

Merging in 3D with 2dx

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Merging in 3D

Single Particle Approach to 2D crystals: Xiangyan Zeng

Maximum Likelihood single particle processing of unit cells eliminates need for well ordered crystals, and eliminates problems from TTF or Coma.

Projective Constraint Optimization: Bryant Gipson, (Raphael Thierry)

Oversampling at low tilt angles produces data in high tilt angles, including full reconstruction of data in missing cone.

(No lattice line interpolation, no lattice line sinc fit. No FFT.)

2dx: Bryant Gipson, Marcel Arheit, Xiangyan Zeng, (Raphael Thierry)

Project Management.

User guidance.

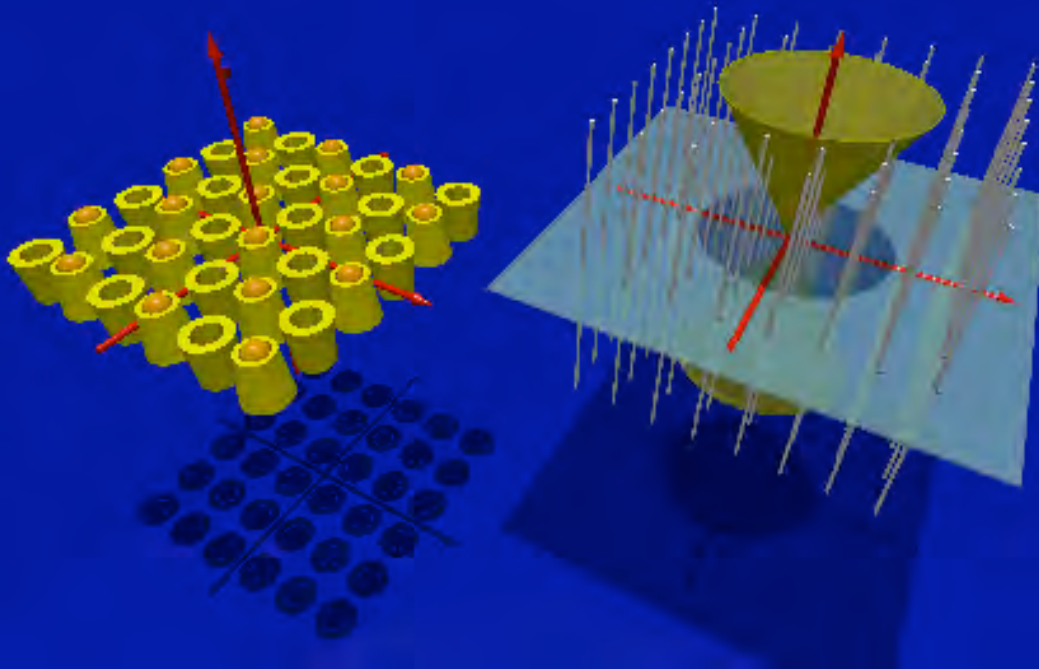
User-friendly tool to use MRC manually or (semi-)automatically.

Platform to combine different approaches and software systems, including MRC, CCP4, ML, Spider, Chimera, (future: IPLT).

The Missing Cone

Real Space

Fourier Space



Diffraction Spots in 2D
Lattice Lines in 3D

File Formats and Flow

ttbox => origtilt => avramphs => f2mtz

ttbox: takes cor\${image}.fft.mrc =====> generates tt\${image}.aph

1: Header

2: H	K	AMP	PHS	IQ	BCK	CTF
1234567890	AII1234567890	Fri	15	Feb	2002,	CCUNBENDE PASS 1
1	1	258.1	360.0	2	59.3	0.0
1	2	57.4	127.0	8	61.9	0.0
1	3	844.6	32.8	1	55.8	0.0

origtilt: takes tt\${image}.aph =====> generates merge.aph

1: Header

2: H	K	Z*	AMP	PHS	NO	IQ WEIGHT	BACK	CTF
1001								
1	1	0.0049	1290.8	-36.3	205051	1 1.00000	63.3	0.000
1	2	0.0054	471.4	-83.3	205051	2 1.00000	68.6	0.000
1	3	0.0059	2625.7	-33.3	205051	1 1.00000	61.1	0.000

File Formats and Flow

ttbox => origtilt => avramphs => f2mtz

avramphs (keyname ph) =====> (kl (rt.2) and others)

avrg.hkl

1: Header

2: H K L AMP PHS FOM

```

1001
1 1 0 258 -36 99.000
1 2 0 942. -82 98.200
1 3 0 525 133 99.000
    
```

Web site: 2dx.org

f2mtz:

takes avrg.hkl

====>

generates avrg.mtz

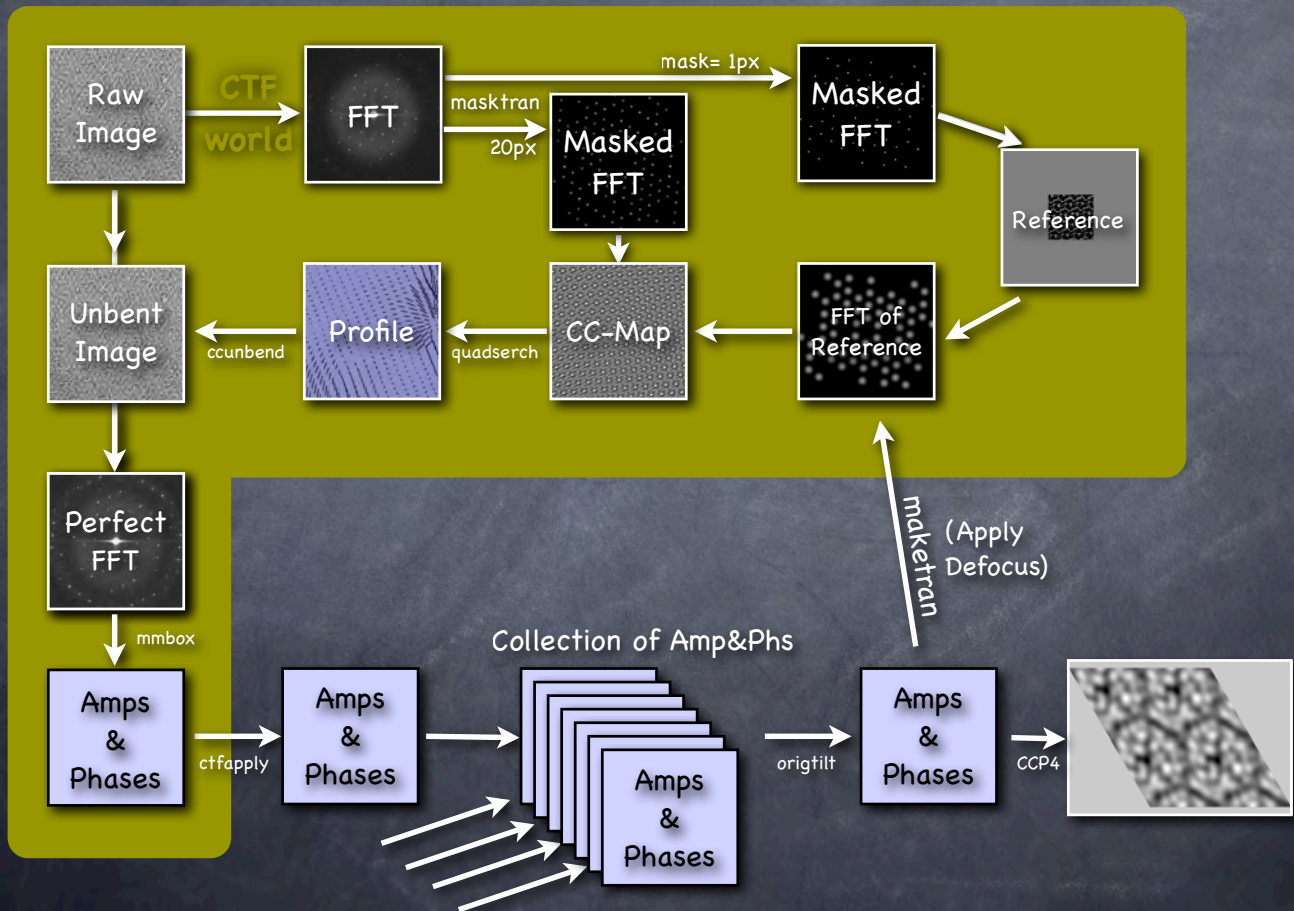
avrg.mtz

(binary)

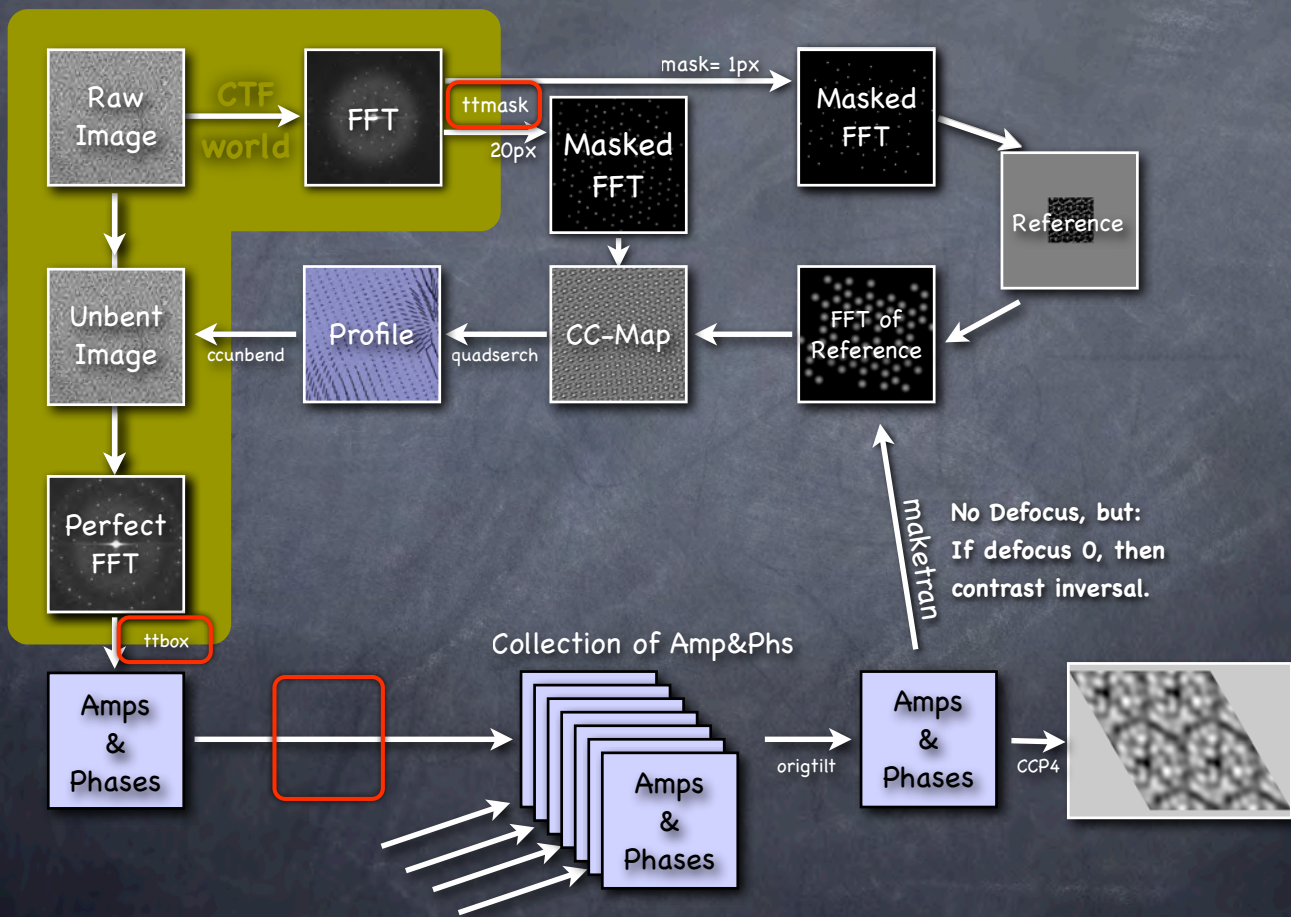
LABOUT H K L FP PHIB FOM

CTYPOUT H H H F P W

Algorithm Non-tilted



Algorithm Tilted



Merging Script

ttbox => origilt => avramphs => f2mtz

origilt: takes many *.aph =====> generates merge.aph

```
origilt.exe << eot
7 0 F F 1 98.0,98.0 400.00000 90.0 0 15      ! ISPG,NPRG,NTL,NBM,ILST,A,B,W,ANG,IPL,MNRF
1001 0 30 5 1 F F 0.75                      ! IRUN,LHMN,LHMX,IQMX,IBXPHS,NREFOUT,NSHFTIN,RFACAMP
100 DUMMY
/usr/local/2dx/2dx_image/proc/dummy.aph
00326401 Merging, Mon 24 Feb 2003
../AQP2-00/gAII00326401/APH/cormAII00326401.nolimit.aph
F
0.0 0.0 0      ! TAXA,TANGL,IORIGT
-162.29,-163.91 0.01 0.00125 0 1.0 0 0 0 1 0 ! OH,OK,STEP,WIN,SGNXCH,SCL,ROT,REV,CTFREV,ROT90,REVHND
2.0,200.0 0.00,0.00      ! cs,kv,tx,ty
200.00 6.00      ! resolution limits
00326402 Merging, Mon 24 Feb 2003
../AQP2-00/gAII00326402/APH/cormAII00326402.nolimit.aph
F
0.0 0.0 0      ! TAXA,TANGL,IORIGT
142.42,38.28 0.01 0.00125 0 0.0 0 0 0 1 0 ! OH,OK,STEP,WIN,SGNXCH,SCL,ROT,REV,CTFREV,ROT90,REVHND
2.0,200.0 0.00,0.00      ! cs,kv,tx,ty
200.00 6.00      ! resolution limits
30328305 Merging, Mon 24 Feb 2003
../AQP2-30/AII30328305/APH/cormAII30328305.nolimit.aph
F
73.80 -29.49 0      ! TAXA,TANGL,IORIGT
14.90,133.25 0.01 0.00125 0 0.0 0 0 0 1 0 ! OH,OK,STEP,WIN,SGNXCH,SCL,ROT,REV,CTFREV,ROT90,REVHND
2.0,200.0 0.00,0.00      ! cs,kv,tx,ty
200.00 6.00      ! resolution limits
-1
eot
```