https://bl831.als.lbl.gov/~jamesh/powerpoint/RapiDataXDStutorial_2024.pptx

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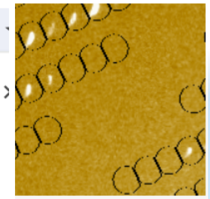
Useful links

https://bl831.als.lbl.gov/~jamesh/powerpoint/?C=M;O=D

Index of /~jamesh/powerpoint

Name	Last modified	Size	Description
Parent Directory		-	
RapiData_XDStutorial..>	2024-04-30 09:21	1.6M	
RapiData_XDStutorial..>	2024-04-30 09:21	1.5M	
fear_no_Spacegroups.mp4	2024-03-13 13:47	326M	
fear_no_Spacegroups.pdf	2024-03-13 09:38	6.9M	
fear_no_Spacegroups...>	2024-03-12 20:27	106M	
Ringberg_tangle_2024..>	2024-02-15 05:54	7.0M	
SIBYLS_tangle_2024.pptx	2024-01-08 11:38	6.0M	
MX_at_ALS_JMH.pptx	2023-12-04 21:18	10M	

Scan QR Code



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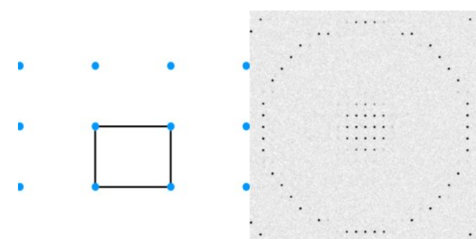
Difficult datasets

The following suggestions apply not only to ... eak or low-resolution, or otherwise difficult macromolecular datasets.

These datasets have few (or few strong, or few well-defined) reflections per frame. Therefore, the multitude of parameters describing the diffraction experiment needs to be reduced (in refinement one would say: to avoid overfitting). This means that some

phasertng

Fear no Space Groups



ELVES

Chapter 7: Tips and Tricks

Neat-o unix commands

...e is the little sentence you type to run unix programs. The text that appears on each line to the left of ...e command prompt. This is a very old convention, but it is incredibly powerful. No graphical ...e close to providing the detailed control that a command line gives you. The only problem with ...hey almost always have obtuse syntax, and novice users have a really hard time figuring out what to ...ended as a quick guide for crystallographers who want to optimize their unix environment without ... all the unix manuals that I have. :)

The unix "shell"

Your "shell" program is probaly tcsh (Turbo-C-shell). All a shell program does is accept your typed commands, find and run the unix program you have invoked, and then prompt you for another command. That's about it. However, the shell is

James Holton's Benchmarks...

Comparison of x-ray programs on different machin...

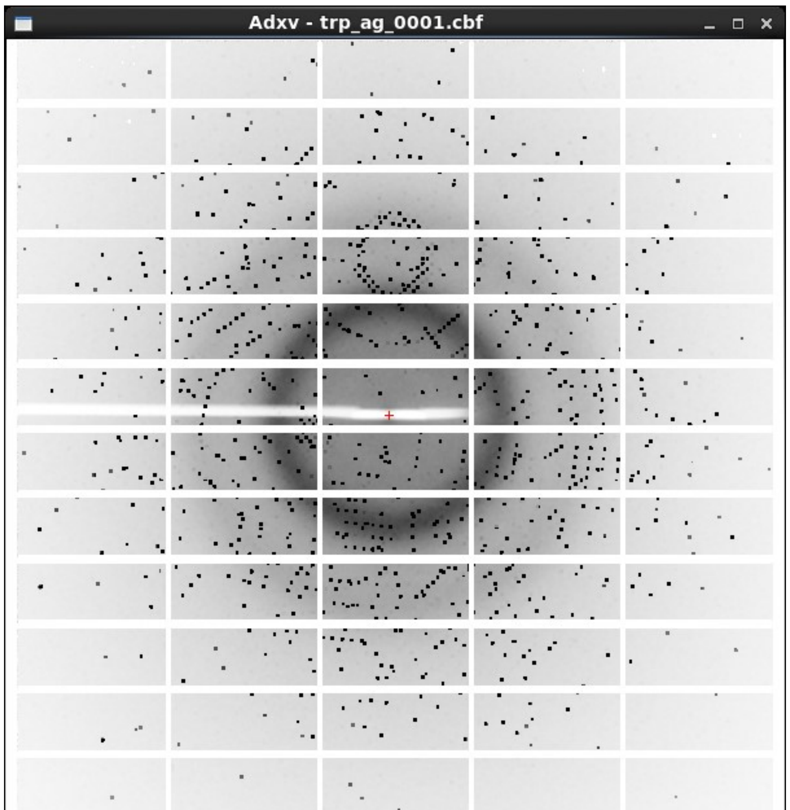
The following tables are a comparison of standard x-ray data-processing ... access to. The machine names have been omitted to protect the innocent. ... "major" process on the machine, and always from a local disk. The exact ... moved from machine to mahcine.

Speed of DIALS

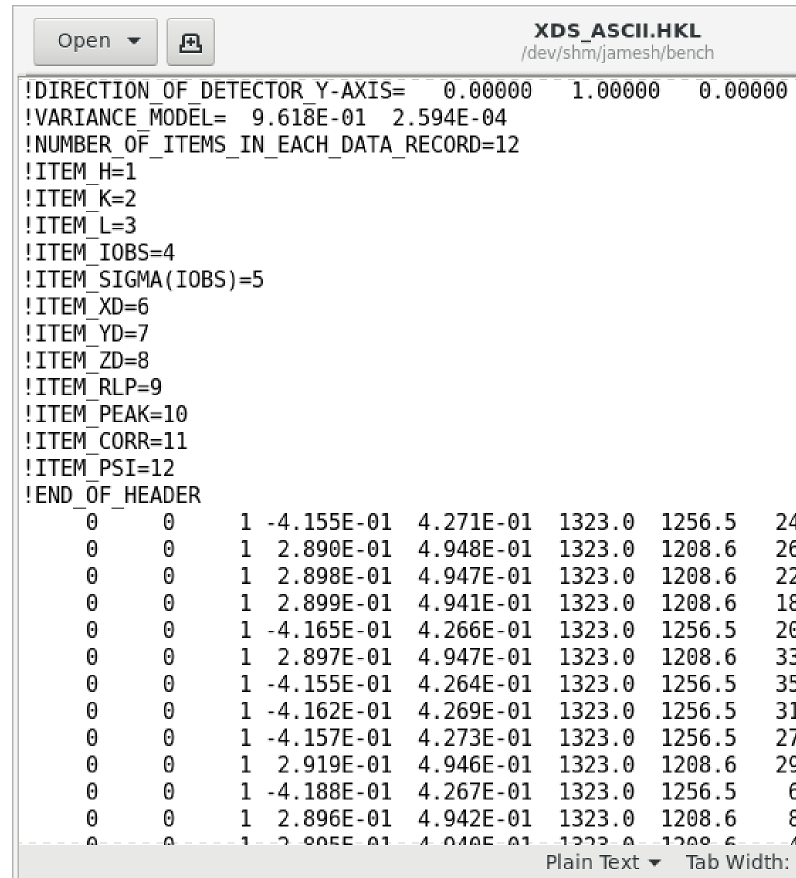
XDS

X-ray diffraction data reduction engine

Diffraction image data



List of spot intensities (text)




```
!DIRECTION_OF_DETECTOR_Y-AXIS=    0.00000    1.00000    0.00000
!VARIANCE_MODEL=  9.618E-01  2.594E-04
!NUMBER_OF_ITEMS_IN_EACH_DATA_RECORD=12
!ITEM_H=1
!ITEM_K=2
!ITEM_L=3
!ITEM_IOBS=4
!ITEM_SIGMA(IOBS)=5
!ITEM_XD=6
!ITEM_YD=7
!ITEM_ZD=8
!ITEM_RLP=9
!ITEM_PEAK=10
!ITEM_CORR=11
!ITEM_PSI=12
!END_OF_HEADER
     0     0     1 -4.155E-01  4.271E-01  1323.0  1256.5   24
     0     0     1  2.890E-01  4.948E-01  1323.0  1208.6   26
     0     0     1  2.898E-01  4.947E-01  1323.0  1208.6   22
     0     0     1  2.899E-01  4.941E-01  1323.0  1208.6   18
     0     0     1 -4.165E-01  4.266E-01  1323.0  1256.5   20
     0     0     1  2.897E-01  4.947E-01  1323.0  1208.6   33
     0     0     1 -4.155E-01  4.264E-01  1323.0  1256.5   35
     0     0     1 -4.162E-01  4.269E-01  1323.0  1256.5   31
     0     0     1 -4.157E-01  4.273E-01  1323.0  1256.5   27
     0     0     1  2.919E-01  4.946E-01  1323.0  1208.6   29
     0     0     1 -4.188E-01  4.267E-01  1323.0  1256.5    6
     0     0     1  2.896E-01  4.942E-01  1323.0  1208.6    8
```

XDS

native user interface: a text file!

Open | Save

XDS.INP
~/xds_tutorial

```
! written by generate_XDS.INP version 0.82 (01-Mar-2018)
JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT
ORGX= 1231.50 ORGY= 1263.50  ! values from frame header; only read by XYCORR, IDXREF

DETECTOR_DISTANCE= 189.16000 !read by XYCORR, IDXREF. Negative if detector normal points to
crystal.
OSCILLATION_RANGE= 0.2000
STARTING_ANGLE= 270.0000
X-RAY_WAVELENGTH= 0.97946
NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_?????.cbf
! REFERENCE_DATA_SET=xxx/XDS_ASCII.HKL ! e.g. to ensure consistent indexing
DATA_RANGE=1 1800
SPOT_RANGE=1 900
! BACKGROUND_RANGE=1 10 ! rather use defaults (first 5 degree of rotation)

SPACE_GROUP_NUMBER=0                   ! 0 if unknown
UNIT_CELL_CONSTANTS= 70 80 90 90 90 90 ! put correct values if known
INCLUDE_RESOLUTION_RANGE=50 0  ! after CORRECT, insert high resol limit; re-run CORRECT
! IDXREF now obeys INCLUDE_RESOLUTION_RANGE and EXCLUDE_RESOLUTION_RANGE to exclude ice-rings

FRIEDEL'S_LAW=FALSE     ! This acts only on the CORRECT step
! If the anom signal turns out to be, or is known to be, very low or absent,
! use FRIEDEL'S_LAW=TRUE instead (or comment out the line); re-run CORRECT

! remove the "!" in the following line:
! STRICT_ABSORPTION_CORRECTION=TRUE
! if the anomalous signal is strong: in that case, in CORRECT.LP the three
! "CHI^2-VALUE OF FIT OF CORRECTION FACTORS" values are significantly> 1, e.g. 1.5
!
! exclude (mask) untrusted areas of detector, e.g. beamstop shadow :
! UNTRUSTED_RECTANGLE= 1800 1950 2100 2150 ! x-min x-max y-min y-max ! repeat
! UNTRUSTED_ELLIPSE= 2034 2070 1850 2240 ! x-min x-max y-min y-max ! if needed
! UNTRUSTED_QUADRILATERAL= x1 y1 x2 y2 x3 y3 x4 y4 ! see documentation
!
! parameters with changes wrt default values:
TRUSTED_REGION=0.0 1.2 ! partially use corners of detector (0 1.4143: use all pixels)
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS=6000. 30000. ! often 7000 or 8000 is ok
```

Generate XDS.INP

This script generates XDS.INP based on a list of frame names supplied on the commandline. It currently works for MarCCD, ADSC, Pilatus, Eiger, some Rigaku and one Bruker detector(s); since this is just a bash script, extension to other detectors should be very easy.

Contents [hide]

Usage

Usage is just (don't forget the quotation marks!):

```
generate_XDS.INP "/home/myname/frms/mydata_1_???.img"
```

XDS supports bzip2-ed frames. Thus, when specifying the frame name parameter of the script, you should leave out any .bz2 extension.

A better image viewer

Adxv

https://www.scripps.edu/tainer/arvai/adxv.html

Adxv - A program to display X-Ray diffraction images

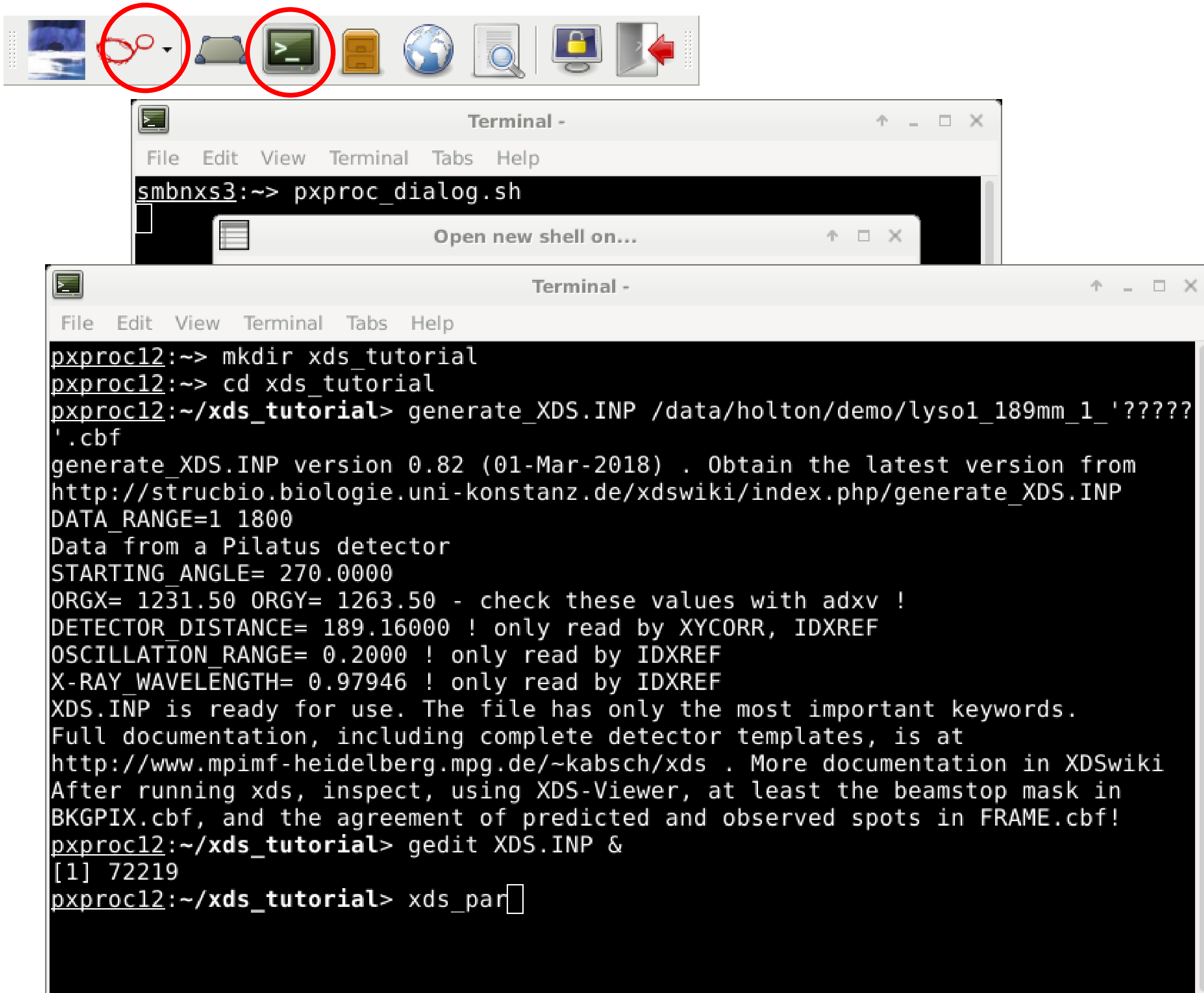
Adxv can be used to display and analyze 2-D area detector data. It is optimized to display X-Ray crystallography diffraction images. The data may be displayed as a 1-D cross section, 2-D image or 3-D surface. Sequential images may be displayed as an animation. The magnification, contrast and color mapping are adjustable. Displayed data may be saved in a variety of formats including ASCII, SMV/IMG, TIFF, JPEG and Postscript. Adxv will run on most versions of Linux and OSX. It is based on X11/Motif so an X-server is required. It will run on Windows if the Cygwin libraries and X-server have been installed.

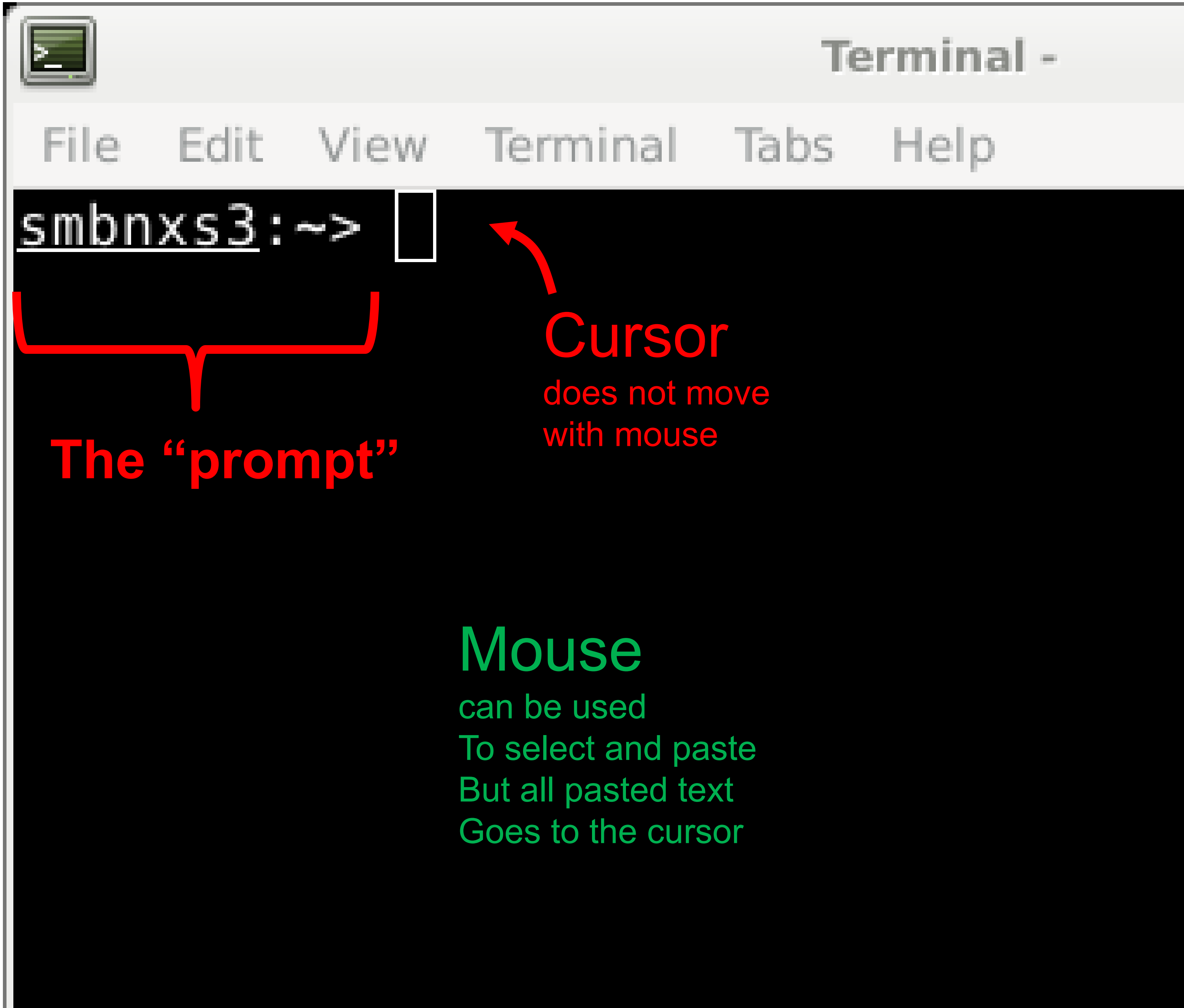
Many common detector and data formats are recognized, including:

- ADSC
- Mar ccd
- Mar image plate (old and new format)
- Raxis II & IV
- Crystallographic Binary Format (CBF)
- XDS .pck files
- European Data Format (EDF)
- Numerical Python (NUMPY)
- Hierarchical Data Format (HDF5)
- Tagged Image File Format (TIFF)
- Raw binary integer and floating point data

XDS

native user interface




Terminal -
File Edit View Terminal Tabs Help
smbnxs3:~>
Cursor
does not move
with mouse
The “prompt”
Mouse
can be used
To select and paste
But all pasted text
Goes to the cursor

too… much… typing!

1) Make sure X11 is running
2) Select some text with mouse
3) Move mouse over to your terminal
4) Hit middle mouse button
5) No keyboard required!

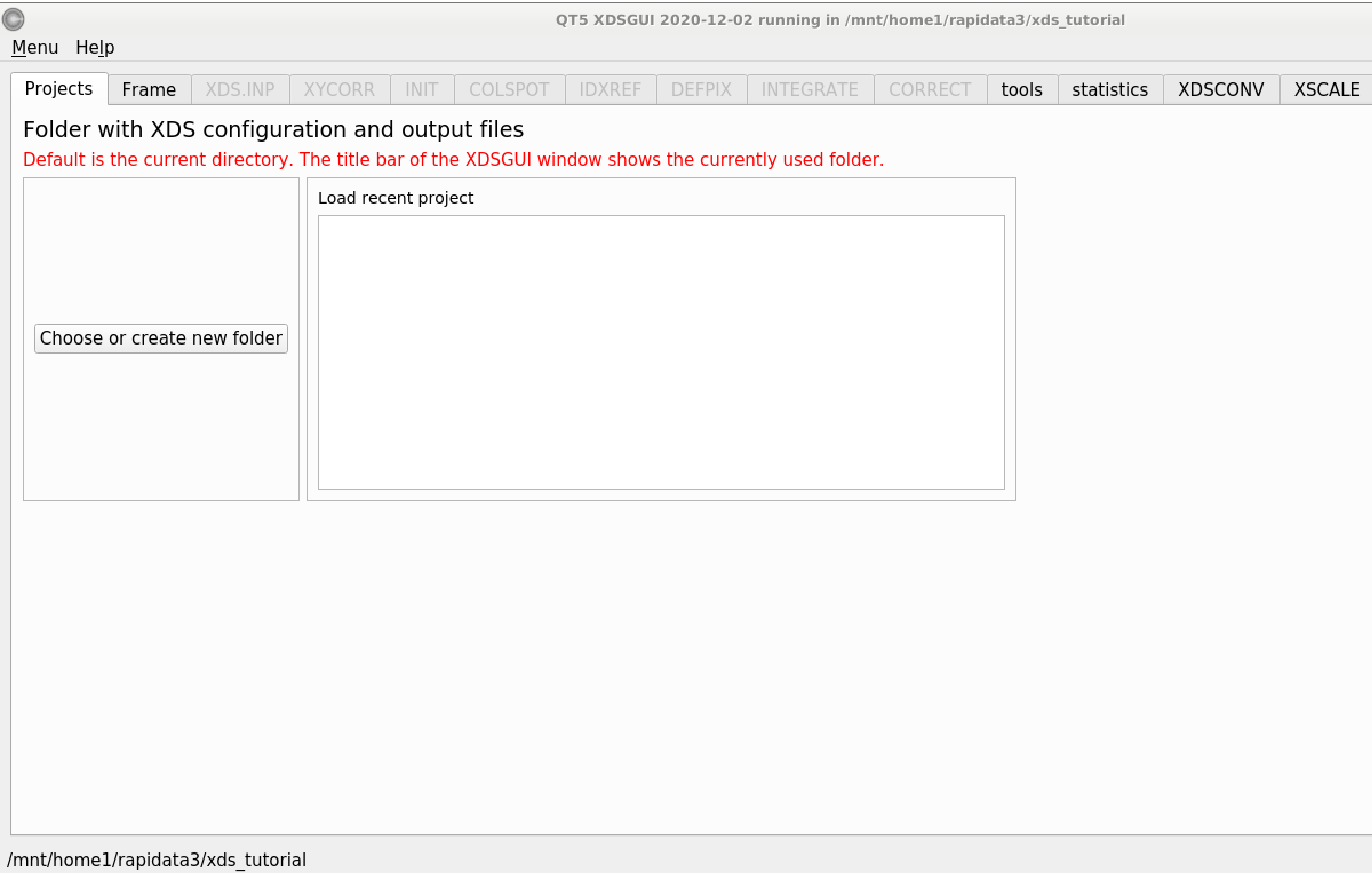
How to start XDS

prompt
Do not type!

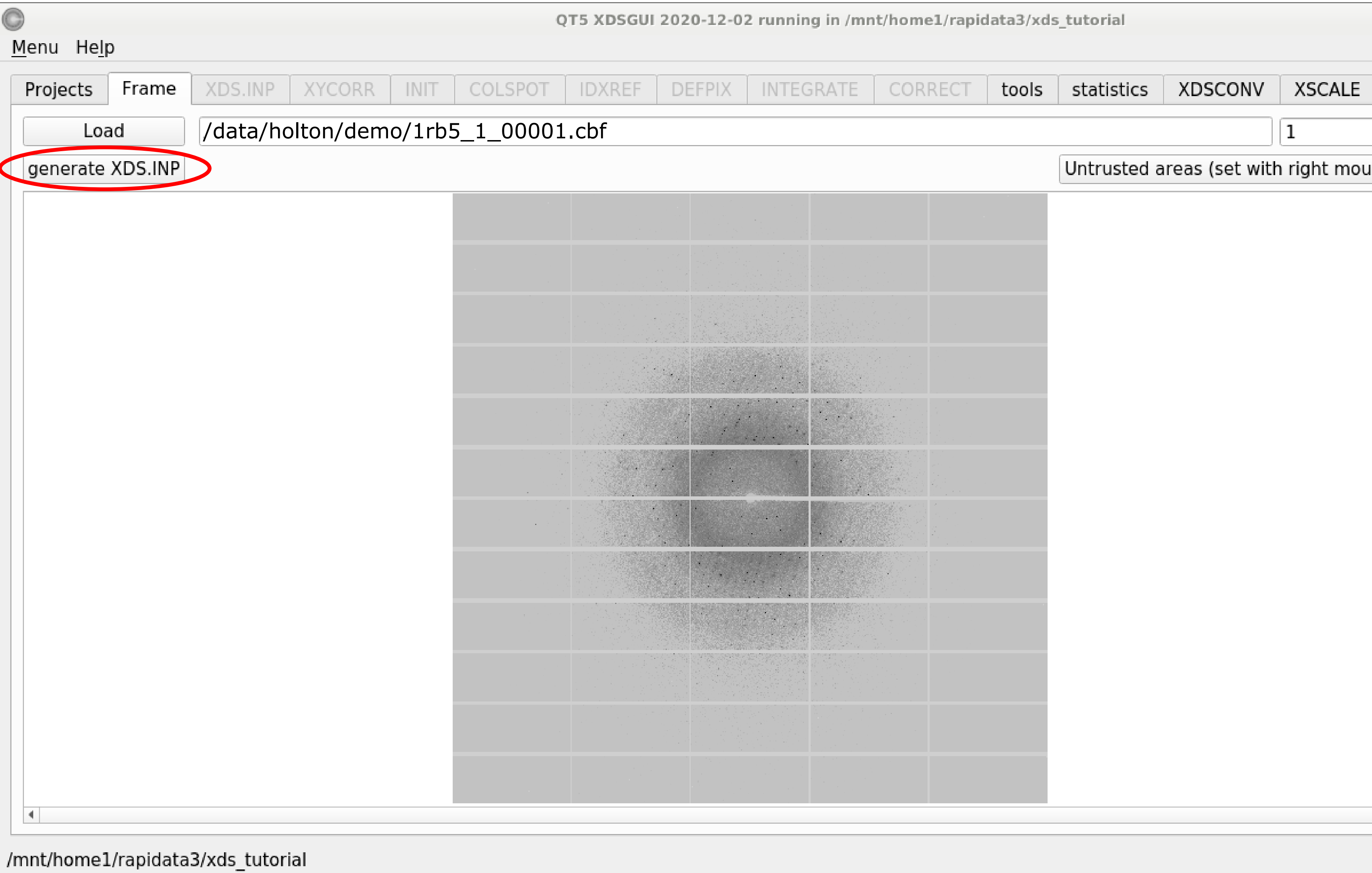
```
ssh pxproc7
proc:~> cd /data/$USER
proc:~> mkdir  xds_tutorial
proc:~> cd  xds_tutorial
proc:~> ln  -sf  /data/holton/demo  .
proc:~> xdsgui
```

Space! · Space! · underscore · Enter · Space! · period!

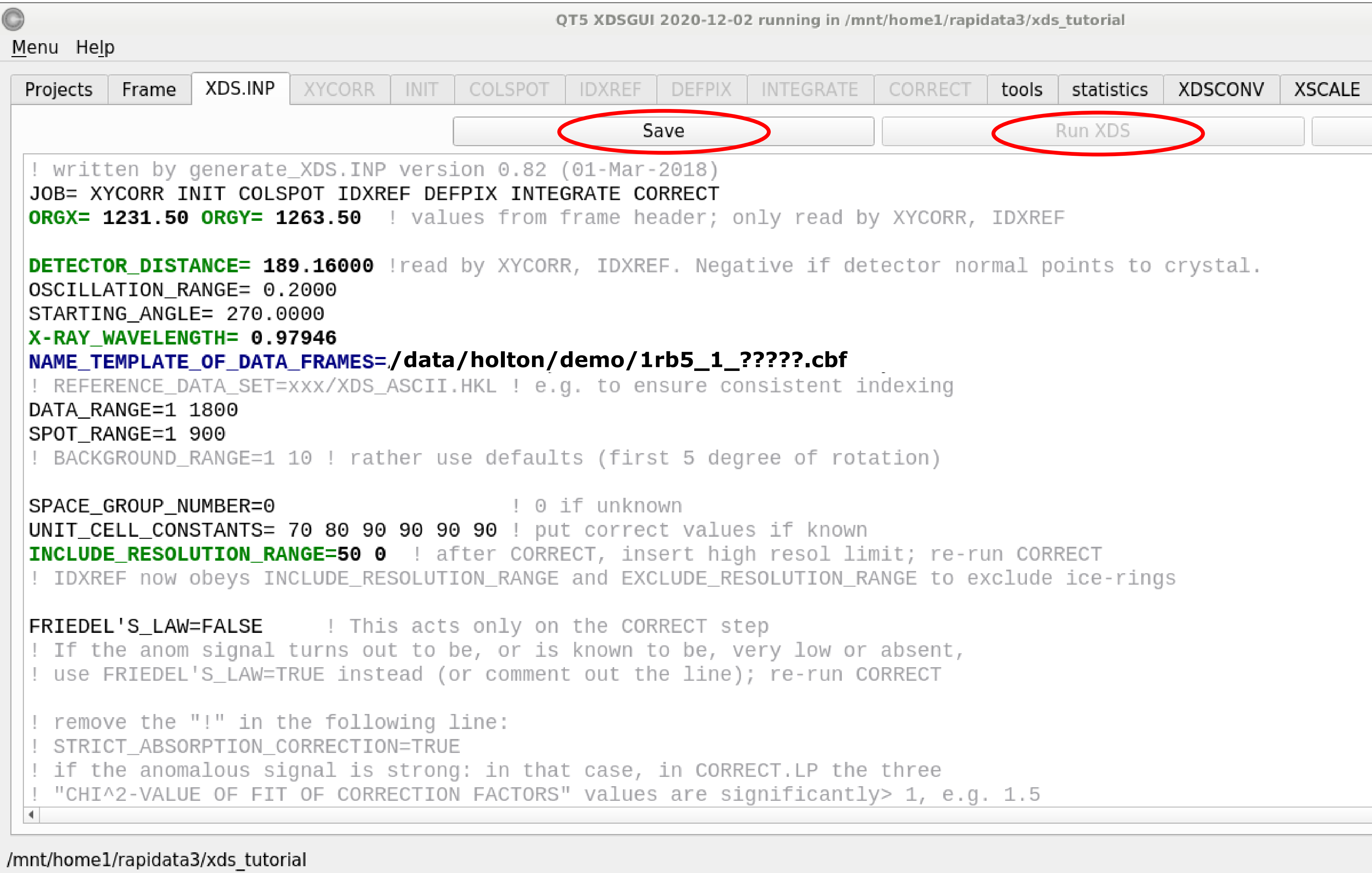
xdsgui – a graphical interface for XDS



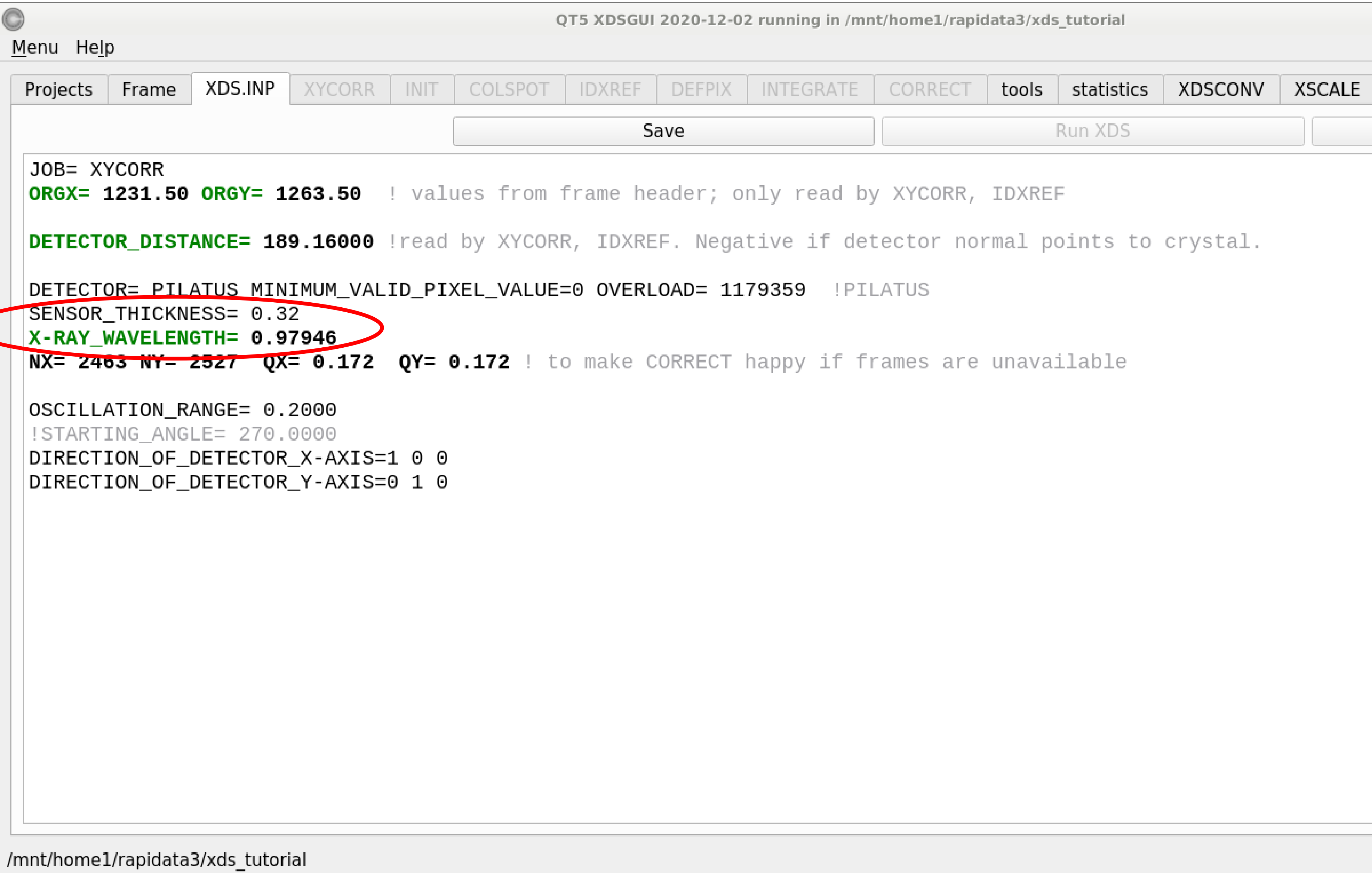
xdsgui – load an image



xdsgui – a GUI for text!



XYCORR– setting things up



INIT – look at the background

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial

Menu Help

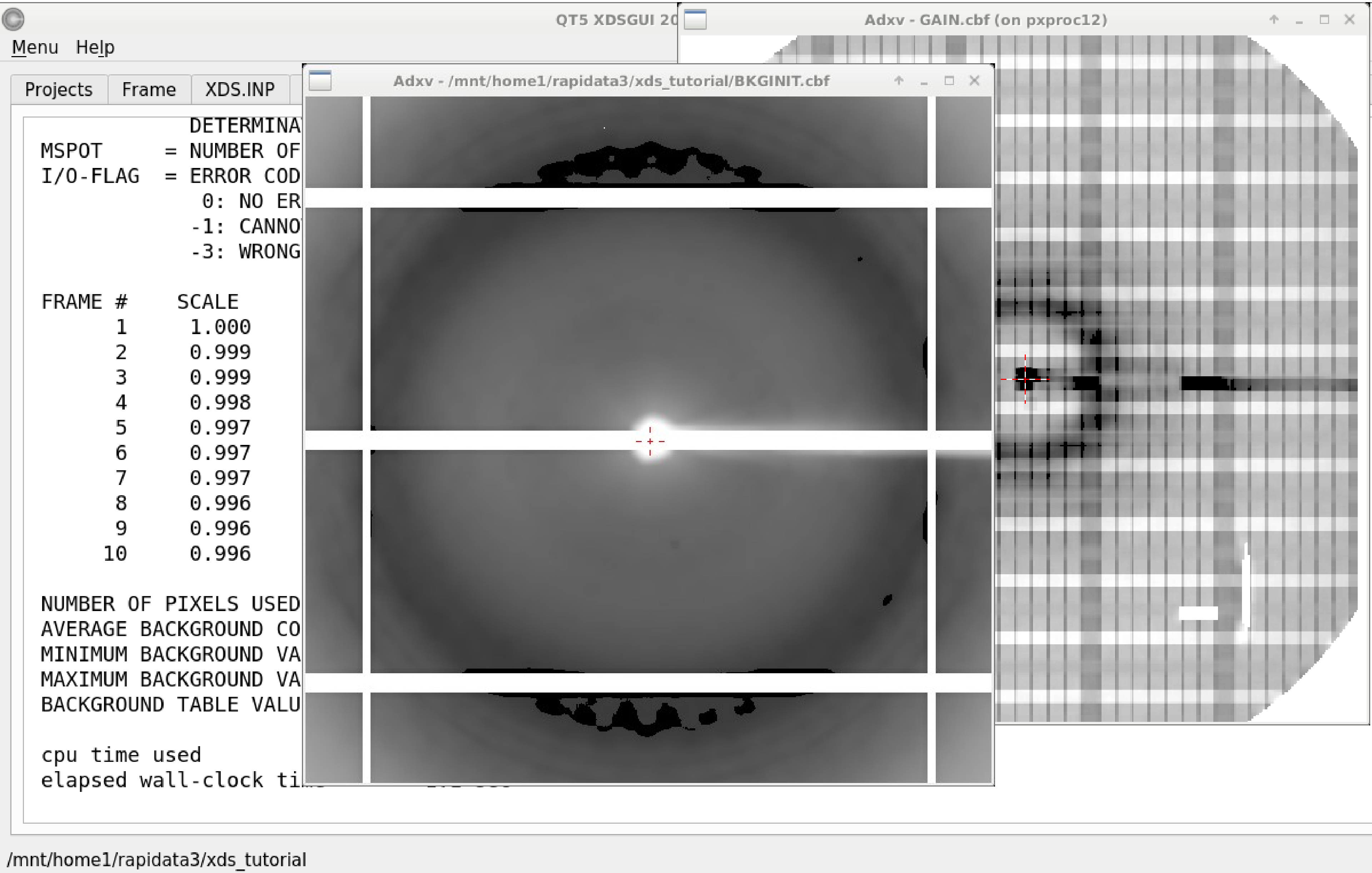
Projects | Frame | XDS.INP | XYCORR | INIT | COLSPOT | IDXREF | DEFPIX | INTEGRATE | CORRECT | tools | statistics | XDSCONV | XSCALE

Save | Run XDS

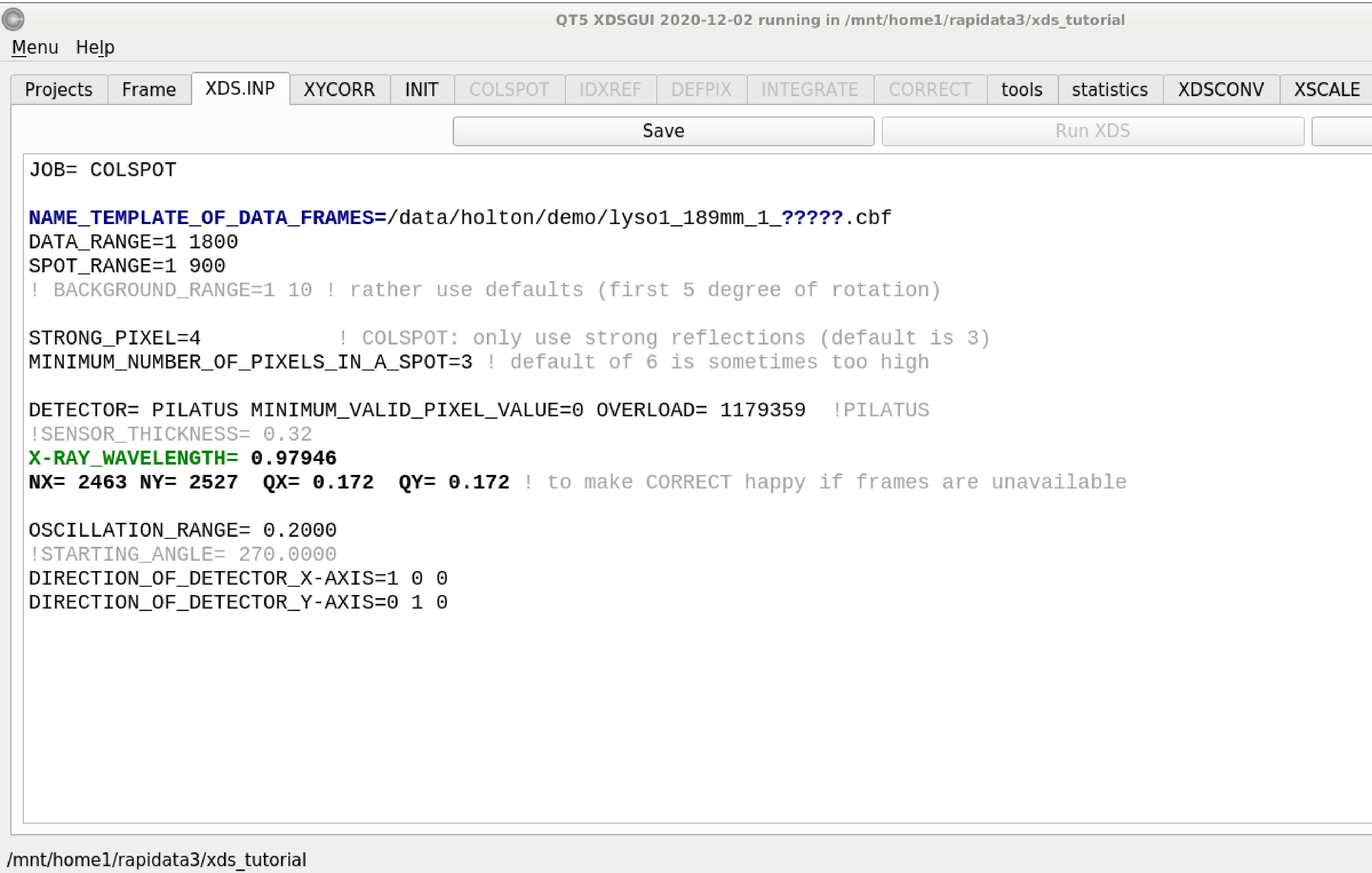
```
JOB= INIT

!DETECTOR_DISTANCE= 189.16000 !read by XYCORR, IDXREF. Negative if detector normal points to crystal.
NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_?????.cbf
DATA_RANGE=1 1800
!SPOT_RANGE=1 900
BACKGROUND_RANGE=1 10 ! rather use defaults (first 5 degree of rotation)

UNTRUSTED_RECTANGLE= 1800 1950 2100 2150 ! x-min x-max y-min y-max ! repeat
UNTRUSTED_ELLIPSE= 2034 2070 1850 2240 ! x-min x-max y-min y-max ! if needed
!UNTRUSTED_QUADRILATERAL= x1 y1 x2 y2 x3 y3 x4 y4 ! see documentation

TRUSTED_REGION=0.0 1.2 ! partially use corners of detector (0 1.4143: use all pixels)




DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD= 1179359  !PILATUS
!SENSOR_THICKNESS= 0.32
X-RAY_WAVELENGTH= 0.97946
NX= 2463 NY= 2527  QX= 0.172  QY= 0.172 ! to make CORRECT happy if frames are unavailable

OSCILLATION_RANGE= 0.2000
!STARTING_ANGLE= 270.0000
DIRECTION_OF_DETECTOR_X-AXIS=1 0 0
DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0
```

/mnt/home1/rapidata3/xds_tutorial

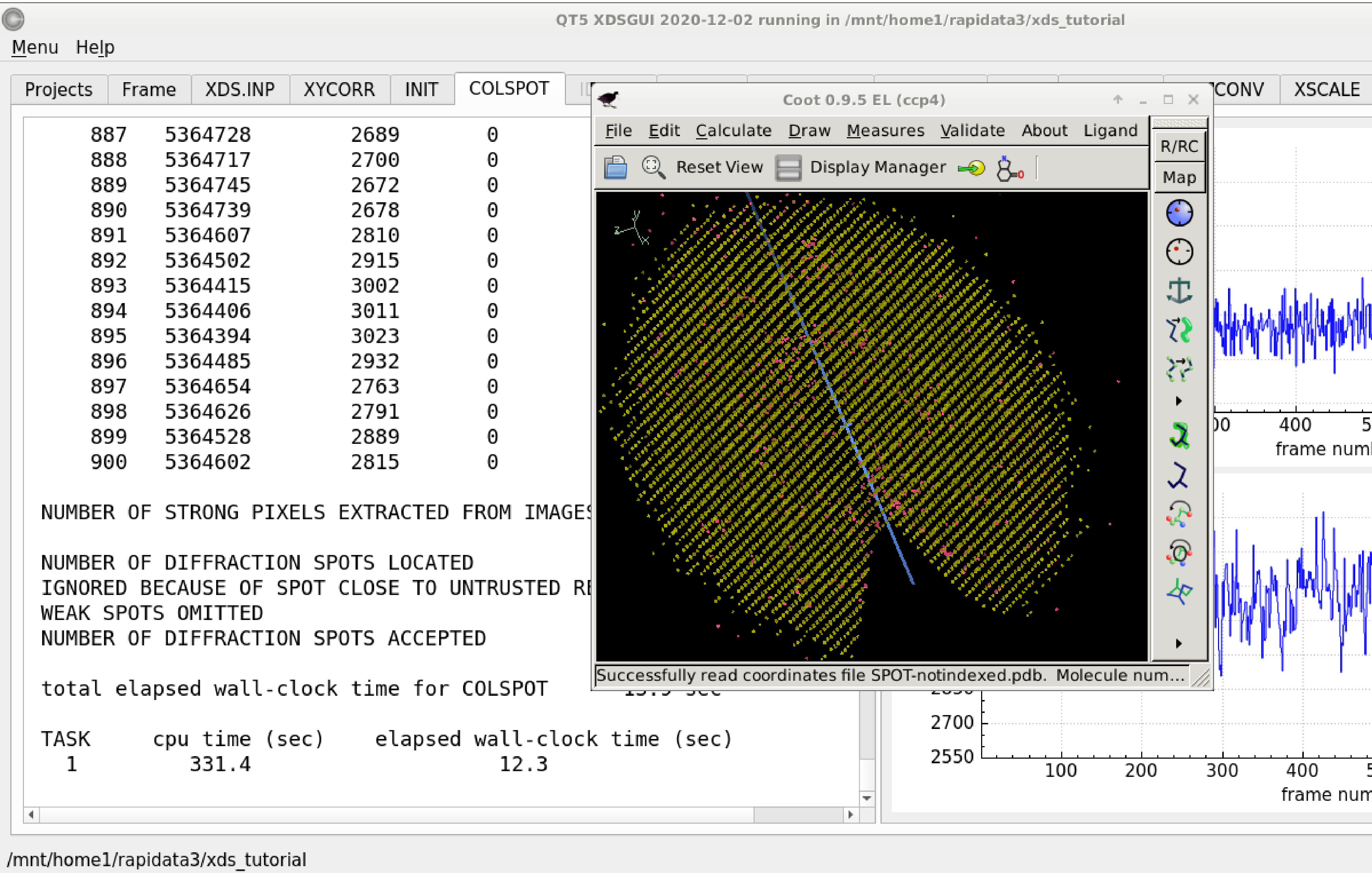
INIT – look at the background



COLSPOT – the spot picker



COLSPOT – the spot picker



IDXREF – auto-indexing

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial

Menu Help

Projects | Frame | XDS.INP | XYCORR | INIT | COLSPOT | IDXREF | DEFPIX | INTEGRATE | CORRECT | tools | statistics | XDSCONV | XSCALE

Save | Run XDS

```
JOB= IDXREF
ORGX= 1231.50 ORGY= 1263.50  ! values from frame header; only read by XYCORR, IDXREF
DETECTOR_DISTANCE= 189.16000 !read by XYCORR, IDXREF. Negative if detector normal points to crystal.
OSCILLATION_RANGE= 0.2000
! STARTING_ANGLE= 270.0000
X-RAY_WAVELENGTH= 0.97946
! NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_?????.cbf
! REFERENCE_DATA_SET=xxx/XDS_ASCII.HKL ! e.g. to ensure consistent indexing
SPOT_RANGE=1 900

SPACE_GROUP_NUMBER= 96                  ! 0 if unknown
UNIT_CELL_CONSTANTS= 78 78 37 90 90 90 ! put correct values if known
INCLUDE_RESOLUTION_RANGE=50 0  ! after CORRECT, insert high resol limit; re-run CORRECT
! EXCLUDE_RESOLUTION_RANGE= 3.93 3.87 !ice-ring at 3.897 Angstrom
TRUSTED_REGION=0.0 1.2 ! partially use corners of detector (0 1.4143: use all pixels)

REFINE(IDXREF)=CELL BEAM ORIENTATION AXIS  ! refine POSITION only if known that header distance inaccurate
! MINIMUM_FRACTION_OF_INDEXED_SPOTS= 0.5

ROTATION_AXIS=1 0 0  ! Australian Synchrotron, SERCAT ID-22 (?), APS 19-ID (?), ESRF BM30A, SPring-8, SSRF BL
INCIDENT_BEAM_DIRECTION=0 0 1          ! only read by IDXREF

DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD= 1179359  !PILATUS
NX= 2463 NY= 2527  QX= 0.172  QY= 0.172 ! to make CORRECT happy if frames are unavailable
DIRECTION_OF_DETECTOR_X-AXIS=1 0 0
DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0
```

/mnt/home1/rapidata3/xds_tutorial

XPARM.XDS

```
 XPARM.XDS     VERSION Feb 5, 2021  BUILT=20210323
     1   270.0000    0.2000  0.999971  0.007404 -0.001831
  0.979460       0.000711       0.000291       1.020970
    96     78.8215     78.8215     37.1784  90.000  90.000  90.000
 36.338257       9.327419     -69.320709
 26.357738      70.532730      23.307367
 30.559622     -16.002089      13.866352
     1      2463      2527    0.172000     0.172000
1231.500000    1263.500000     189.160004
  1.000000       0.000000       0.000000
  0.000000       1.000000       0.000000
  0.000000       0.000000       1.000000
     1        1     2463        1     2527
   0.00      0.00      0.00  1.00000  0.00000  0.00000  0.00000  1.00000  0.00000
```

First image number

Starting phi

Delta-phi

spindle vector

beam vector

wavelen

space group number

unit cell

a b c cell vectors real space

det panels

pixels

pixel size

origin

distance

x y z Detector fast/slow

Panel #

IDXREF – auto-indexing

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial

Menu Help

Projects | Frame | XDS.INP | XYCORR | INI

LATTICE-CHARACTER	BRAVAIS-LATTICE	QUALITY OF FIT					
* 44	aP	0.0					
* 31	aP	0.2					
* 34	mP	1.5					
* 35	mP	1.8					
* 33	mP	2.9					
* 32	oP	3.1					
* 25	mC	4.5					
* 23	oC	4.9					
* 20	mC	5.1					
* 21	tP	6.2					
39	mC	248.6					
38	oC	249.9					
29	mC	250.0					
28	mC	250.9					
37	mC	251.4					
36	oC	252.7					
27	mC	498.8					
19	oI	501.9					
26	oF	622.5					
18	tI	625.6					
1	cF	999.0					
2	hR	999.0					
3	cP	999.0	57.2	78.8	78.8	90.0	90.0
5	cI	999.0	87.2	87.1	111.4	50.3	50.3

Range

Start

BRAVAIS-TYPE	POSSIBLE SPACE-GROUPS FOR PROTEIN CRYS [SPACE GROUP NUMBER,SYMBOL]
aP	[1,P1]
mP	[3,P2] [4,P2(1)]
mC,mI	[5,C2]
oP	[16,P222] [17,P222(1)] [18,P2(1)2(1)2] [19,P2(1)
oC	[21,C222] [20,C222(1)]
oF	[22,F222]
oI	[23,I222] [24,I2(1)2(1)2(1)]
tP	[75,P4] [76,P4(1)] [77,P4(2)] [78,P4(3)] [89,P42 [91,P4(1)22] [92,P4(1)2(1)2] [93,P4(2)22] [94,P4 [95,P4(3)22] [96,P4(3)2(1)2]
tI	[79,I4] [80,I4(1)] [97,I422] [98,I4(1)22]
hP	[143,P3] [144,P3(1)] [145,P3(2)] [149,P312] [150 [152,P3(1)21] [153,P3(2)12] [154,P3(2)21] [168,P [170,P6(5)] [171,P6(2)] [172,P6(4)] [173,P6(3)] [178,P6(1)22] [179,P6(5)22] [180,P6(2)22] [181,P
hR	[146,R3] [155,R32]
cP	[195,P23] [198,P2(1)3] [207,P432] [208,P4(2)32] [213,P4(1)32]
cF	[196,F23] [209,F432] [210,F4(1)32]
cI	[197,I23] [199,I2(1)3] [211,I432] [214,I4(1)32]

/mnt/home1/rapidata3/xds_tutorial

INTEGRATE – measure the spots!

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial

Menu Help

Projects | Frame | XDS.INP | XYCORR | INIT | COLSPOT | IDXREF | DEFPIX | INTEGRATE | CORRECT | tools | statistics | XDSCONV | XSCALE

Save | Run XDS

```
JOB= INTEGRATE
NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_?????.cbf
DATA_RANGE=1 1800
! EXCLUDE_DATA_RANGE= 1000 1100
SPACE_GROUP_NUMBER=0                   ! 0 if unknown
UNIT_CELL_CONSTANTS= 70 70 40 90 90 90 ! put correct values if known
INCLUDE_RESOLUTION_RANGE=50 0  ! after CORRECT, insert high resol limit; re-run CORRECT
!FRIEDEL'S_LAW=FALSE     ! This acts only on the CORRECT step
REFINE(INTEGRATE)= POSITION BEAM ORIENTATION ! AXIS CELL
!NUMBER_OF_PROFILE_GRID_POINTS_ALONG_ALPHA/BETA=13 ! Default is 9 - Increasing may improve data
!NUMBER_OF_PROFILE_GRID_POINTS_ALONG_GAMMA=13      ! accuracy, particularly if finely-sliced on phi,
!BEAM_DIVERGENCE=   0.50204  BEAM_DIVERGENCE_E.S.D.=   0.05020
!REFLECTING_RANGE=  0.65025  REFLECTING_RANGE_E.S.D.=  0.09289

DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD= 1179359  !PILATUS
X-RAY_WAVELENGTH= 0.97946
NX= 2463 NY= 2527  QX= 0.172  QY= 0.172 ! to make CORRECT happy if frames are unavailable
OSCILLATION_RANGE= 0.2000
DIRECTION_OF_DETECTOR_X-AXIS=1 0 0
DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0
```

/mnt/home1/rapidata3/xds_tutorial

CORRECT – scale all the “factors”

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial

Menu Help

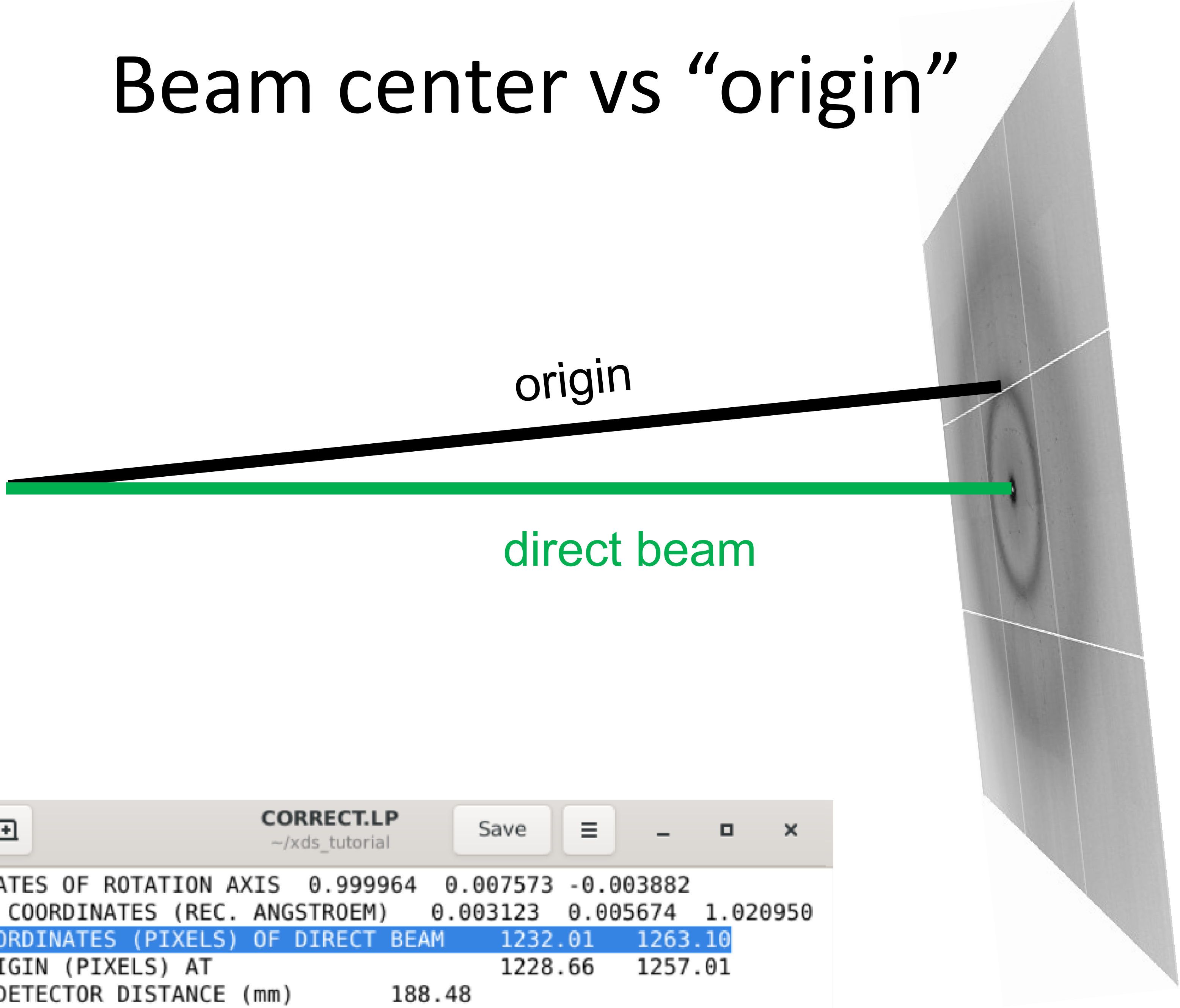
Projects | Frame | XDS.INP | XYCORR | INIT | COLSPOT | IDXREF | DEFPIX | INTEGRATE | CORRECT | tools | statistics | XDSCONV | XSCALE

Save | Run XDS

```
JOB= CORRECT
!NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_?????.cbf
! REFERENCE_DATA_SET=xxx/XDS_ASCII.HKL ! e.g. to ensure consistent indexing
DATA_RANGE=1 1800
! EXCLUDE_DATA_RANGE=1000 1100
SPACE_GROUP_NUMBER=0                   ! 0 if unknown
UNIT_CELL_CONSTANTS= 70 70 40 90 90 90 ! put correct values if known
INCLUDE_RESOLUTION_RANGE=50 0  ! after CORRECT, insert high resol limit; re-run CORRECT
!EXCLUDE_RESOLUTION_RANGE= 3.93 3.87 !ice-ring at 3.897 Angstrom
FRIEDEL'S_LAW=FALSE     ! This acts only on the CORRECT step
! STRICT_ABSORPTION_CORRECTION=TRUE
! REFINE(CORRECT)=CELL BEAM ORIENTATION AXIS POSITION ! Default is: refine everything
FRACTION_OF_POLARIZATION=0.98   ! better value is provided by beamline staff!
POLARIZATION_PLANE_NORMAL=0 1 0        ! only used by CORRECT

DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD= 1179359  !PILATUS
SENSOR_THICKNESS= 0.32
X-RAY_WAVELENGTH= 0.97946
NX= 2463 NY= 2527  QX= 0.172  QY= 0.172 ! to make CORRECT happy if frames are unavailable

OSCILLATION_RANGE= 0.2000
!STARTING_ANGLE= 270.0000
DIRECTION_OF_DETECTOR_X-AXIS=1 0 0
DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0
```

/mnt/home1/rapidata3/xds_tutorial

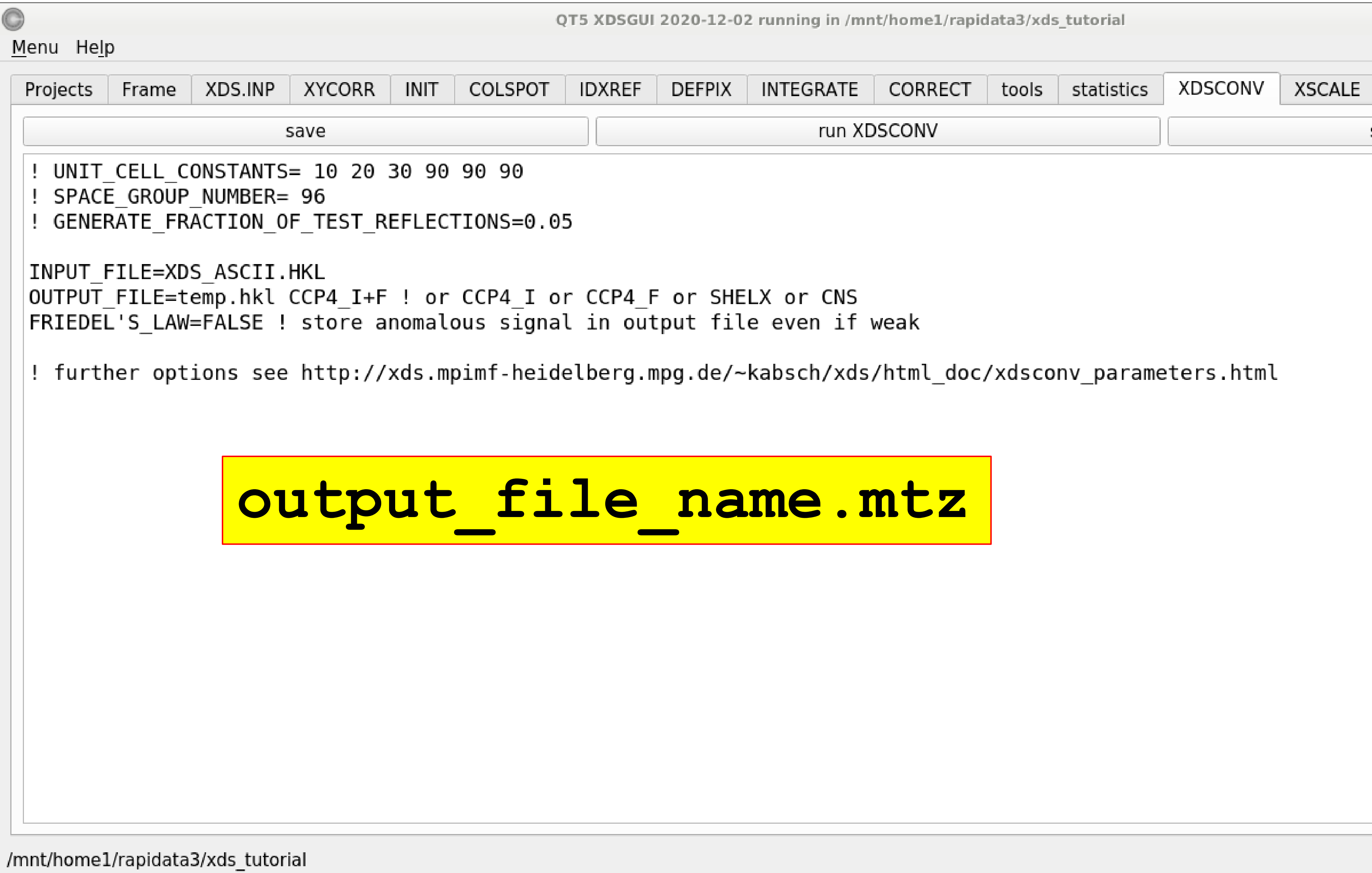
Beam center vs “origin”



CORRECT.LP
~/xds_tutorial

```
LAB COORDINATES OF ROTATION AXIS   0.999964  0.007573 -0.003882
DIRECT BEAM COORDINATES (REC. ANGSTROEM)   0.003123  0.005674  1.020950
DETECTOR COORDINATES (PIXELS) OF DIRECT BEAM     1232.01    1263.10
DETECTOR ORIGIN (PIXELS) AT                      1228.66    1257.01
CRYSTAL TO DETECTOR DISTANCE (mm)       188.48
```

xdsconv – make an “mtz” file



Adding noise

1 + 1 = 1.4

$$\sigma_{total}^2 = \sigma_1^2 + \sigma_2^2$$

Adding noise

$$1^2 + 1^2 = 1.4^2$$

$$3^2 + 1^2 = 3.2^2$$

$$\sigma_{total}^2 = \sigma_1^2 + \sigma_2^2$$

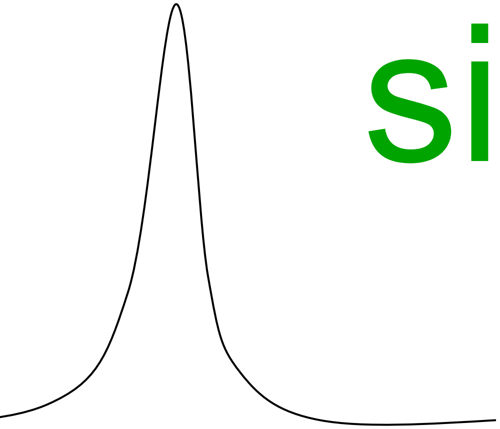
Adding noise

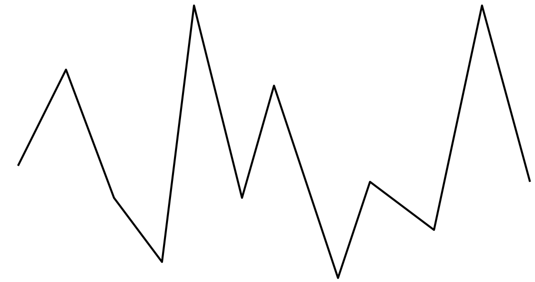
$$1^2 + 1^2 = 1.4^2$$

$$3^2 + 1^2 = 3.2^2$$

$$10^2 + 1^2 = 10.05^2$$

signal *vs* noise





"If you don't have good data, then you must learn statistics."

-James Holton

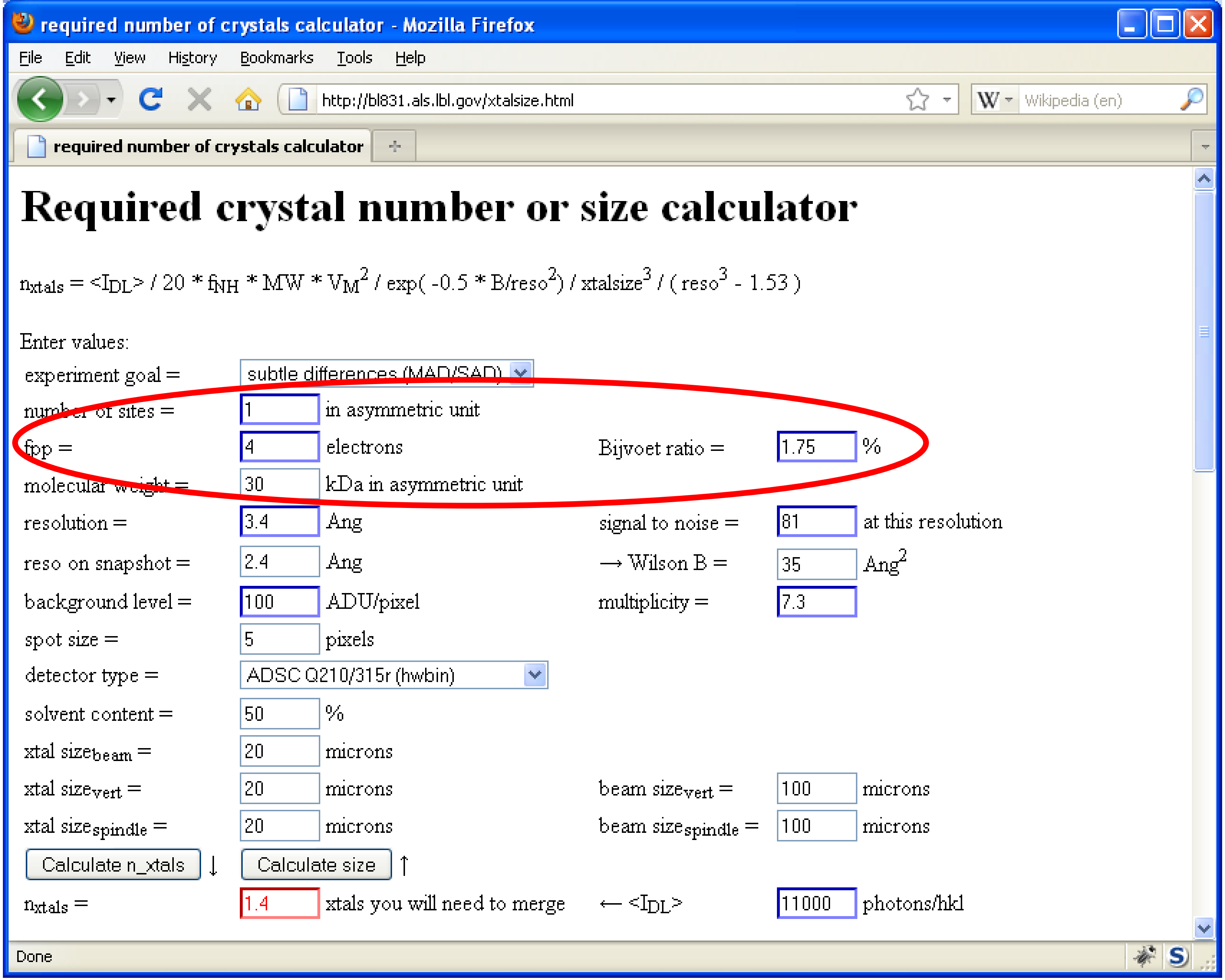
Sources of error for anomalous differences

- Shutter jitter (rms 0.5 ms)
- Beam flicker (0.15%/sqrt(Hz))
- Attenuation correction (< 2%)
- Radiation damage (1%/MGy)
- Detector calibration (3%)

anomalous signal

$$\frac{\Delta F}{F} \approx 1.2\, f'' \sqrt{\frac{\#\ \text{sites}}{\text{MW (Da)}}}$$

Crick, F. H. C. & Magdoff, B. S. (1956) *Acta Crystallogr.* **9**, 901-908.
Hendrickson, W. A. & Teeter, M. M. (1981) *Nature* **290**, 107-113.



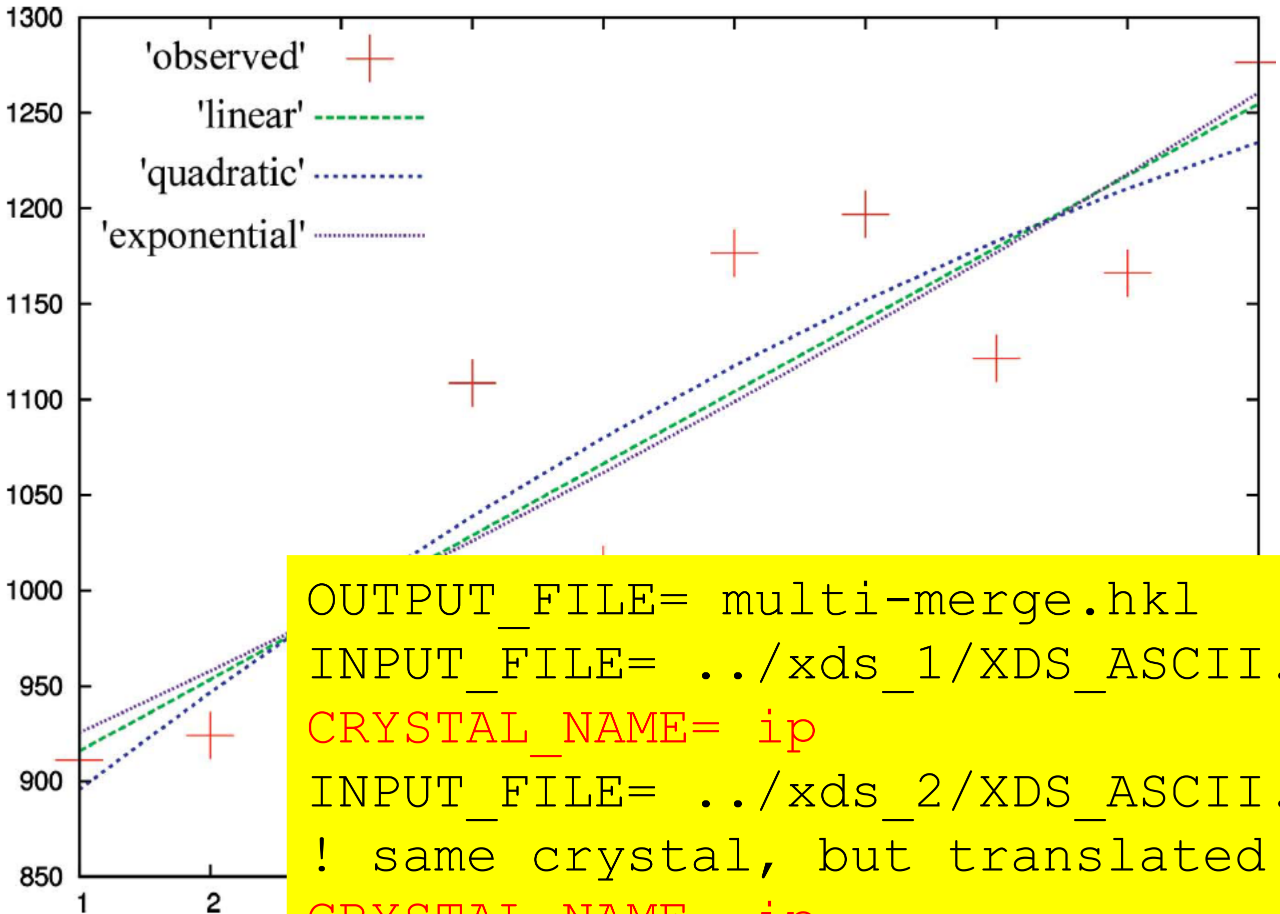
Holton & Frankel (2010) *Acta D* **66** 393-408.

Re-indexing cheat sheet

Space group	Re-indexing
$P4$, ($P4_1$, $P4_3$), $P4_2$, $I4$, $I4_1$	$hkl \rightarrow kh\bar{l}$
$P3$, ($P3_1$, $P3_2$)	$hkl \rightarrow \bar{h}\bar{k}l$
	or $hkl \rightarrow kh\bar{l}$
	or $hkl \rightarrow \bar{k}\bar{h}\bar{l}$
$R3$	$hkl \rightarrow kh\bar{l}$
$P321$, ($P3_121$, $P3_221$)	$hkl \rightarrow \bar{h}\bar{k}l$
$P312$, ($P3_112$, $P3_212$)	$hkl \rightarrow \bar{h}\bar{k}l$
$P6$, ($P6_1$, $P6_5$), ($P6_2$, $P6_4$), $P6_3$	$hkl \rightarrow kh\bar{l}$
$P23$, $P2_13$, ($I23$, $I2_13$), $F23$	$hkl \rightarrow k\bar{h}l$

Dauter, Z. (1999). "Data-collection strategies." Acta Cryst. D **55**(10): 1703-1717.

Zero-dose extrapolation (ZDE)




```
OUTPUT_FILE= multi-merge.hkl
INPUT_FILE= ../xds_1/XDS_ASCII.HKL
CRYSTAL_NAME= ip
INPUT_FILE= ../xds_2/XDS_ASCII.HKL
! same crystal, but translated
CRYSTAL_NAME= ip
```

Figure 2
Example of noisy data points (marked by '+') fitted by a linear (green), a quadratic (blue) and an exponential function (purple). Near 1/4 and near 3/4 of the range, the values of the functions used for fitting coincide.

Diederichs, K. (2006). "Some aspects of quantitative analysis and correction of radiation damage." Acta Cryst. D **62**(1): 96-101.

xscale – final stats

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial

Help

ects | Frame | XDS.INP | XYCORR | INIT | COLSPOT | IDXREF | DEFPIX | INTEGRATE | CORRECT | tools | statistics | XDSCONV | XSCALE | SHELX

save | run xscale | show XSCA

UBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

ESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	COMPARED	I/SIGMA	R-meas	CC(1/2)	Anomal Corr
4.82	15416	1089	1091	99.8%	1.1%	1.8%	15416	145.67	1.2%	100.0*	89*
3.41	24671	1848	1955	94.5%	1.4%	1.9%	24666	140.26	1.5%	100.0*	69*
2.78	36341	2537	2537	100.0%	1.6%	1.9%	36341	132.84	1.7%	100.0*	46*
2.41	37752	3013	3014	100.0%	2.1%	2.1%	37752	106.63	2.2%	100.0*	41*
2.16	46702	3405	3405	100.0%	2.6%	2.4%	46702	96.90	2.7%	100.0*	36*
1.97	51923	3756	3756	100.0%	3.3%	2.9%	51923	78.79	3.4%	100.0*	19*
1.82	51323	4111	4111	100.0%	4.7%	4.0%	51323	54.26	4.9%	99.9*	14*
1.71	57891	4362	4362	100.0%	7.2%	6.3%	57891	38.45	7.5%	99.9*	9
1.61	64156	4680	4680	100.0%	9.8%	9.1%	64156	28.17	10.2%	99.8*	3
1.53	68501	4943	4943	100.0%	14.3%	14.1%	68501	19.31	14.9%	99.7*	3
1.45	64913	5219	5219	100.0%	20.3%	20.4%	64913	13.20	21.2%	99.3*	0
1.39	72865	5446	5447	100.0%	32.4%	33.9%	72865	8.63	33.7%	98.5*	-5
1.34	77152	5660	5660	100.0%	47.7%	50.5%	77152	5.99	49.6%	97.3*	-1
1.29	74358	5893	5893	100.0%	66.2%	70.6%	74358	4.13	69.0%	94.9*	-3
1.25	78139	6102	6103	100.0%	97.4%	105.1%	78139	2.82	101.4%	88.6*	-1
1.21	83395	6304	6304	100.0%	131.6%	143.4%	83395	2.07	136.8%	82.6*	-4
1.17	82112	6550	6551	100.0%	172.1%	189.4%	82112	1.45	179.4%	70.6*	-2
1.14	57381	6701	6701	100.0%	232.2%	256.3%	57381	0.80	247.1%	41.3*	-5
1.11	41788	6847	6918	99.0%	307.2%	341.0%	41689	0.46	335.7%	19.2*	1
1.08	26251	6266	7081	88.5%	456.8%	513.1%	25593	0.22	518.3%	7.1	0
total	1113030	94732	95731	99.0%	2.9%	3.2%	1112268	26.85	3.0%	100.0*	2

ome1/rapidata3/xds_tutorial

XDS: CORRECT.LP or XSCALE.LP

ION

OMPARED	I/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno
3018	33.77	2.3%	99.9*	21*	1.012
4585	22.56	3.6%	99.8*	9	0.914
5327	19.99	4.0%	99.7*	9	0.859
6094	12.27	6.8%	99.3*	-1	0.784
7068	6.01	14.2%	97.8*	-2	0.799
8185	3.10	29.4%	88.8*	-4	0.776
8981	1.90	48.8%	75.9*	2	0.765
5991	1.14	87.3%	53.5*	-2	0.722
2520	0.59	170.4%	21.9*	4	0.693
51769	8.97	9.5%	99.5*	2	0.804

XDS: CORRECT.LP or XSCALE.LP

```
*****************************************************************
   CORRECTION PARAMETERS FOR THE STANDARD ERROR OF REFLECTION I
*****************************************************************


The variance v0(I) of the intensity I obtained from counting st
replaced by v(I)=a*(v0(I)+b*I^2). The model parameters a, b are
minimize the discrepancies between v(I) and the variance estima
sample statistics of symmetry related reflections. This model i
an asymptotic limit ISa=1/SQRT(a*b) for the highest I/Sigma(I)
experimental setup can produce (Diederichs (2010) Acta Cryst D6

     a        b          ISa
3.806E+00  1.080E-04    49.32
```

CCP4: aimless log

```
$TABLE:  Analysis against resolution, XDSdataset:
$GRAPHS:I/sigma, Mean Mn(I)/sd(Mn(I)):0|0.216023x0|137.14:2,13,14:
:Rmerge, Rfull, Rmeas, Rpim v Resolution:0|0.216023x0|1.70834:2,4,5,6,7:
:Average I, RMSdeviation and Sd:0|0.216023x0|1650.8:2,10,11,12:
:Fractional bias:0|0.216023x0|0:2,15:
$$
```

N	1/d^2	Dmid	Rmrg	Rfull	Rcum	Rmeas	Rpim	Nmeas	AvI	RMSdev	sd	I/RMS	Mn(I/sd)	Frc
1	0.0064	12.55	0.020	0.020	0.020	0.021	0.006	13115	1651	57	42	29.2	137.1	
2	0.0191	7.24	0.027	0.027	0.024	0.028	0.008	24753	1171	47	42	25.0	105.2	-
3	0.0318	5.61	0.038	0.038	0.029	0.040	0.012	32197	857	46	43	18.4	79.6	-
4	0.0445	4.74	0.034	0.034	0.031	0.035	0.010	37743	1212	57	53	21.4	91.2	-
5	0.0572	4.18	0.036	0.036	0.032	0.038	0.011	42642	1181	59	57	19.9	83.8	-
6	0.0699	3.78	0.049	0.049	0.036	0.052	0.015	47224	883	59	57	15.1	65.1	-
7	0.0826	3.48	0.065	0.065	0.040	0.068	0.020	51052	685	59	58	11.7	50.9	-
8	0.0953	3.24	0.096	0.096	0.045	0.100	0.029	54636	448	56	56	8.0	35.0	-
9	0.1080	3.04	0.151	0.151	0.050	0.158	0.046	58072	268	53	53	5.1	22.7	-
10	0.1207	2.88	0.229	0.229	0.056	0.240	0.070	60731	171	51	51	3.3	15.4	-
11	0.1334	2.74	0.314	0.314	0.063	0.329	0.097	63807	125	51	51	2.4	11.3	-
12	0.1461	2.62	0.406	0.406	0.070	0.425	0.125	66241	98	51	52	1.9	8.7	-
13	0.1588	2.51	0.537	0.537	0.078	0.562	0.166	68272	76	53	53	1.4	6.5	-

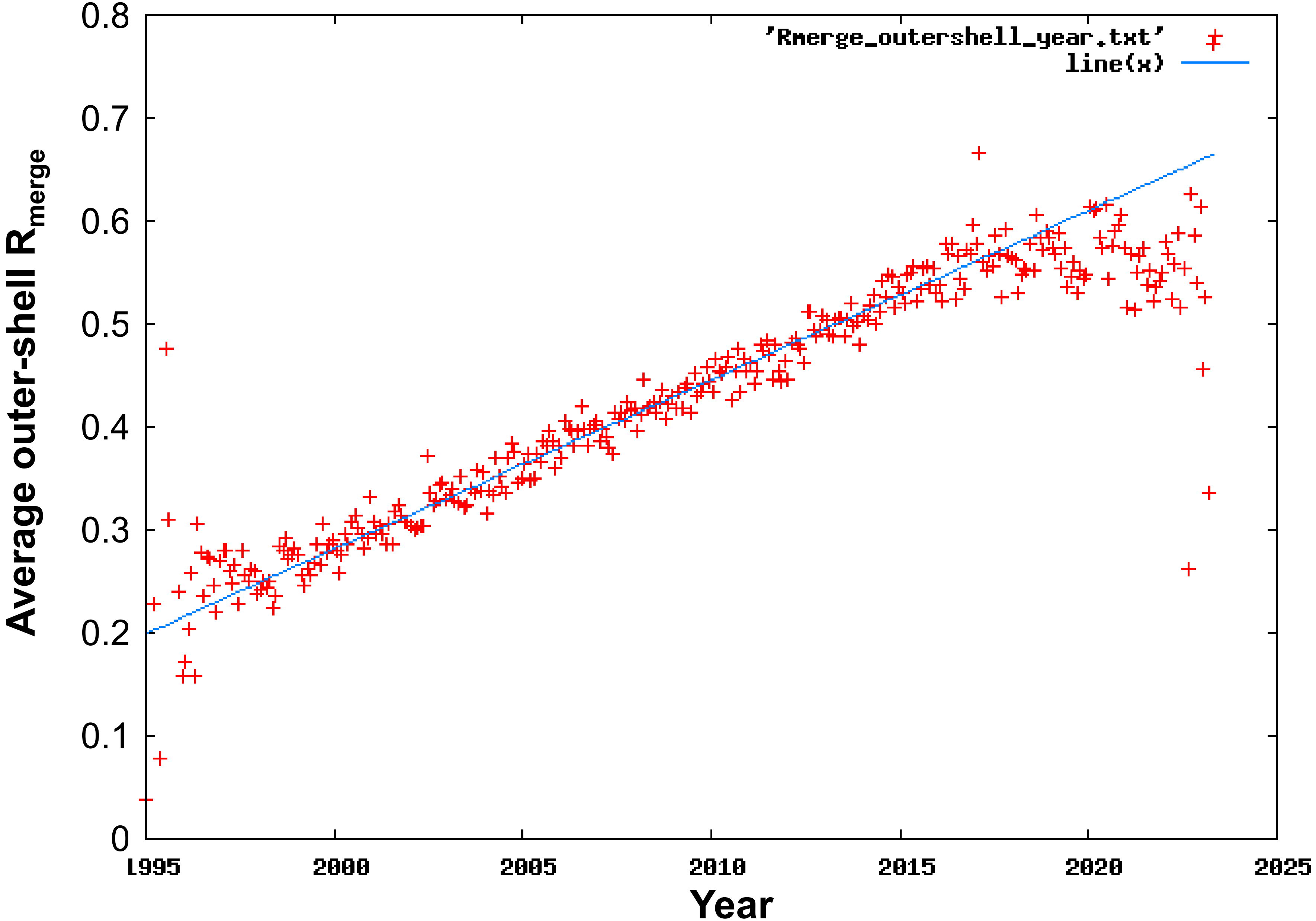
CCP4: aimless log

```
$TABLE:  Correlations CC(1/2) within dataset, XDSdataset:
$GRAPHS: Anom & Imean CCs v resolution:0|0.216023x0|1:2,4,7:
: RMS correlation ratio :0|0.216023x0|2.20344:2,6:
$$
```

N	1/d^2	Dmid	CCanom	Nanom	RCRanom	CC1/2	NImean	$
1	0.0064	12.55	0.659	499	2.203	1.000	669	
2	0.0191	7.24	0.550	975	1.853	1.000	1155	
3	0.0318	5.61	0.527	1295	1.798	1.000	1479	
16	0.1970	2.25	0.037	2123	1.038	0.711	2275	
17	0.2097	2.18	0.043	1682	1.044	0.460	1877	

Resolution cutoff?

R_{merge} at the resolution limit in PDB



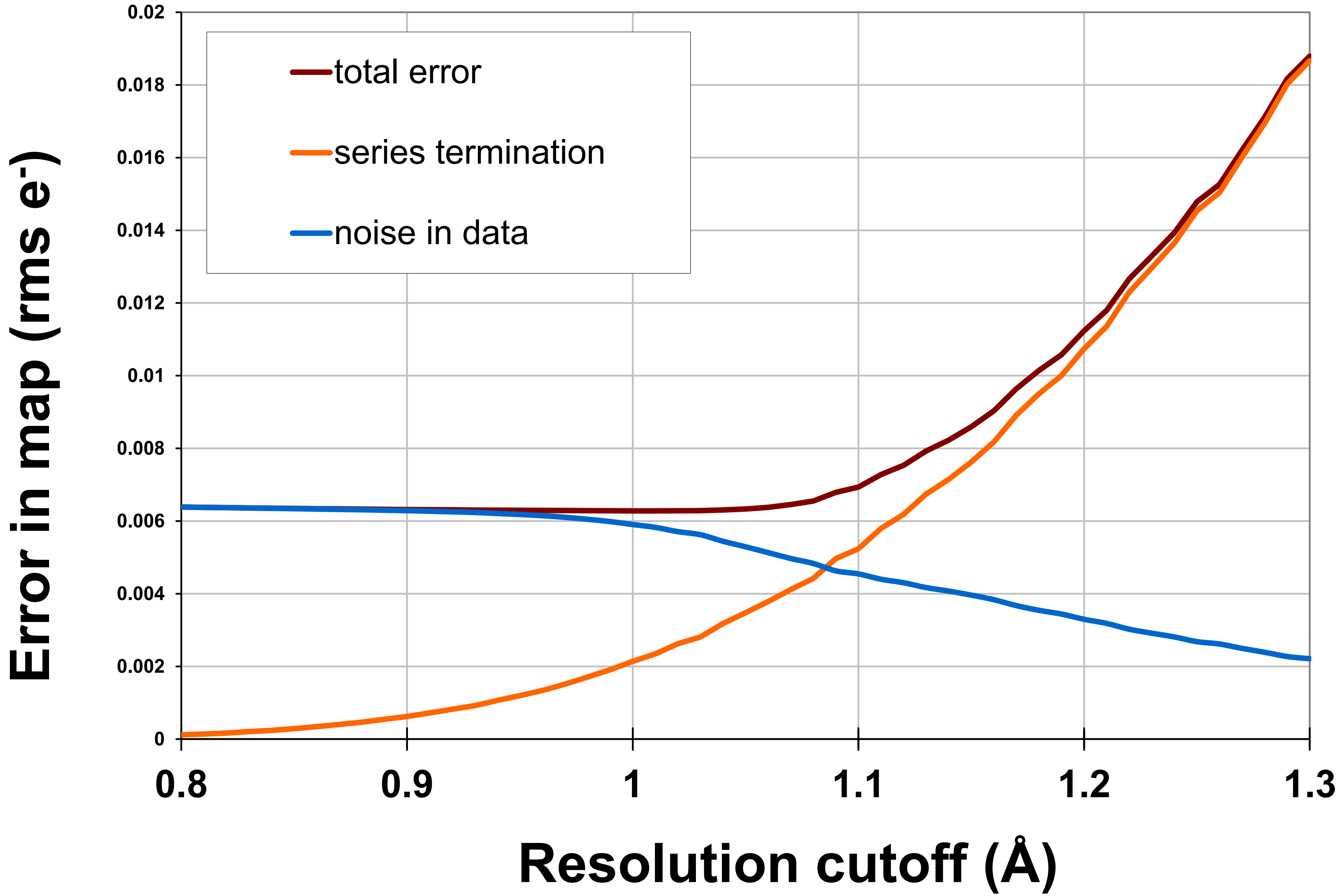
Expected R_{merge} as $I_{obs} \rightarrow 0$

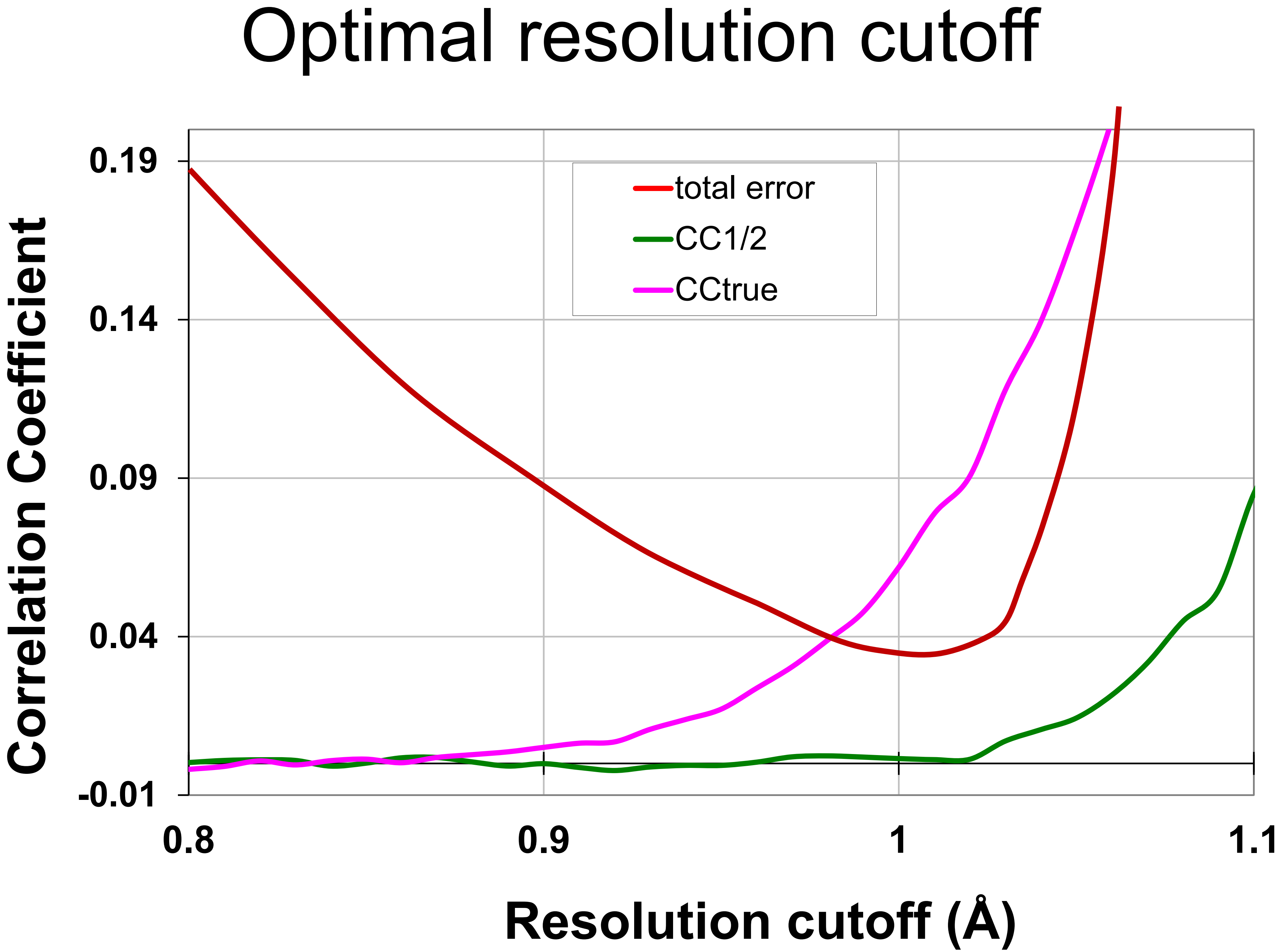
$$R_{merge} = \frac{\sum \left| I_{obs} - \langle I \rangle \right|}{\sum I_{obs}}$$

Optimum resolution cutoff is:

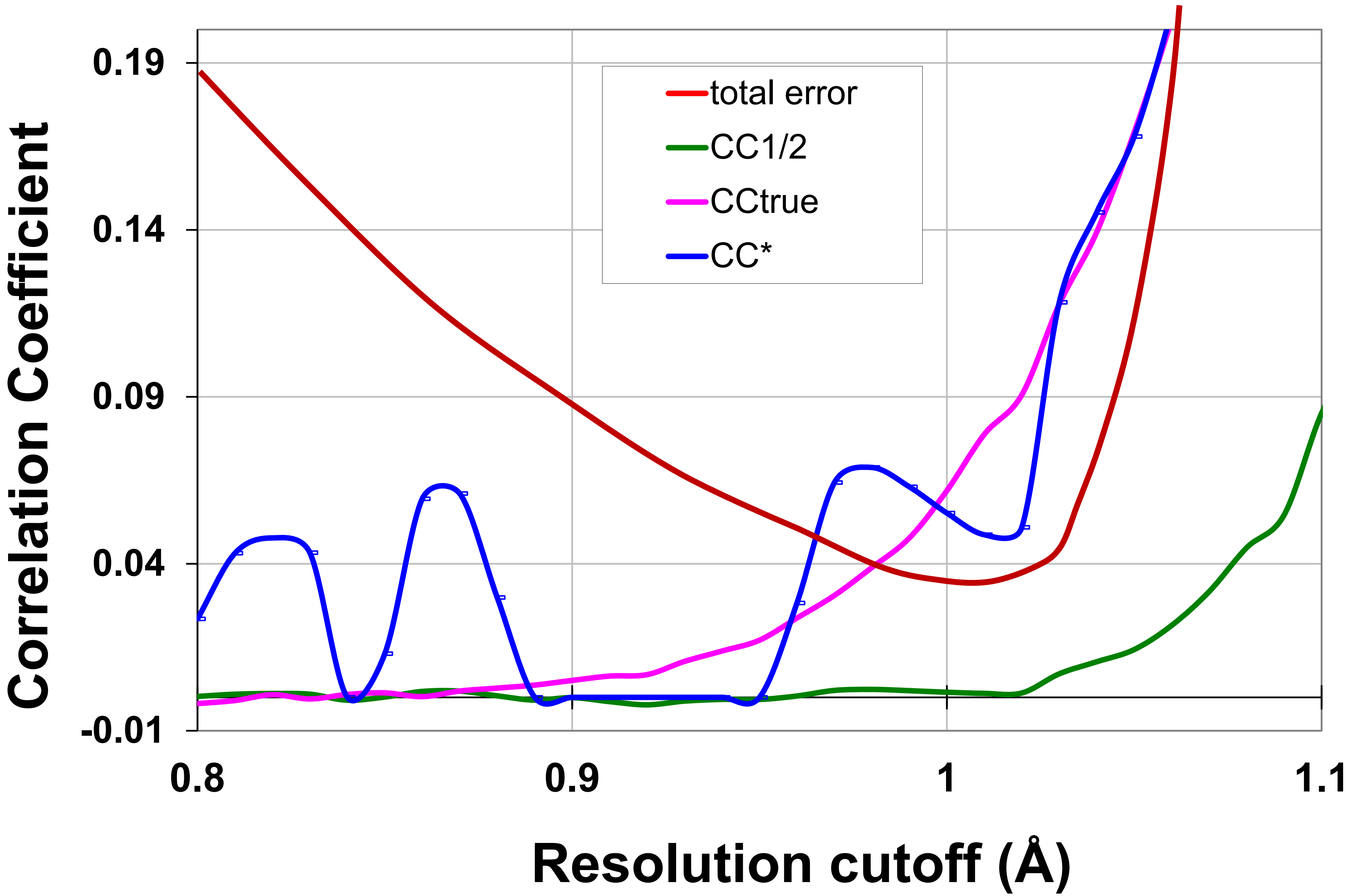
- Too optimistic: add nothing but noise
- Too pessimistic: series-termination error
- Happy medium?
- Simulate:
  - Random atoms, compute F^2
  - Add Gaussian noise, RMS = 1
  - Truncate
  - Subtract “right” map, RMS difference

Optimal resolution cutoff

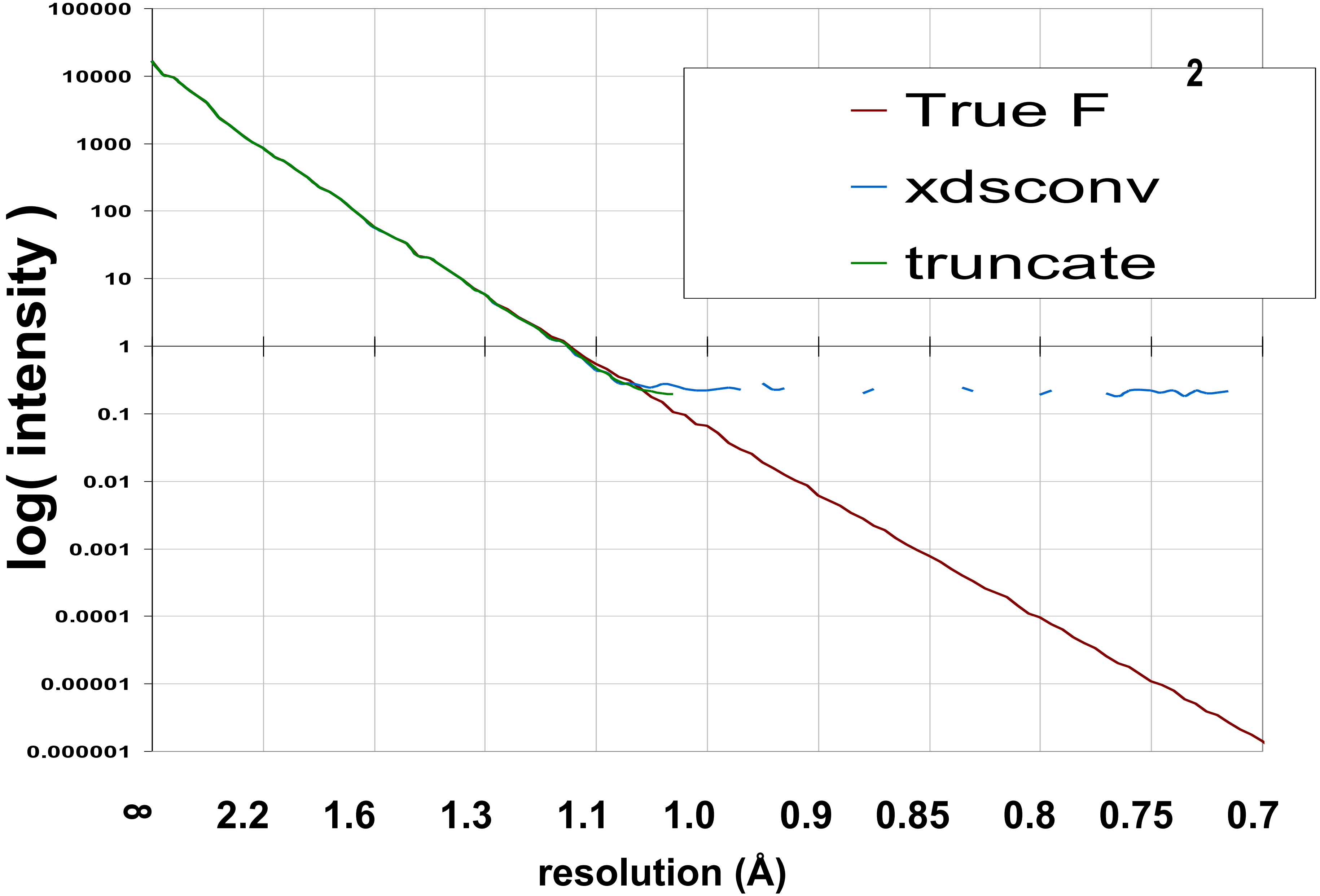



Optimal resolution cutoff
total error
CC1/2
CCtrue
Correlation Coefficient
0.19
0.14
0.09
0.04
-0.01
0.8
0.9
1
1.1
Resolution cutoff (Å)

Optimal resolution cutoff



Wilson Plot

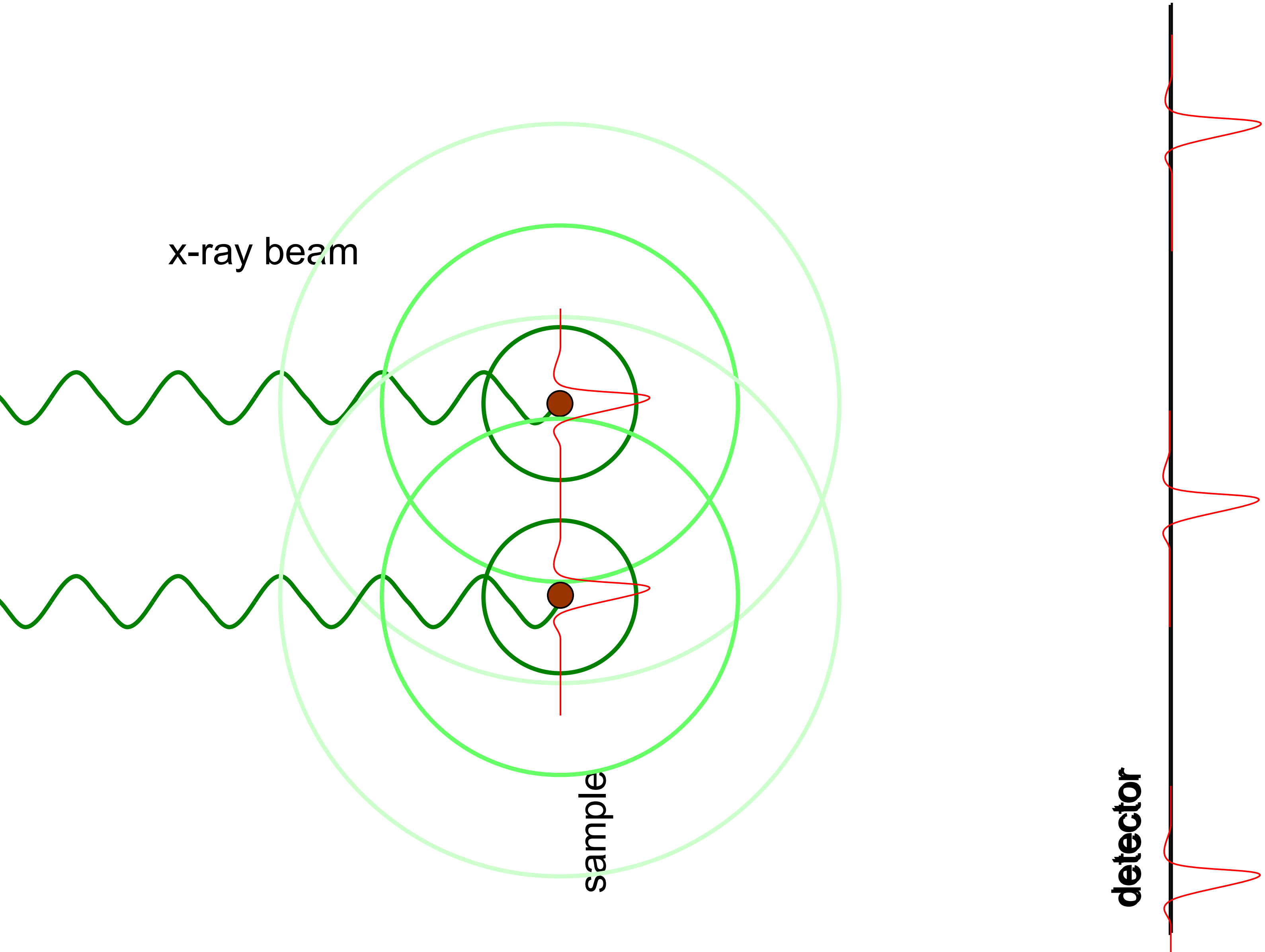


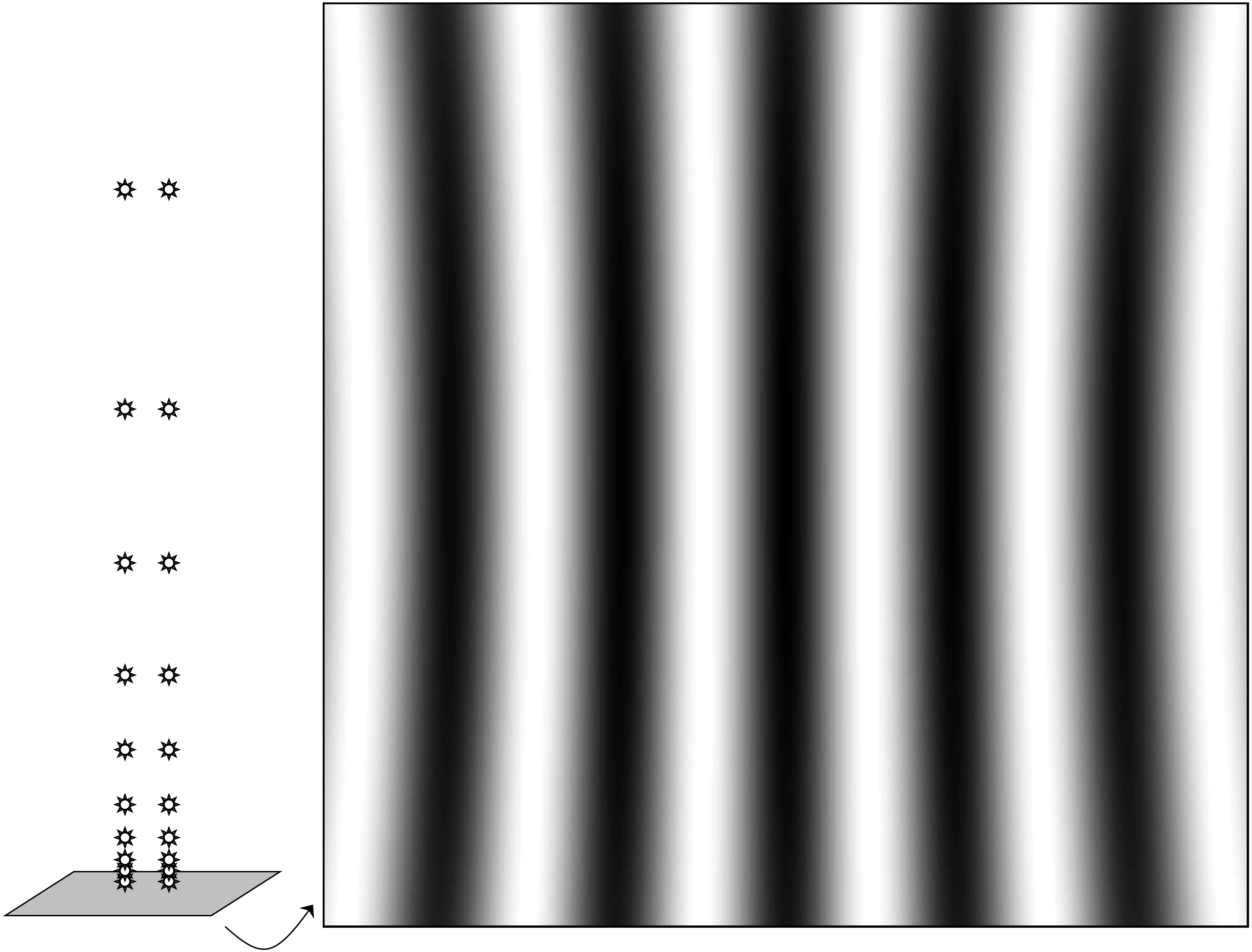
100000
10000
1000
100
10
1
0.1
0.01
0.001
0.0001
0.00001
0.000001
log(intensity)
True F 2
xdsconv
truncate
∞
2.2
1.6
1.3
1.1
1.0
0.9
0.85
0.8
0.75
0.7
resolution (Å)

Optimum resolution cutoff is:

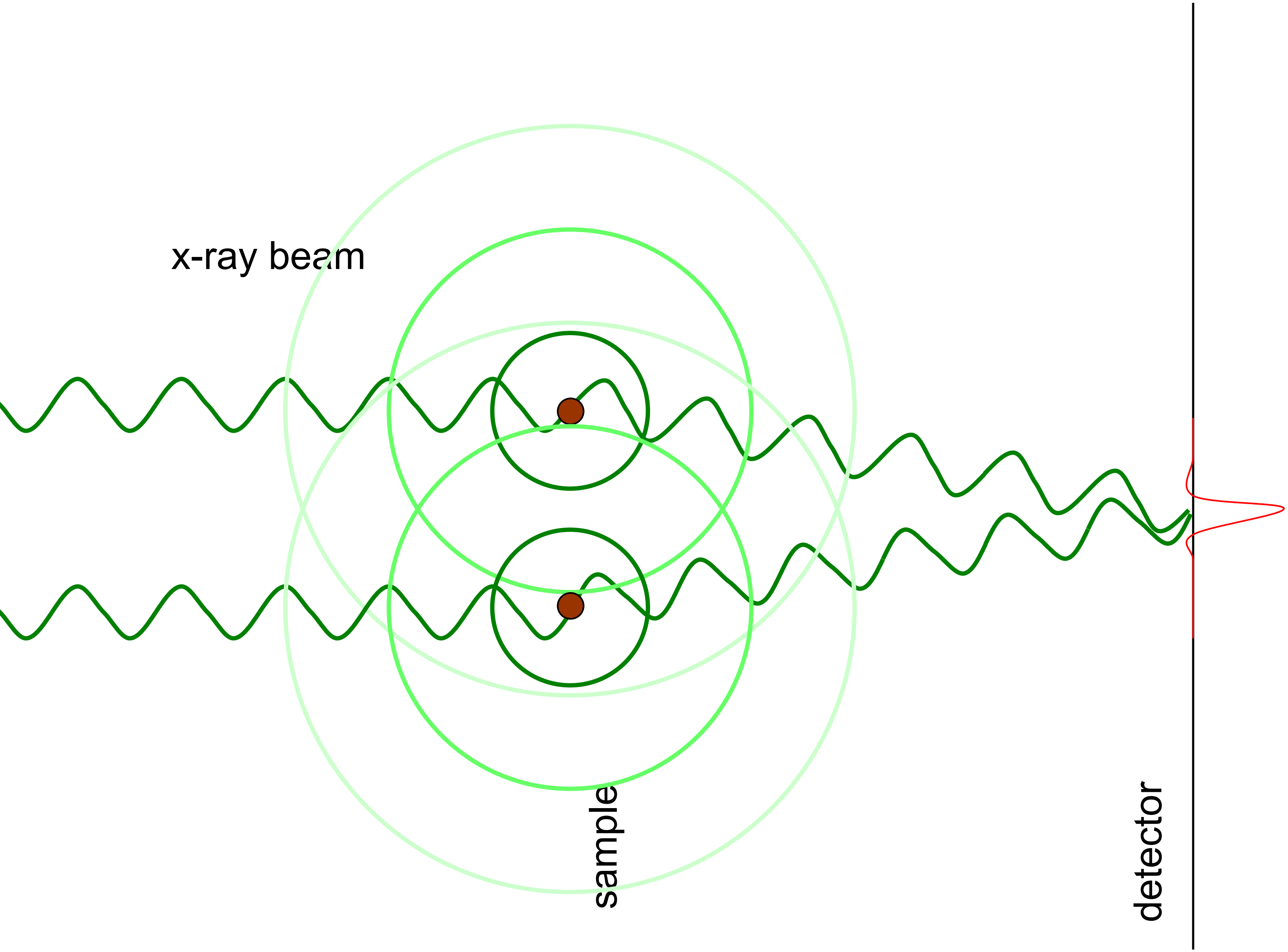
0.0 Å

scattering

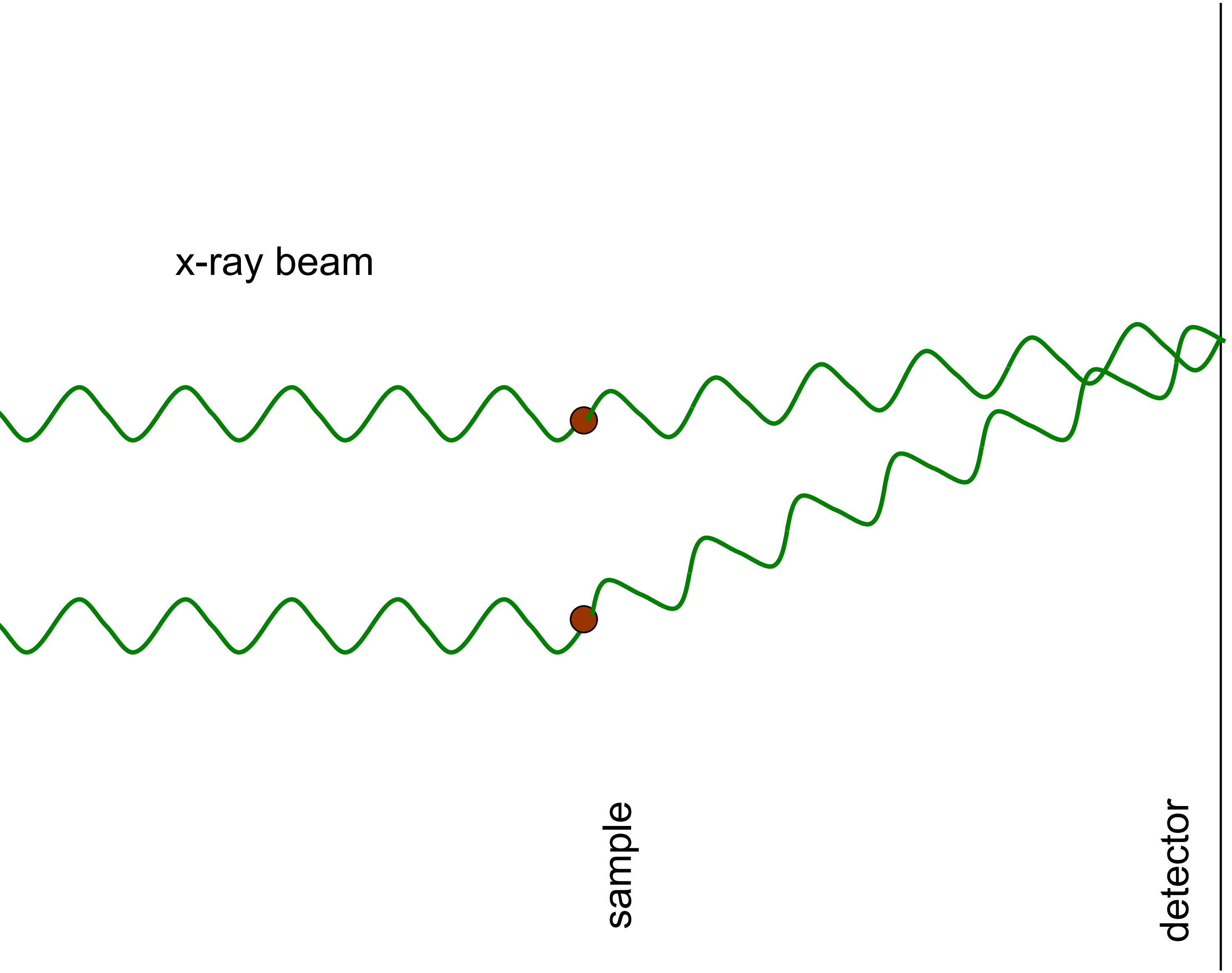




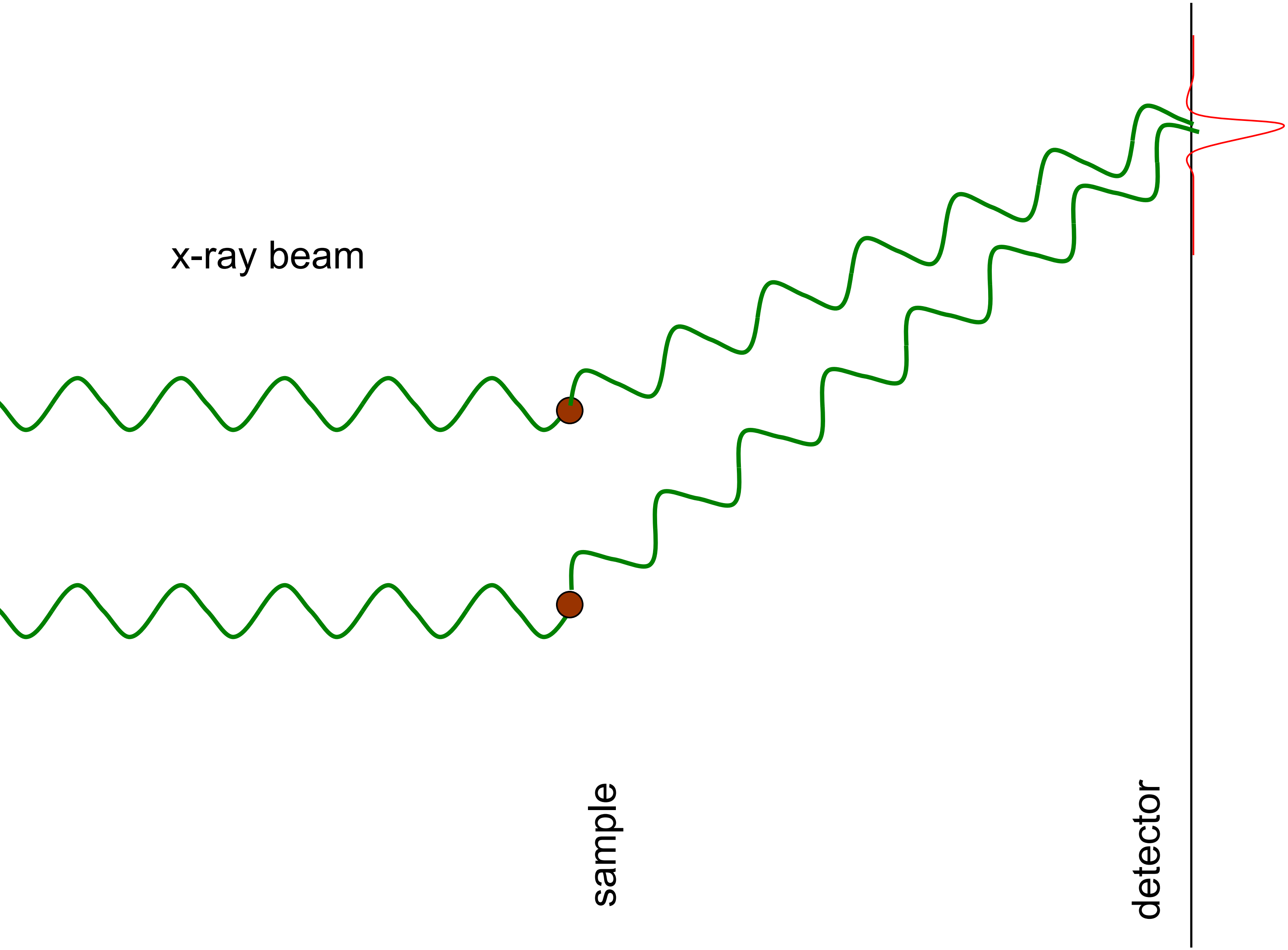
scattering



scattering

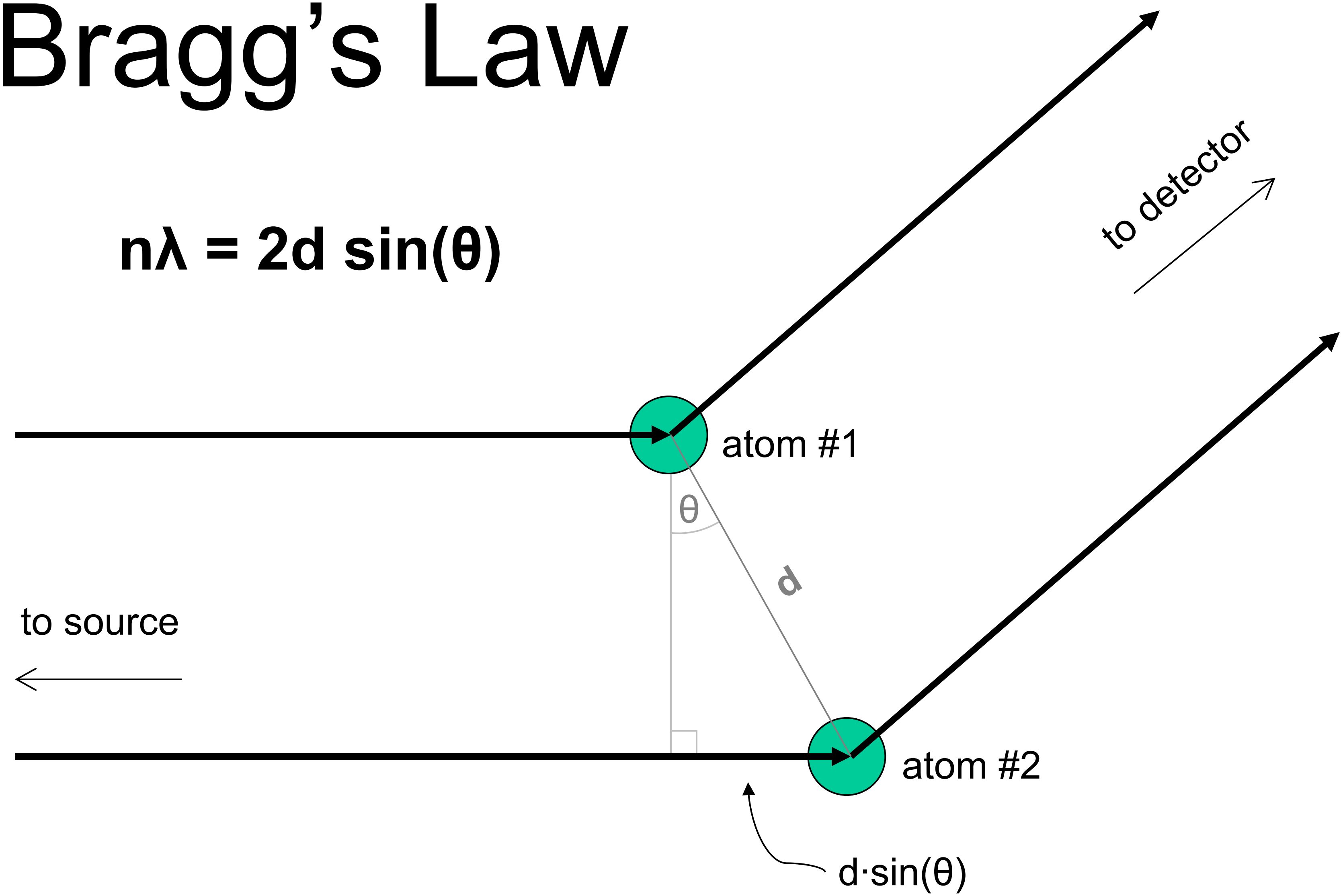


scattering



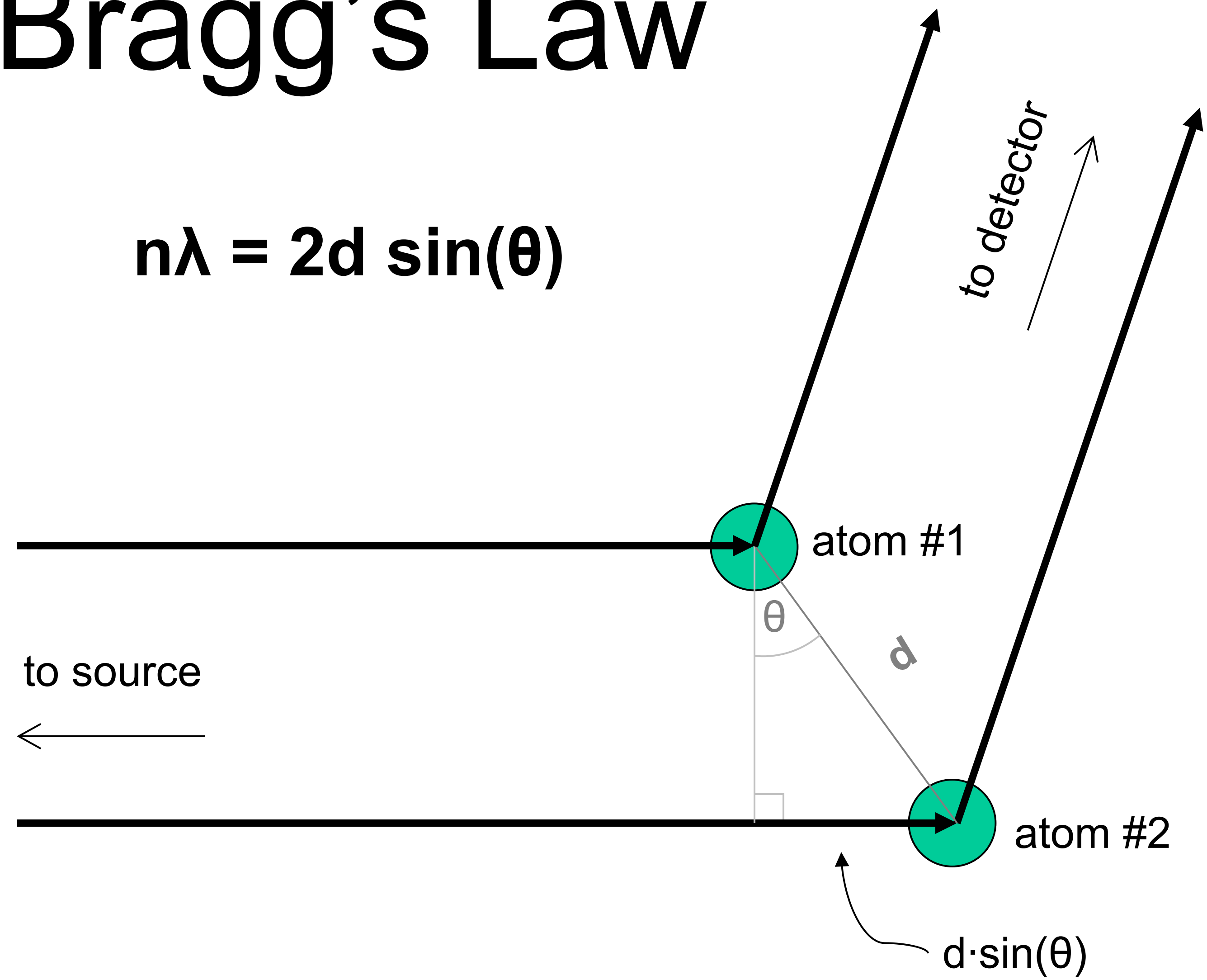
Bragg's Law

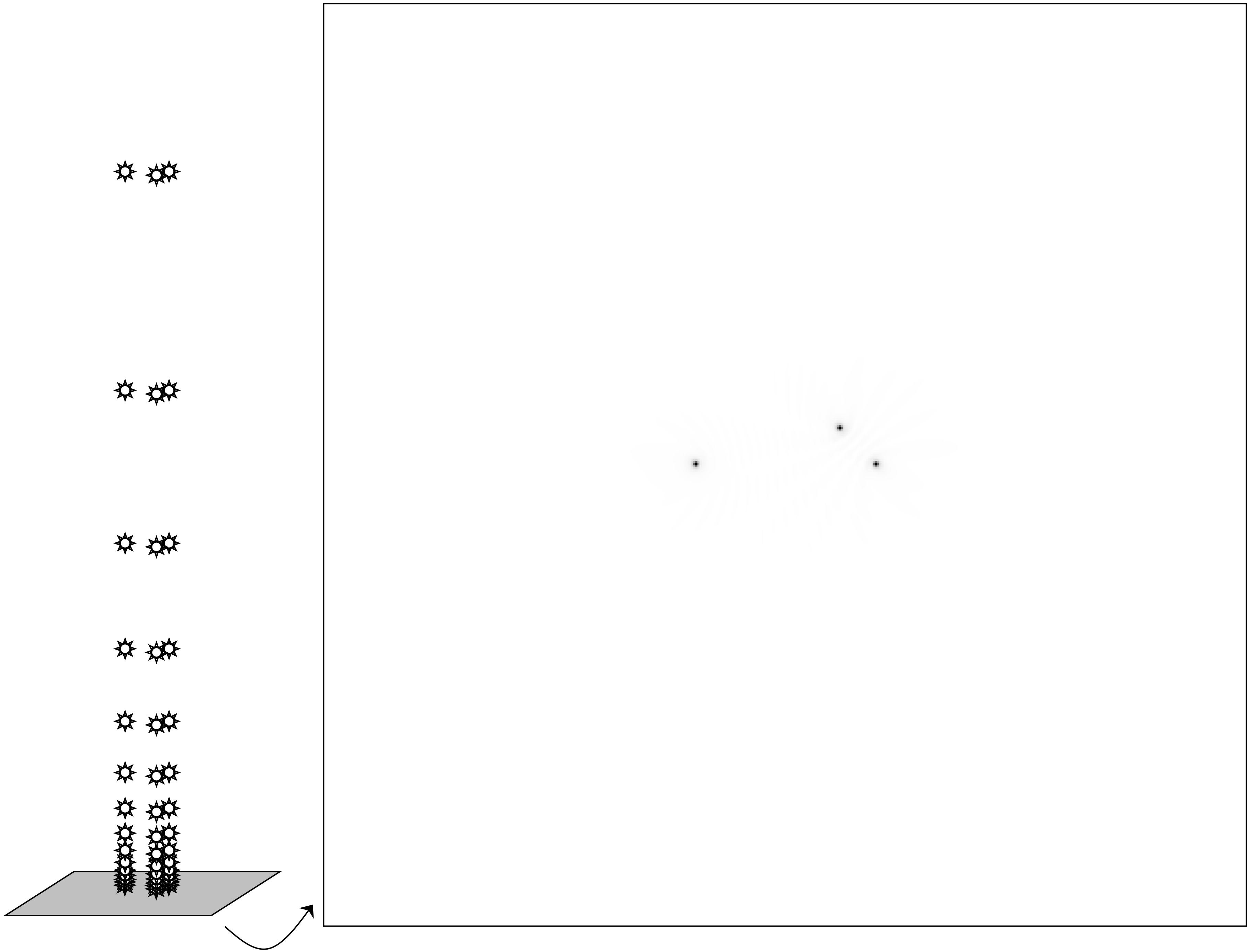
$$n\lambda = 2d \sin(\theta)$$



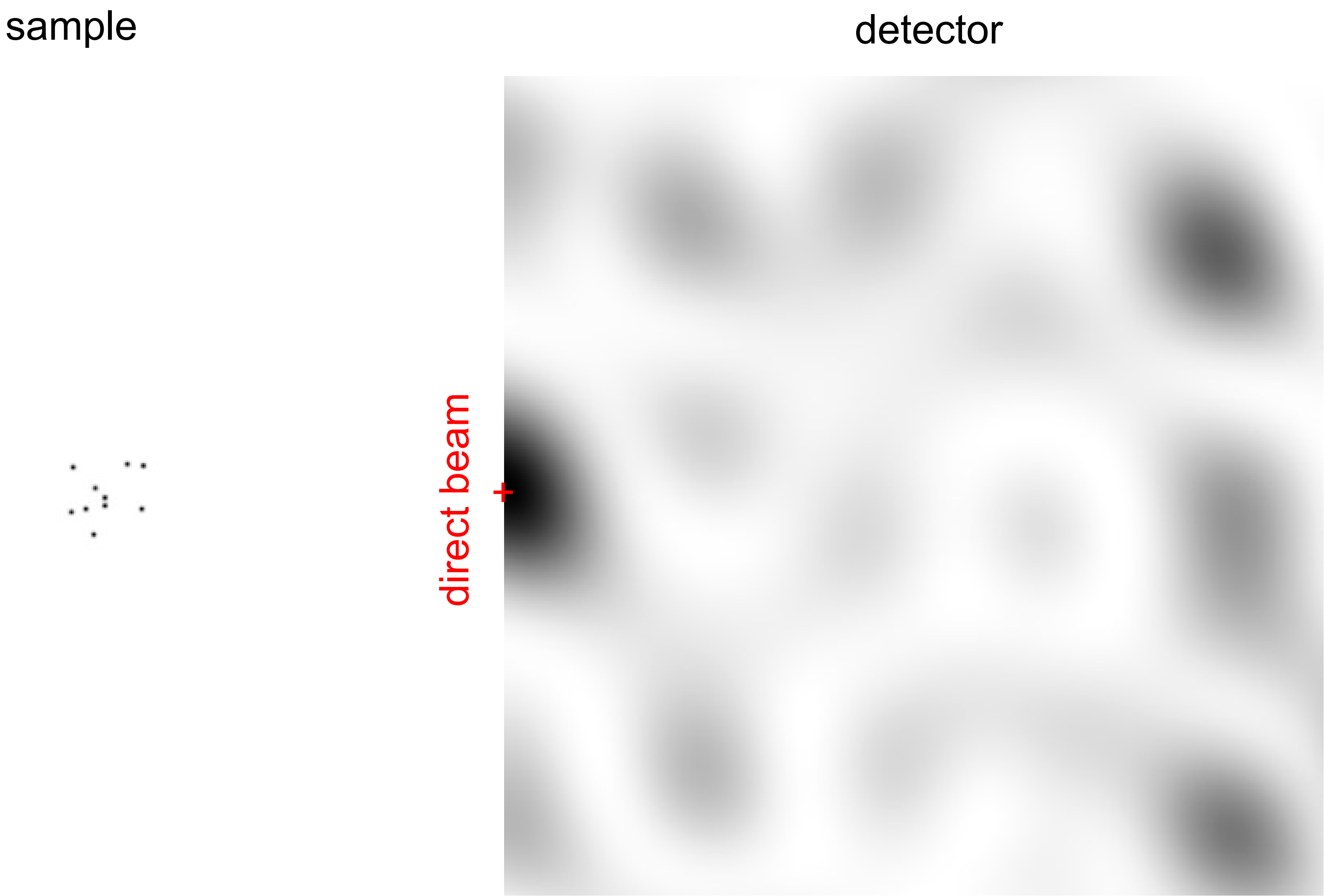
Bragg's Law

$$n\lambda = 2d \sin(\theta)$$



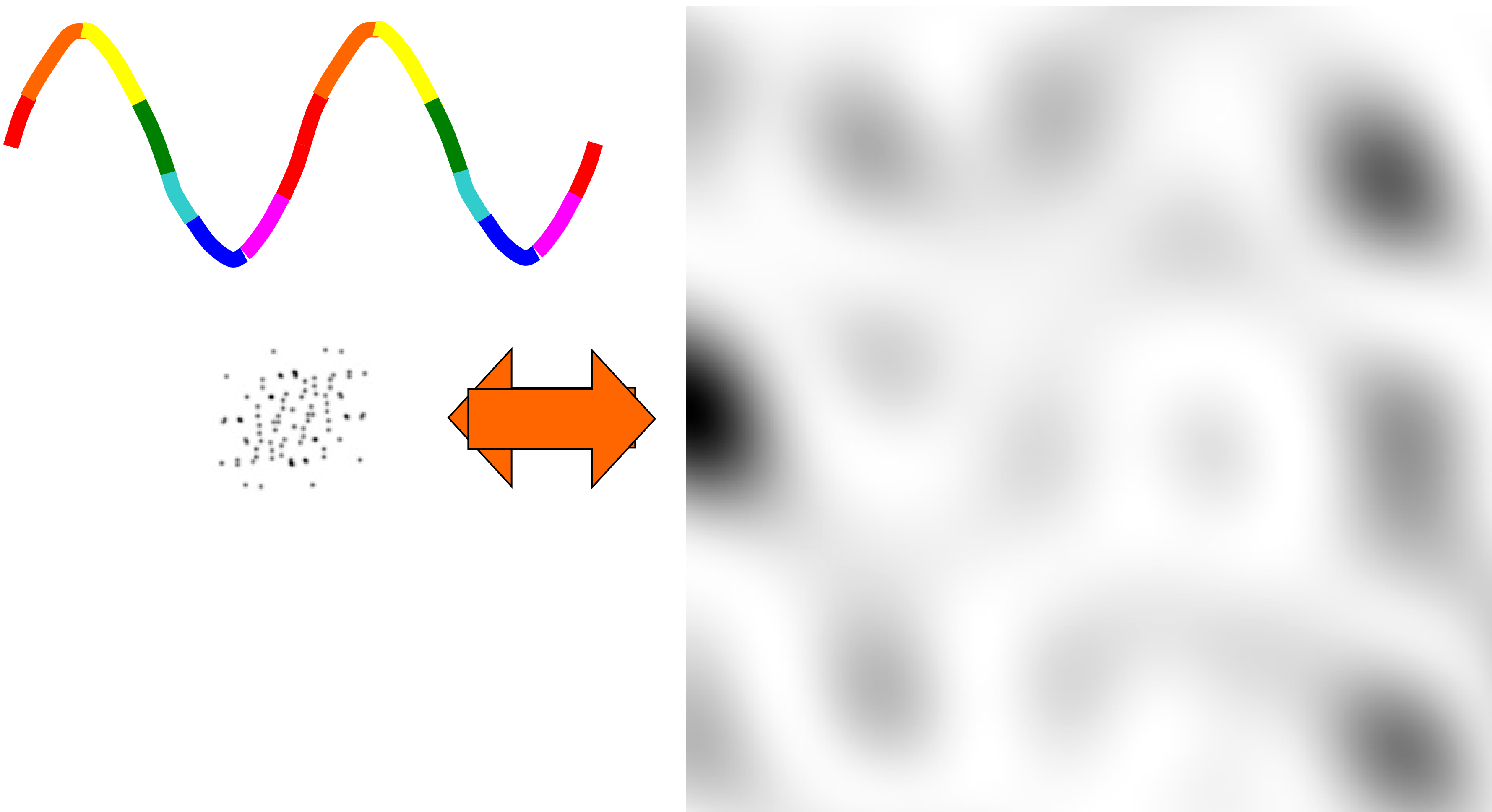


scattering from a structure



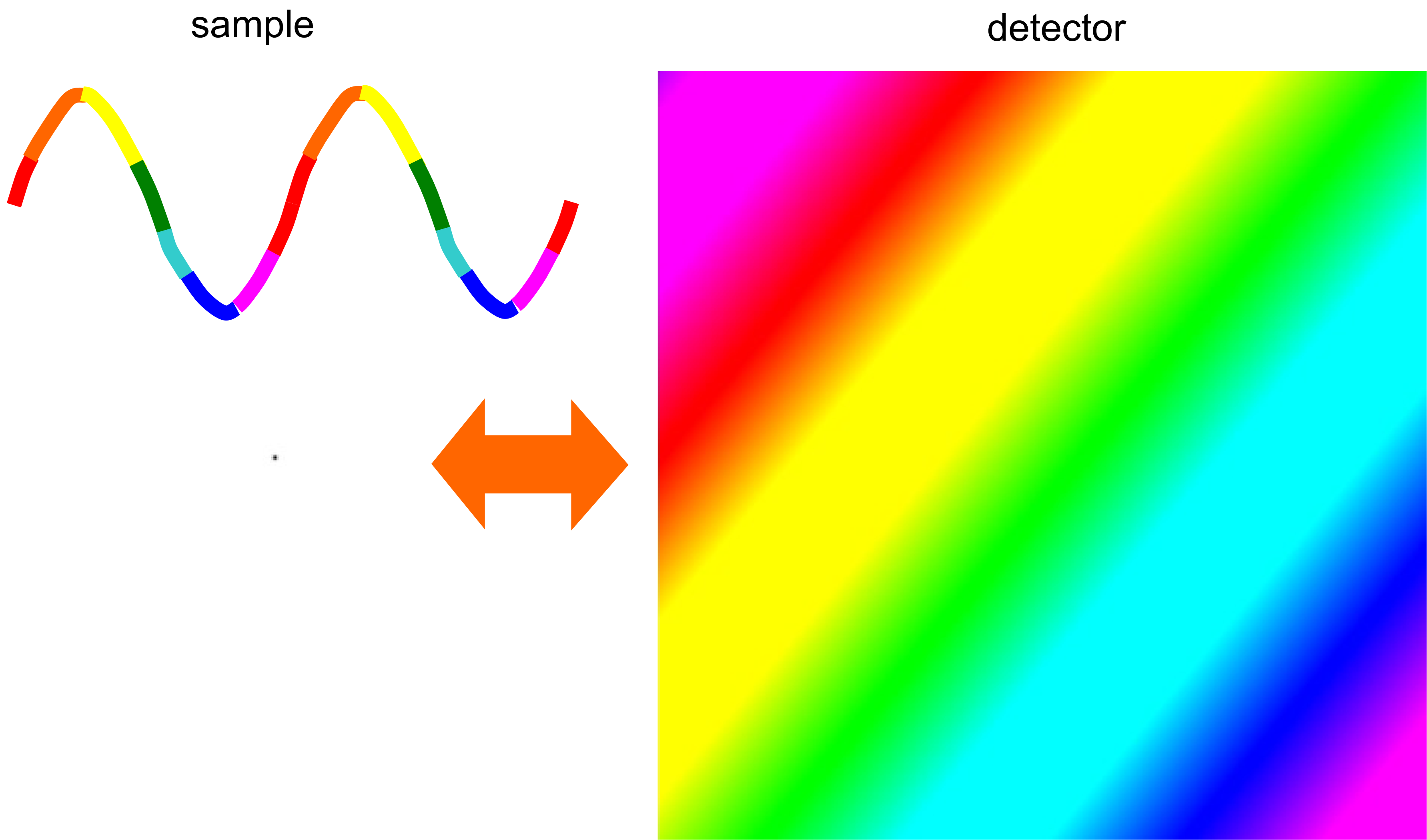
forward inverse Fourier Transform

no phase



scattering Fourier Transform

colored by phase

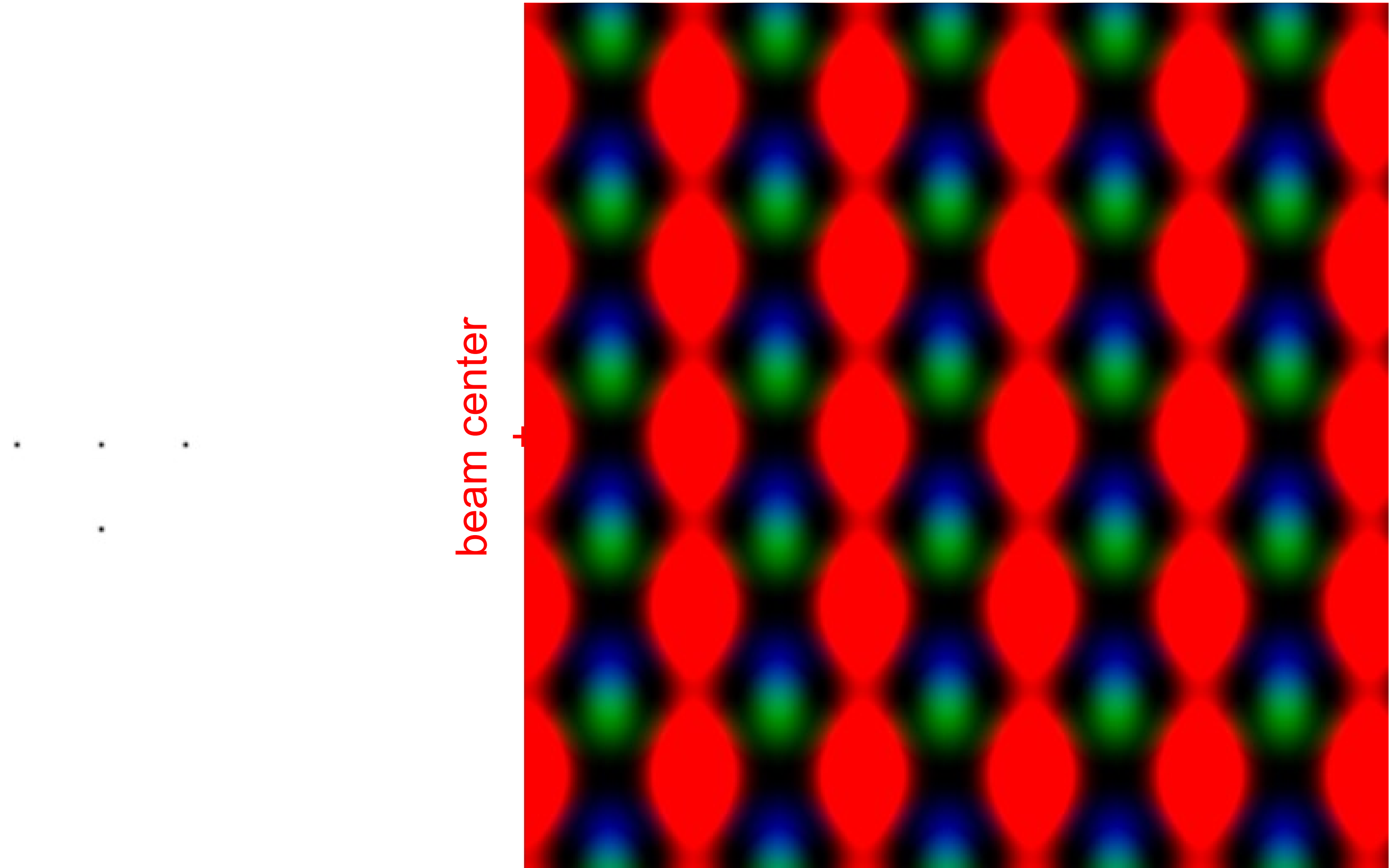


scattering from a lattice

colored by phase

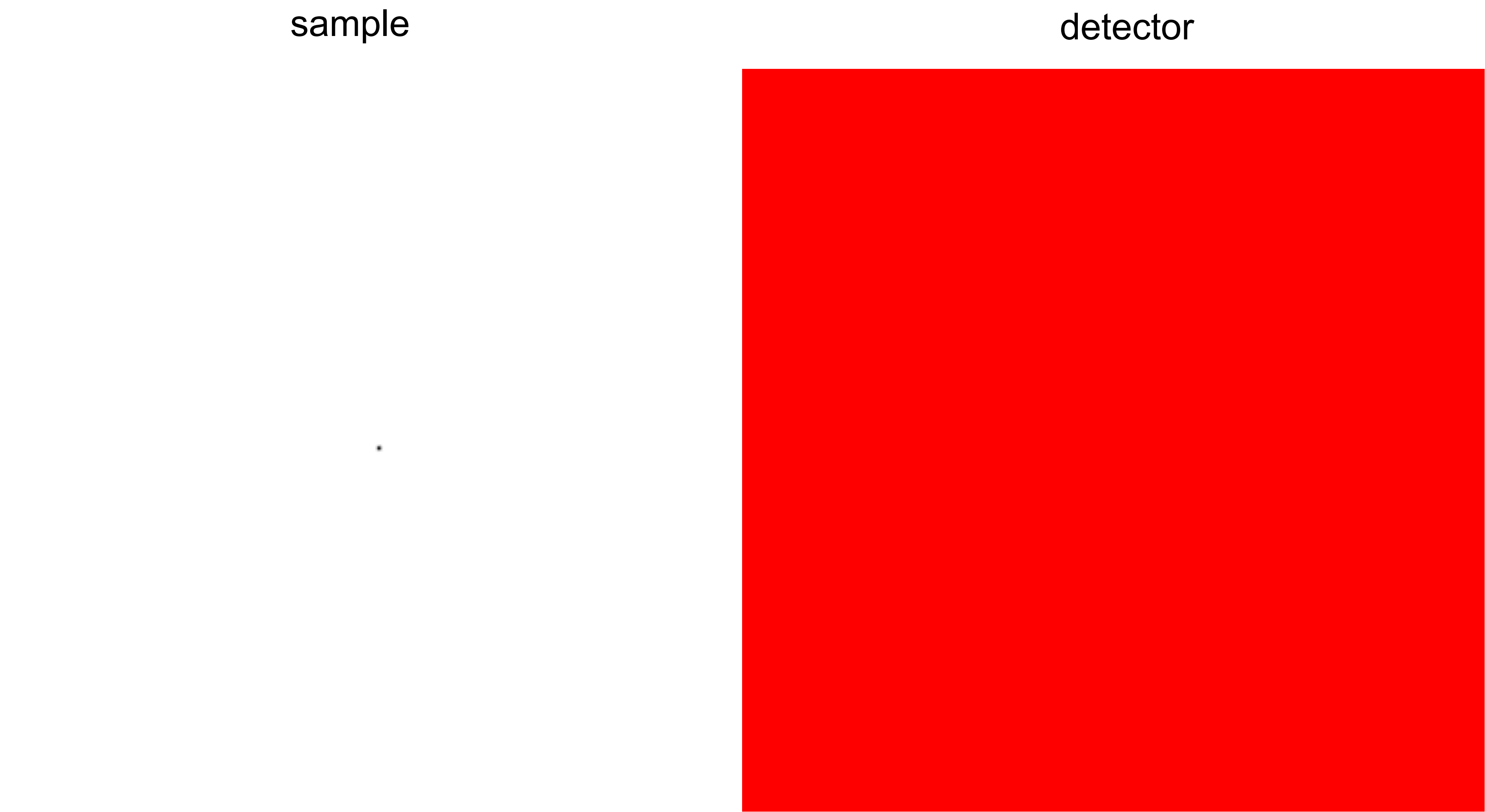
sample

detector



scattering from a lattice

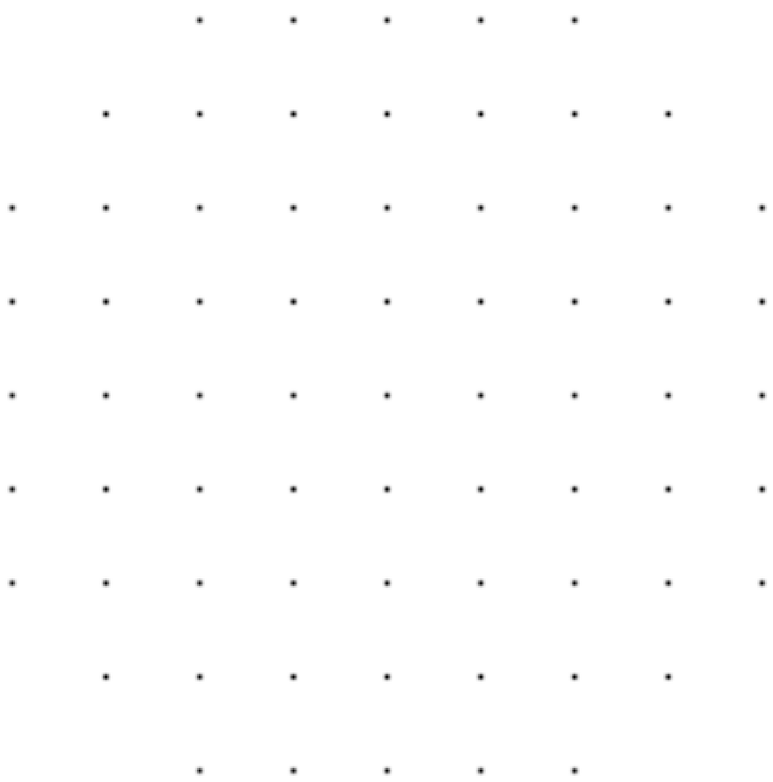
colored by phase



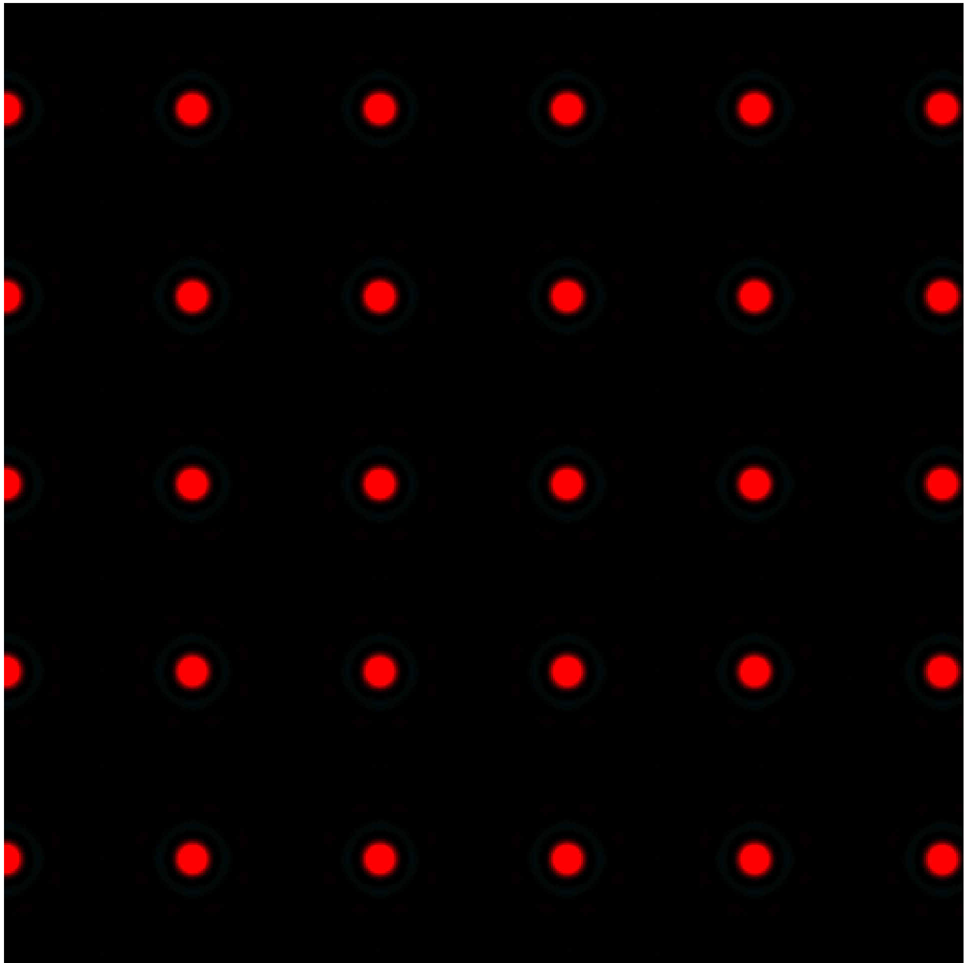
scattering from a lattice

colored by phase

sample



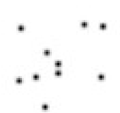
detector



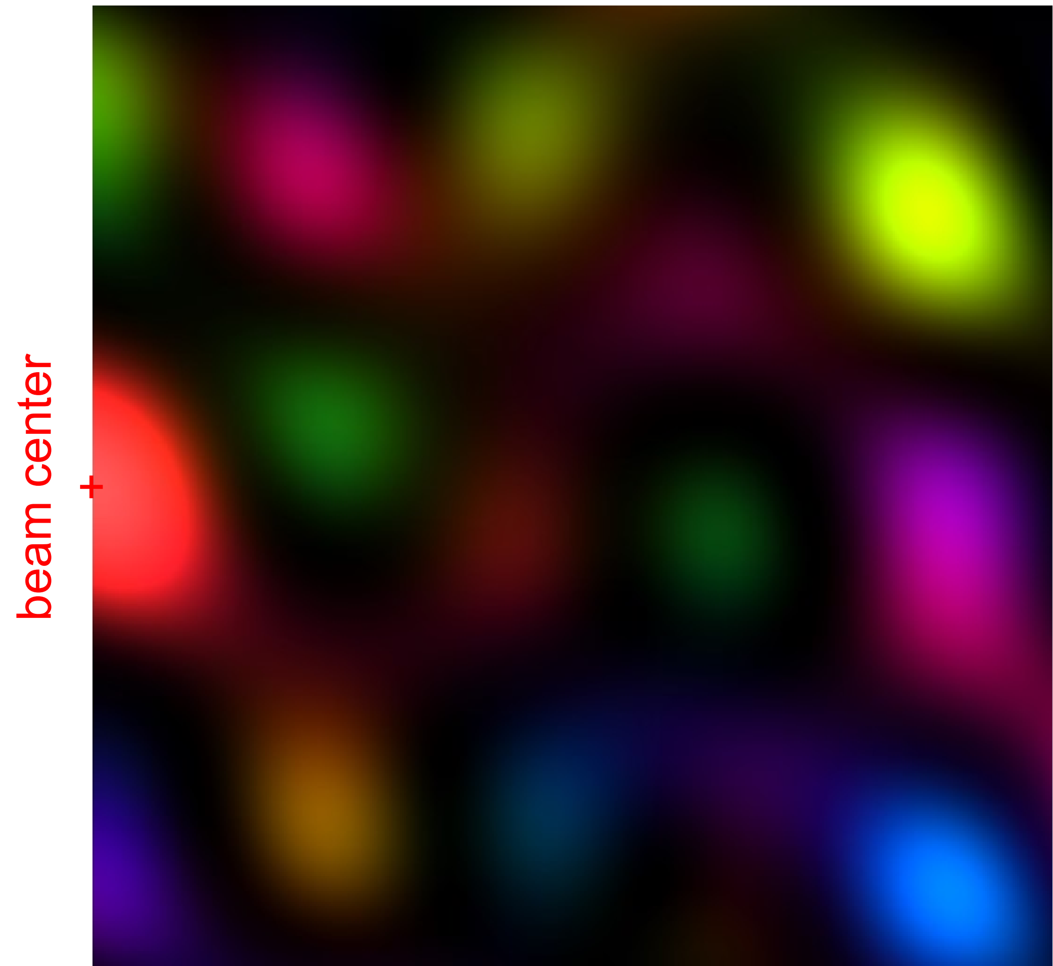
scattering from a crystal structure

colored by phase

sample



detector

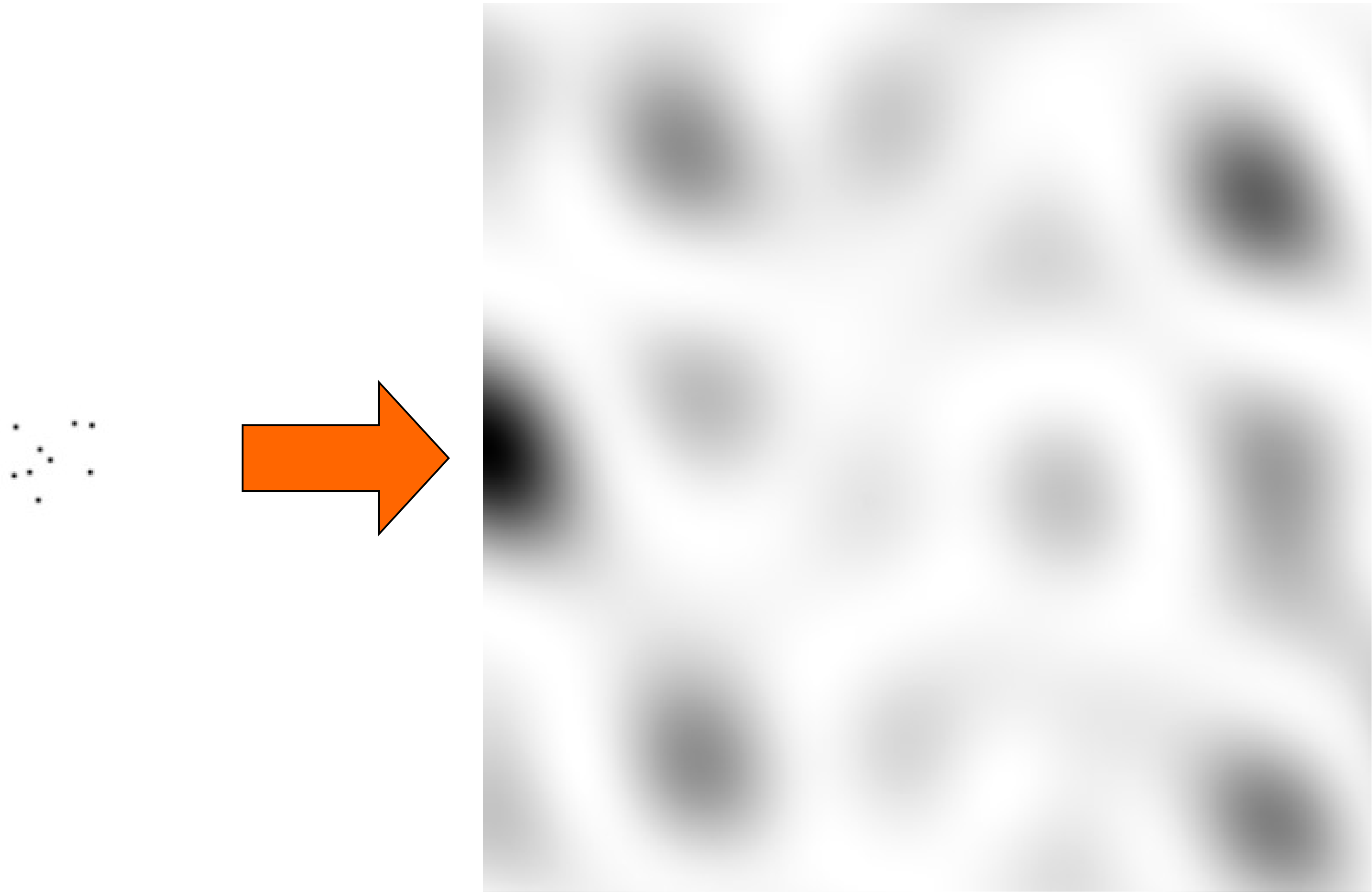


Major Phasing techniques

- Molecular Replacement
- Multiple Isomorphous Replacement
- Multiwavelength Anomalous Diffraction
- Single-wavelength Anomalous Diffraction

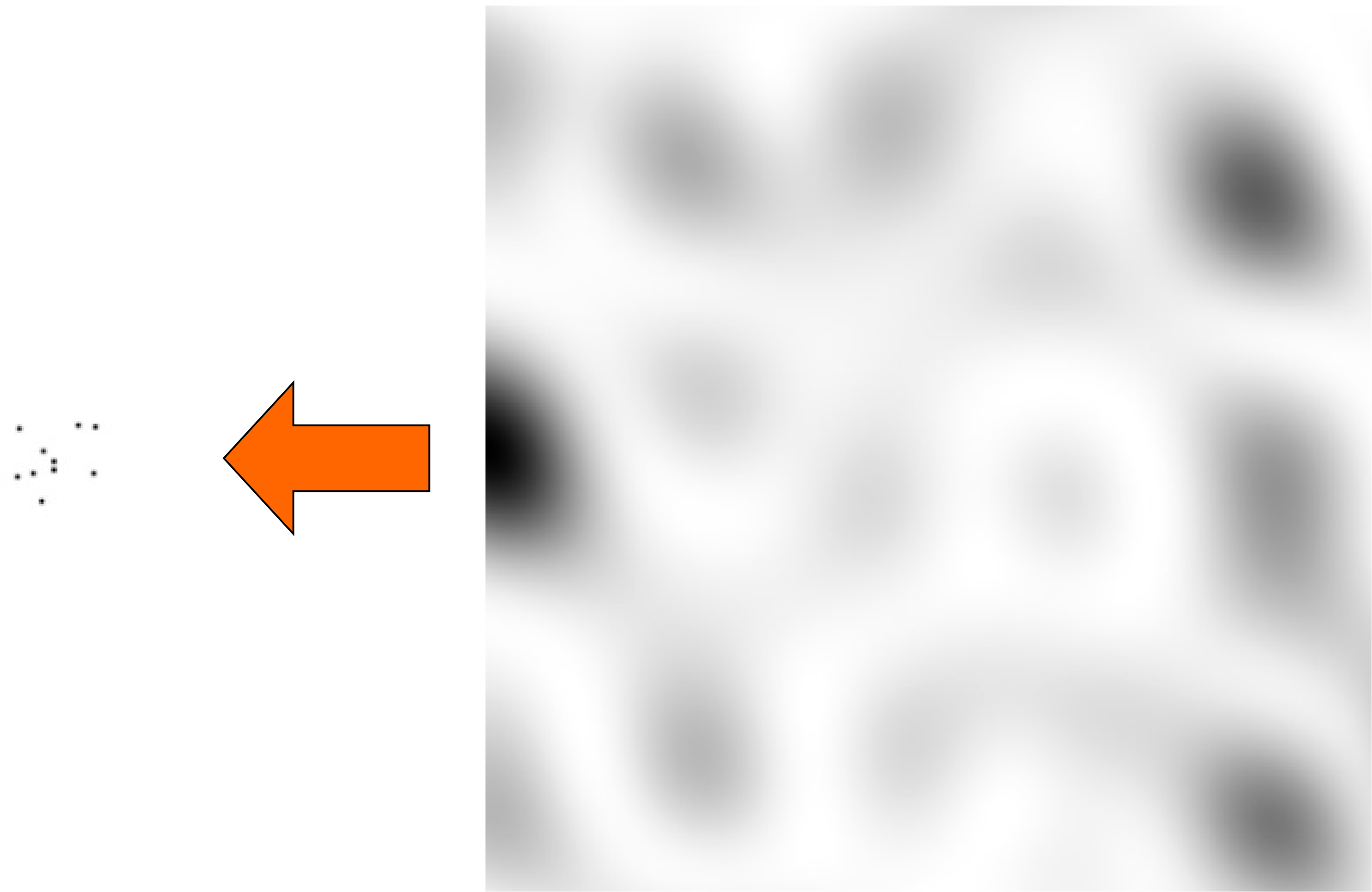
inverse Fourier Transform

no phase



inverse Fourier Transform

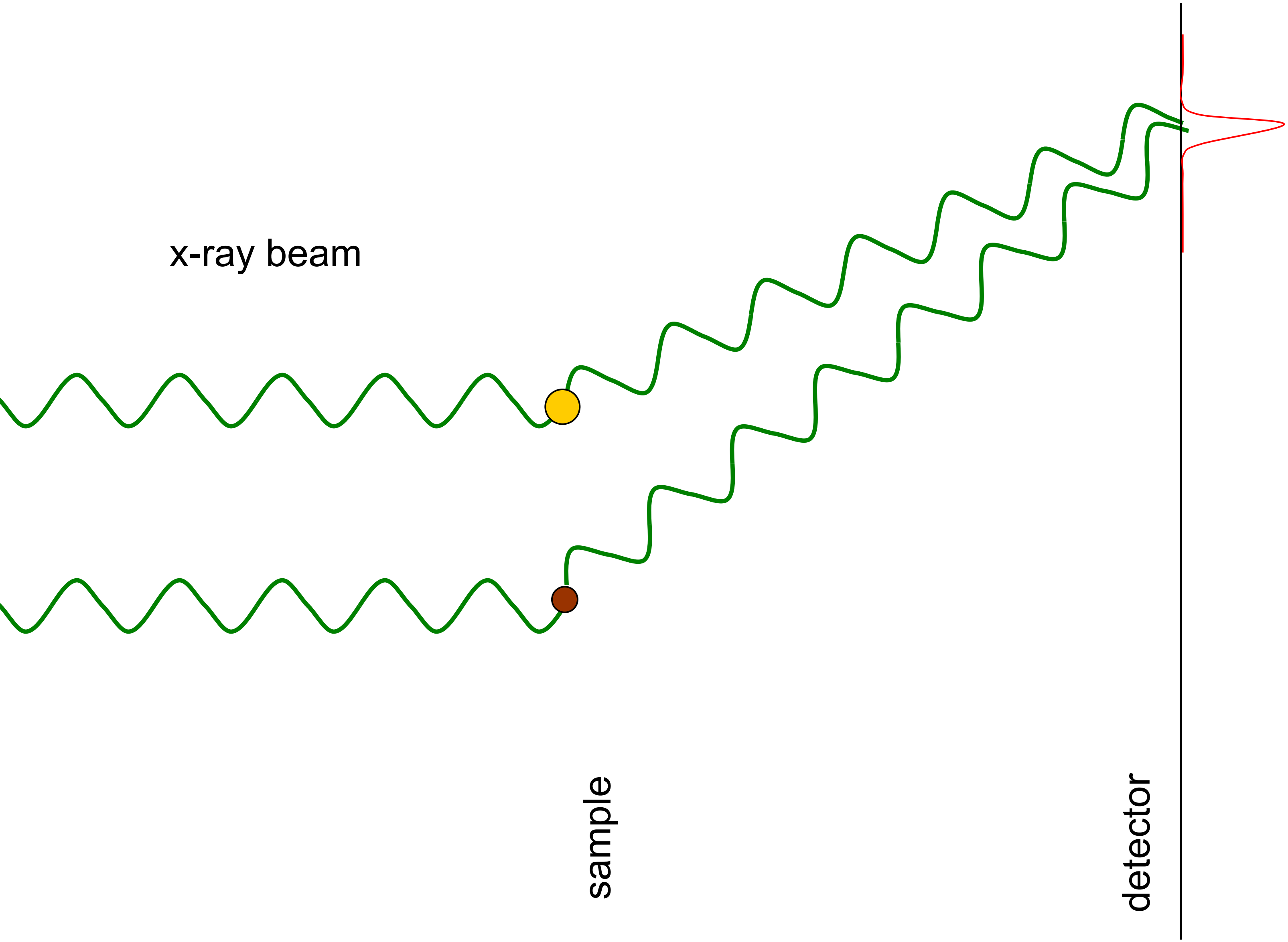
no phase



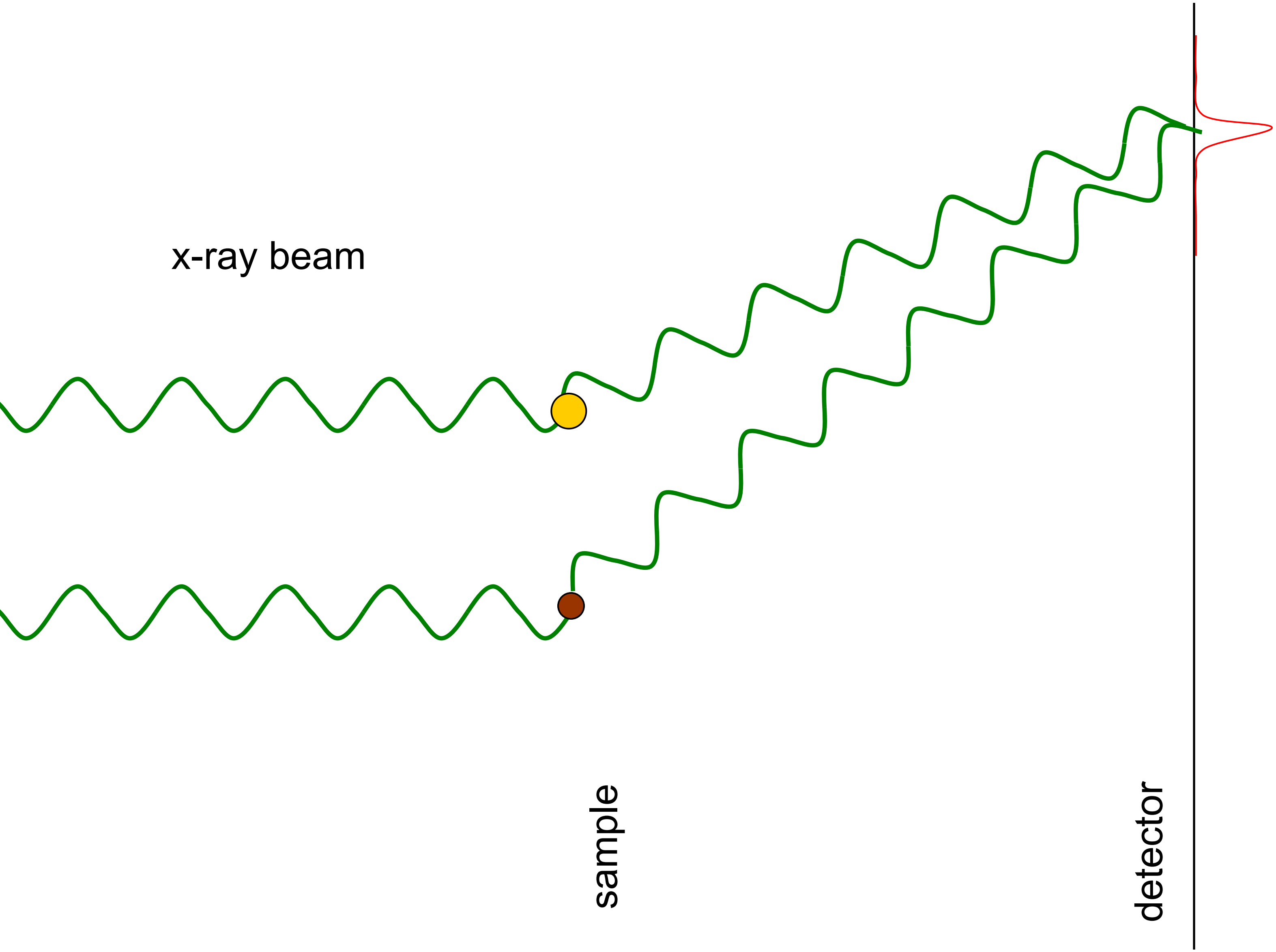
Major Phasing techniques

- Molecular Replacement
- Multiple Isomorphous Replacement
- Multiwavelength Anomalous Diffraction
- Single-wavelength Anomalous Diffraction

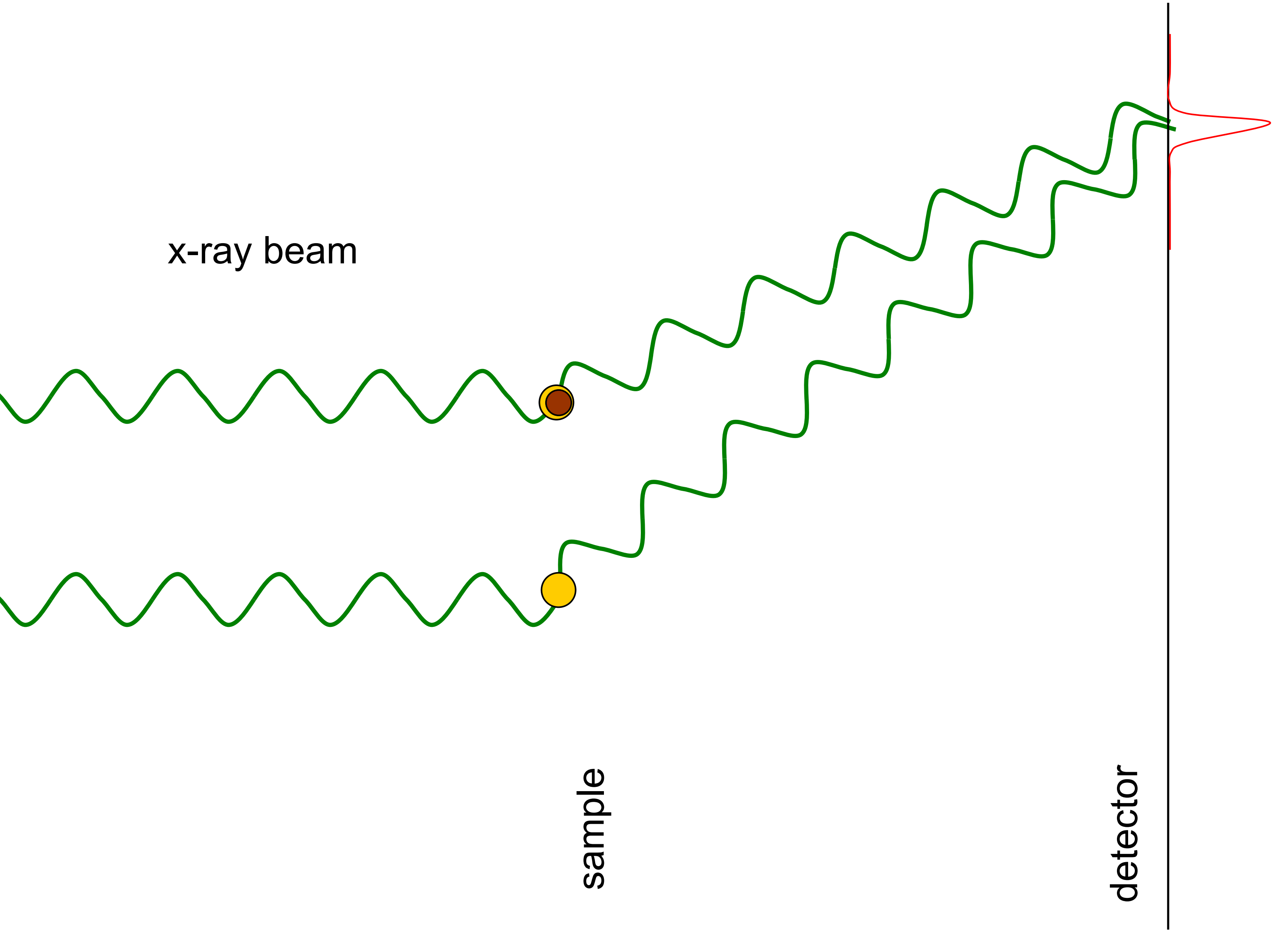
anomalous scattering



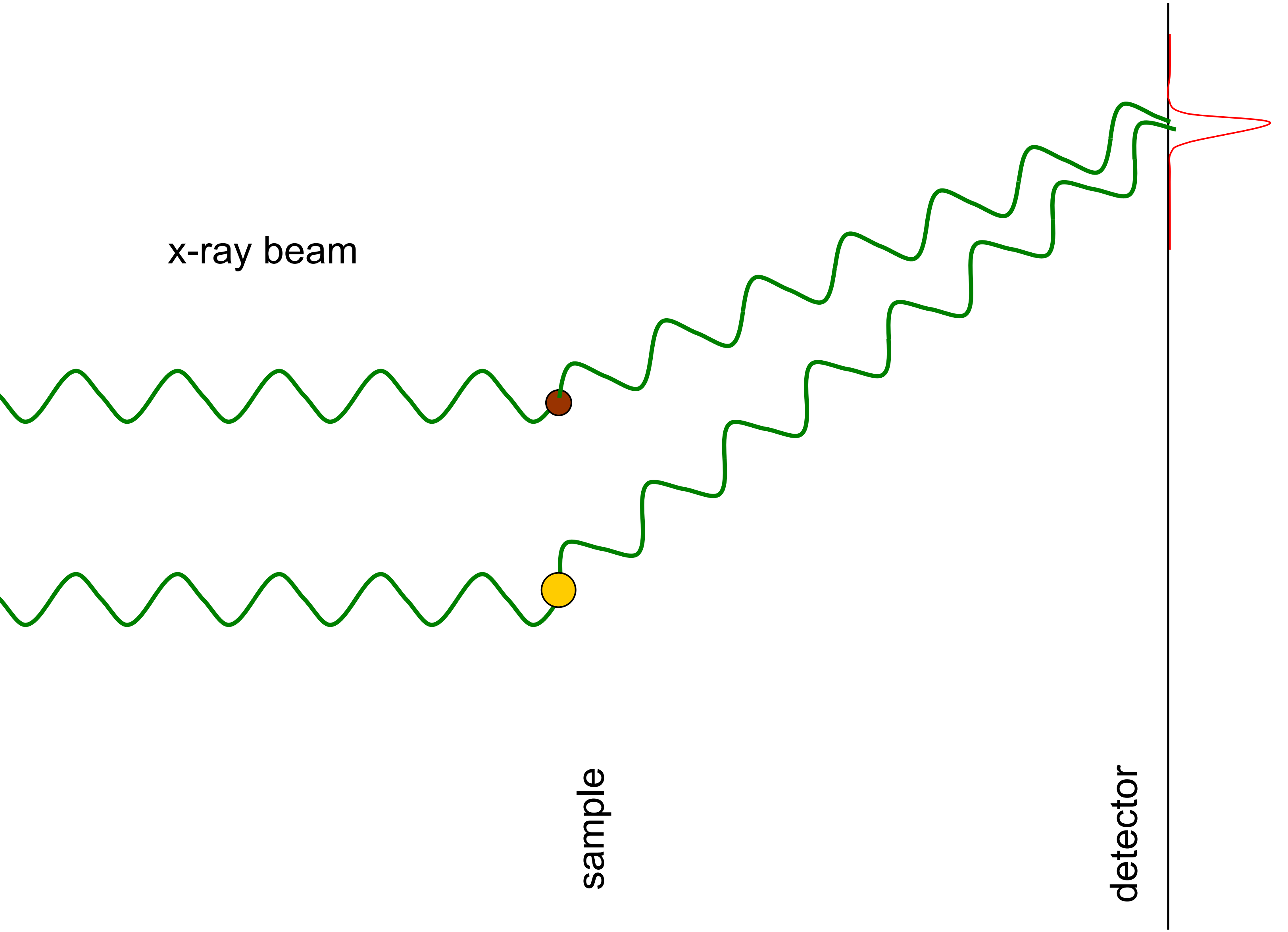
anomalous scattering



anomalous scattering



anomalous scattering



anomalous scattering