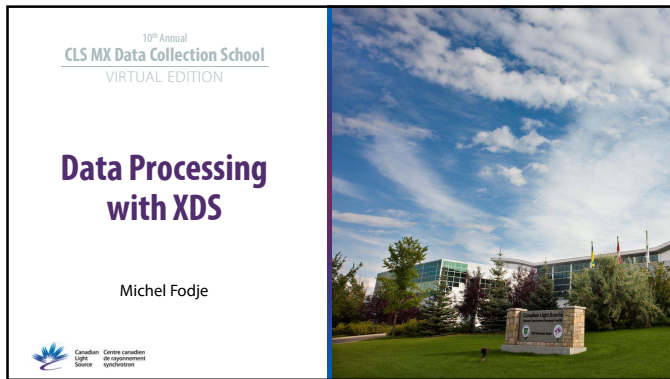




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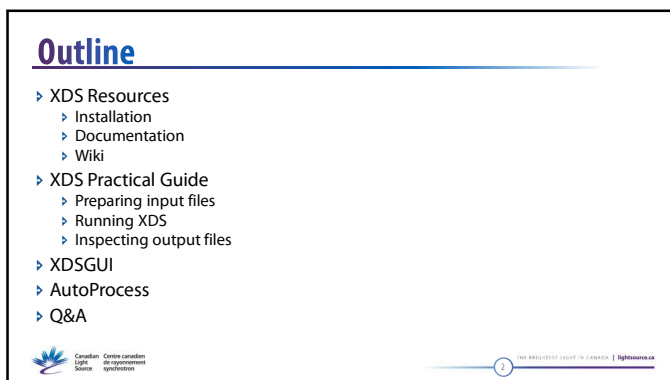
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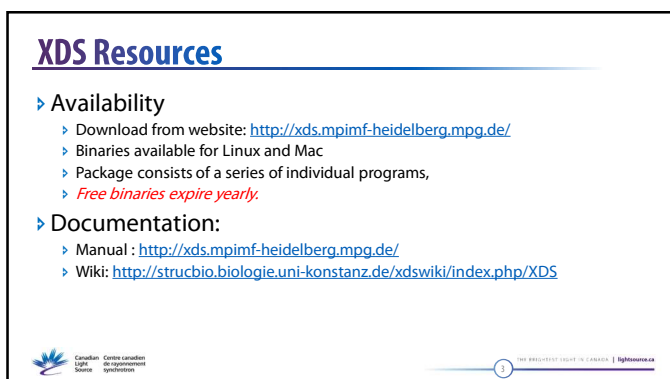
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## XDS Installation

### Linux

```
cd /MyApps
wget ftp://ftp.mpimf-heidelberg.mpg.de/pub/kabsch/XDS-INTEL64_Linux_x86_64.tar.gz
tar xzvf XDS-INTEL64_Linux_x86_64.tar.gz
cd XDS-INTEL64_Linux_x86_64
wget https://strucbio.biologie.uni-konstanz.de/pub/Linux_bin/generate_XDS.INP
chmod a+x generate_XDS.INP
```



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## Third-Party Software

### GUIs

- ▶ XDSgui – <http://strucbio.biologie.uni-konstanz.de/xdswiki/index.php/XDSGUI>
- ▶ XDSi – (P. Kursula J. Appl. Cryst. (2004). 37, 347)
- ▶ XDSapp – (M. Krug, BESSY J. Appl. Cryst. (2012). 45, 568)

### Automation Pipelines

- ▶ AutoProcess (CLS)
- ▶ Xia2 (CCP4)
- ▶ autoPROC (Global Phasing)
- ▶ autoxds (SSRL)
- ▶ XDSme (SOLEIL)

### Image Viewers

- ▶ xds-viewer (<http://xds-viewer.sourceforge.net/>)
- ▶ adxv (<http://www.scripps.edu/tainer/arval/adxv.html>)



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## Programs - XDS

- ▶ Inputs: Sequence of images collected using the rotation method
- ▶ Only assumptions:
  - ▶ Images are adjacent and non-overlapping
  - ▶ Each image covers the same positive rotation range
  - ▶ Incident beam and rotation axis intersect at crystal position
- ▶ Reads input parameters from a file XDS.INP
- ▶ Determines crystal orientation, symmetry
- ▶ Produces a list of corrected integrated intensities from the images
- ▶ XDS accomplishes its function in eight sub-tasks
  - ▶ XYCORR, INIT, COLSPOT, IDXREF, DEPIX, XPLAN, INTEGRATE, CORRECT
- ▶ Each task uses output files from previous tasks and creates new output files



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## XDS – Practical guide

- › Always use a dedicated directory for input and output files.
- › Prepare input file **XDS.INP**
  - › XDS.INP often written by beamline software
  - › Contains data collection and beamline parameters (~30 relevant parameters)
  - › Use *generate\_XDS.INP* script if no XDS.INP available from beamline
- › File format is simple and consist of **keyword=value** pairs.
  - › *Note: keywords includes the '=' without any space between*
  - › Not all parameters are mandatory
  - › Parameters have reasonable defaults were possible
- › Individual tasks can be repeated by modifying **JOB=** parameters
- › Output files will be overwritten, rename/copy them elsewhere to keep



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## Steps/Commands

- › Create a folder for output (for example "xds-proc")
 

```
mkdir xds-proc && cd xds-proc
```
- › Create XDS.INP and update it according to the experiment
 

```
generate_XDS.INP /full/path/to/dataset_?????.img
```
- › Run XDS
 

```
xds_par
```

  - › *Inspect output \*.LP \*.cbf files*
  - › *edit XDS.INP and repeat steps as required.*
- › Generate XSCALE.INP
- › Run XSCALE
 

```
xscale_par
```
- › Generate XDSCONV.INP
- › Run XDSCONV
 

```
xdsconv
```



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## Input file examples – XDS.INP

```
!-XDS.INP-----File generated by auto_process
JOB=ALLIYCONV INPT COLSPOT IDREF DEPIX XPLAN INTEGRATE CORRECT
MAXIMUM_NUMBER_OF_PROCESSORS=32
MAXIMUM_NUMBER_OF_JOBS=4

!-----Dataset parameters-----
X-RAY_WAVELENGTH=1.23984
DETECTOR_DISTANCE=120.0
STARTING_ANGLE=165.0
STARTING_FRAME= 1
OSCILLATION_RANGE=0.80
SPACE_GROUP_NUMBER=1
UNIT_CELL_CONSTANTS= 0 0 0 0 0
NAME_TEMPLATE_OF_DATA_FRAMES=/full/path/to/dataset_?????.img
DATA_RANGE=1 450
BACKGROUND_RANGE=1 10
SPOT_RANGE=1 90
SPOT_RANGE=180 270
FRIEDEL'S_LAW=TRUE

!-----Beamline parameters-----
W=4006 NY=4006
QX=0.87324 QY=0.87324
ORGX=2000 ORGY=2046

DETECTOR=CCDCHES
MINIMUM_VALID_PIXEL_VALUE= 1
STRONG_PIXEL= 5
OVERLOAD=65535
TRUSTED_RESOLUTION=0.00 1.414
TEST_RESOLUTION_RANGE= 75.0 0.0
TOTAL_SPINDLE_ROTATION_RANGES= 10 180 10
STARTING_ANGLES_OF_SPINDLE_ROTATION= 0 180 5
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 6000 30000
INCLUDE_RESOLUTION_RANGE=50.0 0.0
ROTATION_AXIS= 1.0 0.0 0.0
INCIDENT_BEAM_DIRECTION=0.0 0.0 1.0
FRACTION_OF_POLARIZATION=0.95
POLARIZATION_PLANE_NORMAL= 0.0 1.0 0.0
DIRECTION_OF_DETECTOR_X-AXIS= 1.000 0.000 0.000
DIRECTION_OF_DETECTOR_Y-AXIS= 0.000 1.000 0.000
```



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## Checking

- › Always inspect the self-documented \*.LP files from each step.
  - › IDXREF.LP should indicate that there is a clear indexing solution for the lattice
  - › INTEGRATE.LP should show well defined 3D spot profiles.
  - › Completeness, outliers, systematic absences if present, I/sigma, R-factors and other statistics are reported within CORRECT.LP
- › \*.cbf files can be inspected with *xds-viewer*, *adxv*, or *imgview* (at CLS)
  - › FRAME.cbf shows an overlay of the predicted profile on last image integrated. Spots should be clearly within the circles.
  - › BKGPIX.cbf should show that beam-stop is masked properly
- › CORRECT.LP
  - › Shutter Statistics
  - › R-factors, CC<sub>1/2</sub>, I/sigma, ISa should be more than 20



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## XDS tasks

| Task    | Description                                                                                                                                                    | Input files                                                                              | Output files                                                     |
|---------|----------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|------------------------------------------------------------------|
| XYCORR  | Calculates lookup tables for spatial corrections at each pixel position required to correct for geometrical distortions of the detector image                  | XDS.INP                                                                                  | XYCORR.LP<br>X-CORRECTIONS.cbf<br>Y-CORRECTIONS.cbf<br>FRAME.cbf |
| INIT    | Determines lookup tables required for classifying a pixel as background or part of a reflection                                                                | XDS.INP<br>X-CORRECTIONS.cbf<br>Y-CORRECTIONS.cbf                                        | INIT.LP<br>BKGINT.cbf<br>BLANK.cbf<br>GAIN.cbf                   |
| COLSPOT | Locates strong diffraction spots in subset of data and saves their centroids. Too many strong ice rings will introduce false spots and the next task may fail. | XDS.INP<br>X-CORRECTIONS.cbf<br>Y-CORRECTIONS.cbf<br>BKGINT.cbf<br>BLANK.cbf<br>GAIN.cbf | COLSPOT.LP<br>SPOT.XDS                                           |



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## XDS tasks

| Task   | Description                                                                                                     | Input files         | Output files                      |
|--------|-----------------------------------------------------------------------------------------------------------------|---------------------|-----------------------------------|
| IDXREF | Finds the orientation, metric and symmetry of crystal lattice. Assigns indices to diffraction spots in SPOT.XDS | XDS.INP<br>SPOT.XDS | IDXREF.LP<br>SPOT.XDS<br>XPRM.XDS |

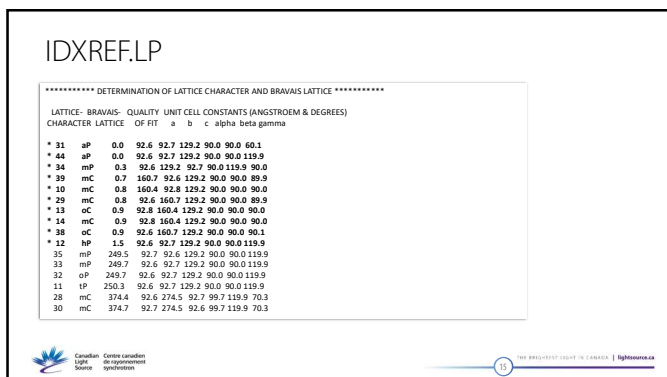
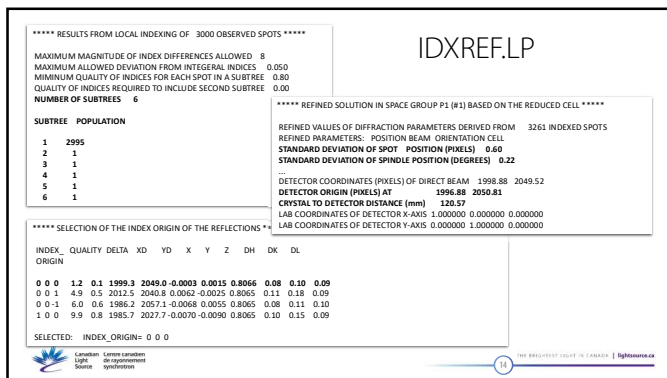
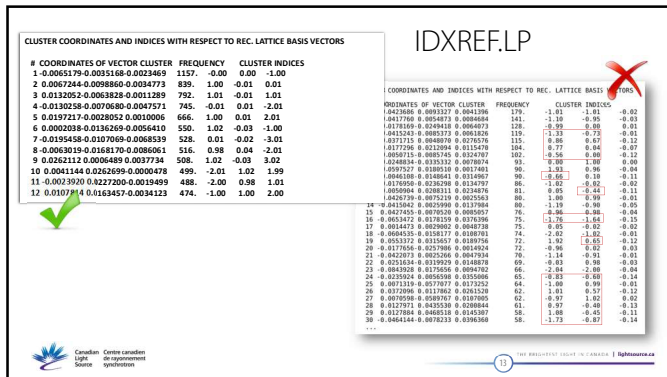
- › **Very important task!**
- › Output SPOT.XDS will contain indices next to each reflection
- › Un-indexed reflections will contain 0, 0, 0 as indices
- › Potential problems
  - › Difference-vector clusters deviate significantly from integral values (due to too many alien spots or wrong input parameters)
  - › Wrong index origin, (due to wrong beam center)
  - › Not enough reflections indexed (due to alien spots or satellites)
- › Troubleshooting:
  - › Try changing SPOT\_RANGE=, REFINE(IDXREF)=
  - › Check ORGX=, ORGY=, or Rerun IDXREF with different index origins suggested in IDXREF.LP
  - › Repeat COLSPOT task with different peak search parameters
  - › Specify Space group and Cell parameters



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## XDS tasks

| Task         | Description                                                                                                                                                            | Input files                                                                                                                                   | Output files                                                             |
|--------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|
| <b>DEFPX</b> | Finds and masks untrusted regions in the background file <code>BKGINT.cbf</code> as well as regions outside the included resolution range                              | <code>XDS.INP</code><br><code>X-CORRECTIONS.cbf</code><br><code>Y-CORRECTIONS.cbf</code><br><code>BKGINT.cbf</code><br><code>XPARM.XDS</code> | <code>DEFPX.LP</code><br><code>BKGPIX.cbf</code><br><code>ABS.cbf</code> |
| <b>XPLAN</b> | Estimates the completeness for each starting angle, total rotation and resolution based on refined crystal orientation and symmetry. Used for planning data collection | <code>XDS.INP</code><br><code>XPARM.XDS</code><br><code>BKGPIX.cbf</code><br><code>X-CORRECTIONS.cbf</code><br><code>Y-CORRECTIONS.cbf</code> | <code>XPLAN.LP</code>                                                    |



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## XDS tasks

| Task             | Description                                                                                                                                                                                                                                                                         | Input files                                                                                                                                                                                       | Output files                                                                      |
|------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|
| <b>INTEGRATE</b> | Uses diffraction parameters in <code>XPARM.XDS</code> to predict reflection positions in all images. Determines the intensity of each reflection in the images and saves them to <code>INTEGRATE.HKL</code> . Periodically refines diffraction parameters using strong reflections. | <code>XDS.INP</code><br><code>X-CORRECTIONS.cbf</code><br><code>Y-CORRECTIONS.cbf</code><br><code>BLANK.cbf</code><br><code>BKGPIX.cbf</code><br><code>GAIN.LCBF</code><br><code>XPARM.XDS</code> | <code>INTEGRATE.LP</code><br><code>INTEGRATE.HKL</code><br><code>FRAME.cbf</code> |

### ► Potential problems

- Off-centered profiles
  - Incorrectly predicted spots
  - Mis-indexing
- Crystal slippage, or change in incident beam direction
- Reflections extending to edge of profile
  - Incorrect input parameters for beam divergence and reflecting range
- Many unintegrated reflections
  - Incorrect diffraction parameters in `XPARM.XDS`



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```

IMAGE IER SCALE  NBKG NOVU NEWHALD NSTRONG NREJ  SIGMAB SIGMAR
1 0 1.006 16234201 0 15352 3111 4 0.06024 0.0976
2 0 1.000 16233310 0 15332 3128 4 0.06056 0.09939
3 0 1.004 16239611 0 15383 3124 3 0.06053 0.09965
4 0 1.001 16242211 0 15390 3096 2 0.06043 0.09898
5 0 1.004 16229677 0 15470 3153 2 0.06063 0.09798
6 0 1.001 16217104 0 15412 3186 4 0.06119 0.09858
7 0 1.005 16235773 0 15348 3089 3 0.06118 0.09888
8 0 1.011 16246209 0 15422 3041 1 0.06125 0.09896
9 0 1.011 16235276 0 15436 3090 0 0.06161 0.09925
10 0 1.000 16238660 0 15371 3088 1 0.06197 0.09829
11 0 0.996 16250094 0 15410 2964 2 0.06250 0.09874
12 0 0.996 16240255 0 15413 3006 3 0.06310 0.09750
13 0 1.008 16230900 0 15408 3030 0 0.06406 0.09630
14 0 0.999 16251593 0 15368 2950 1 0.06266 0.09837
15 0 0.990 16223799 0 15374 3067 2 0.06430 0.09684
16 0 0.993 16230604 0 15485 3051 5 0.06337 0.09710
17 0 0.993 16238069 0 15384 2995 4 0.06343 0.09765
18 0 1.009 16231665 0 15409 3005 0 0.06523 0.09614
19 0 0.988 16243754 0 15359 2982 0 0.06407 0.09862
20 0 0.981 16222628 0 15509 3036 2 0.06511 0.09679
21 0 0.971 16223825 0 15389 3047 1 0.06517 0.09676
    
```

INTEGRATE.LP

```

71146 OUT OF 71416 REFLECTIONS ACCEPTED FOR REFINEMENT
REFINED PARAMETERS: POSITION BEAM ORIENTATION CELL
STANDARD DEVIATION OF SPOT POSITION (PIXELS) 0.90
STANDARD DEVIATION OF SPINDLE POSITION (DEGREES) 0.12
SPACE GROUP NUMBER 178
UNIT CELL PARAMETERS 92.748 92.748 129.223 90.000 90.000 120.000
REC. CELL PARAMETERS 0.012450 0.012450 0.007739 90.000 90.000 60.000
COORDINATES OF UNIT CELL A-AXIS -47.530 -45.288 -65.514
COORDINATES OF UNIT CELL B-AXIS -38.013 82.456 -18.926
COORDINATES OF UNIT CELL C-AXIS 108.572 58.801 38.120
CRYSTAL ROTATION OFF FROM INITIAL ORIENTATION -0.008 -0.008 0.006
(Shown as x,y,z components of rotation axis X angle (degrees))
CRYSTAL MOSAICITY (DEGREES) 0.098
LAB COORDINATES OF ROTATION AXIS 0.999999 -0.001413 -0.003997
DIRECT BEAM COORDINATES (REC. ANGSTROMS) 0.001277 0.000166 0.800555
DETECTOR COORDINATES (PIXELS) OF DIRECT BEAM 1998.89 2049.59
DETECTOR ORIGIN (PIXELS) AT 1996.28 2049.26
CRYSTAL TO DETECTOR DISTANCE (mm) 120.45
LAB COORDINATES OF DETECTOR X-AXIS 1.000000 0.000000 0.000000
LAB COORDINATES OF DETECTOR Y-AXIS 0.000000 1.000000 0.000000
    
```



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\*\*\*\*\* ANSWARE THREE DIMENSIONAL PROBLEMS OF INTEGRATION SOLUTIONS \*\*\*\*\*

\*\*\*\*\* Q.1 \*\*\*\*\*

Find the volume of the solid bounded by the planes  $x = 0$ ,  $y = 0$ ,  $z = 0$  and  $x + y + z = 1$ .

**Solution:**

The solid is a tetrahedron with vertices at  $(0, 0, 0)$ ,  $(1, 0, 0)$ ,  $(0, 1, 0)$  and  $(0, 0, 1)$ . The volume is given by:

$$V = \int_0^1 \int_0^{1-x} \int_0^{1-x-y} dz dy dx$$

$$= \int_0^1 \int_0^{1-x} (1-x-y) dy dx$$

$$= \int_0^1 \left[ (1-x)y - \frac{y^2}{2} \right]_0^{1-x} dx$$

$$= \int_0^1 \left( (1-x)(1-x) - \frac{(1-x)^2}{2} \right) dx$$

$$= \int_0^1 \left( (1-x)^2 - \frac{(1-x)^2}{2} \right) dx$$

$$= \int_0^1 \frac{(1-x)^2}{2} dx$$

$$= \frac{1}{2} \int_0^1 (1-x)^2 dx$$

$$= \frac{1}{2} \left[ -\frac{(1-x)^3}{3} \right]_0^1$$

$$= \frac{1}{2} \left( 0 - \left( -\frac{1}{3} \right) \right)$$

$$= \frac{1}{2} \cdot \frac{1}{3}$$

$$= \frac{1}{6}$$

The volume of the solid is  $\frac{1}{6}$  cubic units.

\*\*\*\*\* Q.2 \*\*\*\*\*

Find the volume of the solid bounded by the planes  $x = 0$ ,  $y = 0$ ,  $z = 0$  and  $x + y + z = 2$ .

**Solution:**

The solid is a tetrahedron with vertices at  $(0, 0, 0)$ ,  $(2, 0, 0)$ ,  $(0, 2, 0)$  and  $(0, 0, 2)$ . The volume is given by:

$$V = \int_0^2 \int_0^{2-x} \int_0^{2-x-y} dz dy dx$$

$$= \int_0^2 \int_0^{2-x} (2-x-y) dy dx$$

$$= \int_0^2 \left[ (2-x)y - \frac{y^2}{2} \right]_0^{2-x} dx$$

$$= \int_0^2 \left( (2-x)(2-x) - \frac{(2-x)^2}{2} \right) dx$$

$$= \int_0^2 \left( (2-x)^2 - \frac{(2-x)^2}{2} \right) dx$$

$$= \int_0^2 \frac{(2-x)^2}{2} dx$$

$$= \frac{1}{2} \int_0^2 (2-x)^2 dx$$

$$= \frac{1}{2} \left[ -\frac{(2-x)^3}{3} \right]_0^2$$

$$= \frac{1}{2} \left( 0 - \left( -\frac{8}{3} \right) \right)$$

$$= \frac{1}{2} \cdot \frac{8}{3}$$

$$= \frac{4}{3}$$

The volume of the solid is  $\frac{4}{3}$  cubic units.

# INTEGRATE.LP

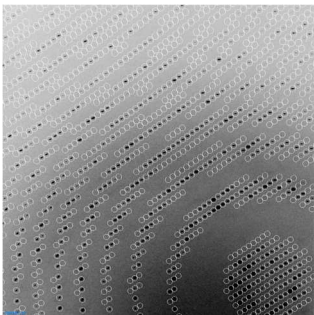
|    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|
| 0  | 0  | 0  | 0  | -1 | 0  | 0  |
| 0  | 33 | 0  | 3  | 2  | 0  | 2  |
| 0  | 29 | 29 | 18 | 46 | 2  | 0  |
| 0  | 33 | 11 | 12 | 27 | 23 | 12 |
| 53 | 58 | 39 | 38 | 88 | 25 | 12 |
| 19 | 34 | 32 | 63 | 48 | 48 | 36 |
| 0  | -2 | 3  | 15 | 27 | 37 | 31 |
| 0  | 28 | 35 | 17 | -6 | 4  | 0  |
| 0  | 0  | 0  | 32 | 31 | 15 | 0  |

|   |    |    |    |    |    |    |
|---|----|----|----|----|----|----|
| 0 | 0  | 0  | 0  | 0  | 0  | 0  |
| 0 | 0  | 0  | 0  | 0  | 0  | 0  |
| 0 | 0  | 0  | 0  | 0  | 0  | 0  |
| 0 | 0  | 0  | 0  | 0  | 0  | 0  |
| 0 | 0  | 0  | 0  | 0  | 0  | 0  |
| 0 | 5  | 0  | 2  | 12 | 4  | 0  |
| 0 | -4 | 3  | 15 | 37 | 49 | 57 |
| 0 | 19 | 13 | 15 | 45 | 13 | -9 |
| 0 | 0  | 8  | 43 | 26 | 0  | 0  |

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[illegible]

FRAME.cbf

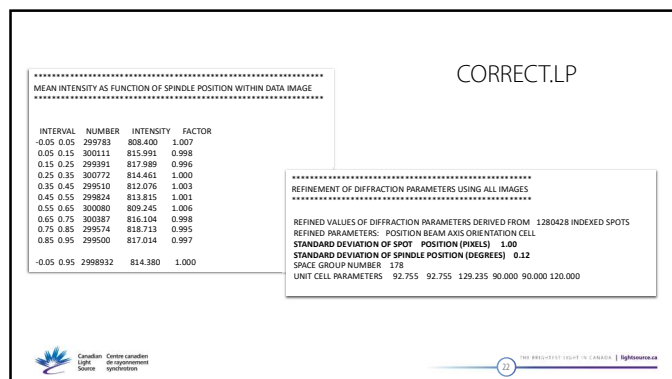
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[illegible]

| XDS tasks      |                                                                                                                                                                                                                                                                                                  |                                                                                  |                                                                                                                                                                             |
|----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Task           | Description                                                                                                                                                                                                                                                                                      | Input files                                                                      | Output files                                                                                                                                                                |
| <b>CORRECT</b> | Applies correction factors to intensities and standard deviations determined from INTEGRATE. Determines space group (without screw-axis). If unknown and refines cell parameters. Saves corrected intensities in XDS_ASCII.HKL. Calculates a Wilson plot and cumulative intensity distributions. | XDS.INP<br>INTEGRATE.HKL<br>REMOVE.HKL<br>X-CORRECTIONS.cbf<br>Y-CORRECTIONS.cbf | CORRECT.LP<br>XDS_ASCII.HKL<br>GXPARM.XDS<br>GX-CORRECTIONS.cbf<br>DY-CORRECTIONS.cbf<br>GX-CORRECTIONS.cbf<br>GY-CORRECTIONS.cbf<br>ABSORP.cbf<br>DECIAY.cbf<br>MODPIX.cbf |

[illegible]




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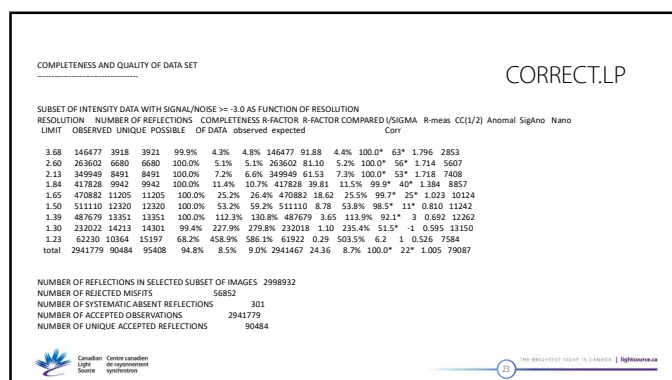
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## Programs – XSCALE & XDSCONV

### ▸ XSCALE

- Input: list of corrected integrated intensities from XDS
- Corrects data for absorption effects, detector variations, radiation damage
- Places data sets on a common scale
- Optionally merges into unique reflection sets
- Calculates statistics for evaluating quality of the data
- Input parameters specified in [XSCALE.INP](#)

### ▸ XDSCONV

- Input: list of reflection intensities from XSCALE or XDS
- Converts reflection data into formats required by other structure determination software: CNS, CCP4, SHELX, ..
- Input parameters specified in [XDSCONV.INP](#)




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## Input file examples

### XSCALE.INP

```
RESOLUTION_SHELLS= 10 6 5 4 3 2.9 2.8
SPACE_GROUP_NUMBER=179
UNIT_CELL_CONSTANTS= 85.71 85.71 145.34 90 90 120

OUTPUT_FILE=D22-rh.ahk1 FRIEDEL'S_LAM=FALSE
STRICT_ABSORPTION_CORRECTION=TRUE
INPUT_FILE= ../xds_rh_2008/XDS_ASCII.HKL XDS_ASCII 50 2.8

OUTPUT_FILE=D22-ip.ahk1
FRIEDEL'S_LAM=FALSE
STRICT_ABSORPTION_CORRECTION=TRUE
INPUT_FILE= ../xds_ip_2008/XDS_ASCII.HKL XDS_ASCII 50 2.8
```

### XDSCONV.INP

```
INPUT_FILE=D22-rh.ahk1
OUTPUT_FILE=D22-rh.hkl SHELX
FRIEDEL'S_LAM=FALSE
```



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## Optimization and Further processing

- › Sometimes, it may help to repeat the last three steps

- › Set "JOB= DEPIX INTEGRATE CORRECT"

- › Copy GXPARM to XPARM
- › Copy the suggested parameters from INTEGRATELP
- › Repeat integration in correct space group

- › Other programs

- › XDSSTAT – calculates extra statistics
- › Rd – for diagnosing radiation damage
- › R-factors and per frame
- › POINTLESS(CCP4)
- › automatic space-group determination
- › Identifies screw axes
- › conversion to MTZ

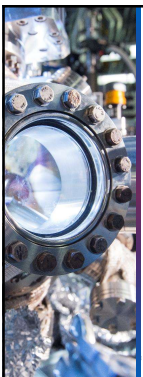
```
***** SUGGESTED VALUES FOR INPUT PARAMETERS *****
BEAM_DIVERGENCE= 0.54954 BEAM_DIVERGENCE_E.S.D.= 0.05495
REFLECTING_RANGE= 0.83218 REFLECTING_RANGE_E.S.D.= 0.11888
```



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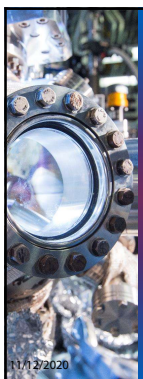


## XDS GUI Demo

Graphical User Interface for XDS

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## AutoProcess

Automated Processing using XDS

11/12/2020

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## What is AutoProcess

- ▶ A software program written in Python, with a series of command line utilities for automated processing:
  - ▶ **auto.process** – full data processing pipeline
  - ▶ **auto.symmetry** – space group determination and refinement
  - ▶ **auto.strategy** – data-collection strategy determination
  - ▶ **auto.scale** – scaling

python

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## Features

- ▶ Determines input parameters and experiment geometry from image header
- ▶ Automates all the steps for data reduction from images to reflection files for various data reduction schemes
  - ▶ Single Native or Anomalous datasets
  - ▶ MAD datasets
  - ▶ multi-pass data on a single crystal
  - ▶ multi-crystal data sets
- ▶ Determines optimal strategy for data collection from a few screening frames
- ▶ Scoring for comparing crystals during screening.

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## Features

- ▶ Graphical HTML output with plots and tables
- ▶ Input and output files are preserved, for manual optimization if needed.
- ▶ Optimization of workload on cluster for very fast parallel processing.
- ▶ MxDC and MxLIVE Integration
- ▶ Automatic resolution of some pathologies that affect indexing
  - ▶ Multiple Lattices or split crystals
  - ▶ Spots too weak, or too many strong spots
- ▶ Optimization using refined spot-profile parameters and orientation matrix.
- ▶ Makes sure multiple datasets are processed in the same setting
- ▶ Optimization of anomalous signal



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## AutoProcess Demo



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