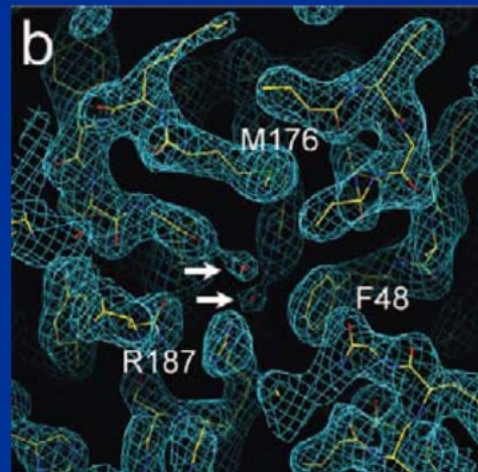
MRC software for real-space images

Henderson & Unwin (1975) Nature 257, 28-32

Gonen et. al. (2005) Nature 438, 633-8

History

- Developed over 30 yrs by a number of people
- Written in Fortran
- image2000
    - image format compatible with ccp4
    - plots in postscript format

http://www.tonh.net/museum/plotter.html

What it includes

- Densitometry
- General processing
    - LABEL, FFTRANS, TWOFILE
- Two-dimensional crystals
- Electron diffraction patterns
- Helical structures
- Icosahedral viruses
- Rotational averaging and filtering
- General display
    - XIMDISP

Crowther, Henderson and Smith (1996) JSB 116, 9-16

MRC image/transform Format

- The MRC file
  - Header is of 1024 bytes long
  - Space for 10 of 80 byte text labels
  - Data records.

http://www.tonh.net/museum/bigtape.html

- MODE   data type :
  - 0   image : signed 8-bit bytes range -128 to 127
  - 1   image : 16-bit halfwords
  - 2   image : 32-bit reals
  - 3   transform : complex 16-bit integers
  - 4   transform : complex 32-bit reals

- No compression!

Example MRC Program Header

```
C LATLINPRESCAL : program to correct image amplitudes for effects of CTF and
C                          to C calculate appropriate weights for output to LATLINE.
C
C vx 1.0 RH 18.9.93 original program fused from READBOTH + SCALIMAMP
C vx 1.1 RH 25.7.95 debug of WTFACTOR on move to Dec Alpha
C vx 1.2 AS 07.07.2003 changed IFILM to 10 digits
C*****************************************************************************
C Control cards:
C
C        Card 1:   NSER,ZMIN,ZMAX (*)
C                          serial number on ORIGTILT input
C                          and ZSTAR limits to be passed on to LATLINE.
C        Card 2:   IQMAX (*)
C                          maximum value of IQ for spots to be used
C
C        INPUT file is raw file straight from ORIGTILT : on unit FOR001
C        OUTPUT has the format required by LATLINE : on unit FOR003
C
C*****************************************************************************
```

http://www.rdrop.com/~jimw/j-hist.shtml#History

Documentation

- **Most recent reference:**
  - Crowther, Henderson and Smith (1996) JSB 116, 9-16
- **Docs on 2dx.org**
  - documentation from MRC (Tony Crowther, Richard Henderson and Jude Smith)
  - program source headers
  - image/FT formats
  - Electron crystallography-steps and program annotation (Vinzenz Unger and Anchi Cheng)

Slide by Anchi Cheng, 2010