*International Tables for Crystallography* (2006). Vol. G, Section 5.6.4, pp. 552–554.



```
int cbf_get_detector_normal (cbf_detector detector,
     double *normal1, double *normal2,
     double *normal3);
int cbf_get_pixel_coordinates (cbf_detector detector,
     double index1, double index2,
     double *coordinate1, double *coordinate2,
     double *coordinate3);
int cbf_get_pixel_normal (cbf_detector detector,
     double index1, double index2,
     double *normal1, double *normal2,
     double *normal3);
int cbf_get_pixel_area (cbf_detector detector,
     double index1, double index2,
     double *area, double *projected_area);
```

`cbf_construct_detector` uses data from the categories DIFFRN, DIFFRN_DETECTOR, DIFFRN_DETECTOR_ELEMENT, DIFFRN_DETECTOR_AXIS, AXIS, ARRAY_STRUCTURE_LIST and ARRAY_STRUCTURE_LIST_AXIS to construct a geometric representation of detector element *element_number* and initializes the `cbf_detector` handle, *detector*. `cbf_free_detector` frees the detector structure; `cbf_get_beam_center` calculates the location at which the beam intersects the detector surface, either in terms of the pixel indices (*index1, index2*) along the slow and fast detector axes, respectively, or the displacement in millimetres along the slow and fast axes (*center1, center2*); `cbf_get_detector_distance` and `cbf_get_detector_normal` calculate the distance of the sample from the plane of the detector surface and the normal vector of the detector at pixel $(0, 0)$, respectively; `cbf_get_pixel_coordinates`, `cbf_get_pixel_normal` and `cbf_get_pixel_area` calculate the coordinates, normal vector, and area and apparent area as viewed from the sample position of the pixel with the given indices, respectively.

## 5.6.3. Compression schemes

Two schemes for lossless compression of integer arrays (such as images) have been implemented in this version of *CBFlib*:

(i) an entropy-encoding scheme using canonical coding;

(ii) a *CCP4*-style packing scheme.

Both encode the difference (or error) between the current element in the array and the prior element. Parameters required for more sophisticated predictors have been included in the compression functions and will be used in a future version of the library.

### 5.6.3.1. Canonical-code compression

The canonical-code compression scheme encodes errors in two ways: directly or indirectly. Errors are coded directly using a symbol corresponding to the error value. Errors are coded indirectly using a symbol for the number of bits in the (signed) error, followed by the error itself.

At the start of the compression, *CBFlib* constructs a table containing a set of symbols, one for each of the $2^n$ direct codes from $-2^{n-1}$ to $2^{n-1}-1$, one for a stop code and one for each of the $maxbits - n$ indirect codes, where $n$ is chosen at compression time and *maxbits* is the maximum number of bits in an error. *CBFlib* then assigns to each symbol a bit code, using a shorter bit code for the more common symbols and a longer bit code for the less common symbols. The bit-code lengths are calculated using a Huffman-type algorithm and the actual bit codes are constructed using the canonical-code algorithm described by Moffat *et al.* (1997).

Table 5.6.3.1. *Structure of compressed data using the canonical-code scheme*

| Byte | Value |
|---|---|
| 1 to 8 | Number of elements (64-bit little-endian number) |
| 9 to 16 | Minimum element |
| 17 to 24 | Maximum element |
| 25 to 32 | (Reserved for future use) |
| 33 | Number of bits directly coded, $n$ |
| 34 | Maximum number of bits encoded, *maxbits* |
| $35$ to $35 + 2^n - 1$ | Number of bits in each direct code |
| $35 + 2^n$ | Number of bits in the stop code |
| $35 + 2^n + 1$ to $35 + 2^n + maxbits - n$ | Number of bits in each indirect code |
| $35 + 2^n + maxbits - n + 1 \ldots$ | Coded data |

Table 5.6.3.2. *Structure of compressed data using the CCP4-style scheme*

| Value in bits 3 to 5 | Number of bits in each error |
|---|---|
| 0 | 0 |
| 1 | 4 |
| 2 | 5 |
| 3 | 6 |
| 4 | 7 |
| 5 | 8 |
| 6 | 16 |
| 7 | 65 |

| Byte | Value |
|---|---|
| 1 to 8 | Number of elements (64-bit little-endian number) |
| 9 to 16 | Minimum element (currently unused) |
| 17 to 24 | Maximum element (currently unused) |
| 25 to 32 | (Reserved for future use) |
| 33 . . . | Coded data |

The structure of the compressed data is described in Table 5.6.3.1.

### 5.6.3.2. *CCP4*-style compression

The *CCP4*-style compression writes the errors in blocks. Each block begins with a 6-bit code. The number of errors in the block is $2^n$, where $n$ is the value in bits 0 to 2. Bits 3 to 5 encode the number of bits in each error. The data structure is summarized in Table 5.6.3.2.

## 5.6.4. Sample templates

The construction of CBF/imgCIF files can be simplified using templates. A template is itself an imgCIF file populated with data entries but without any binary sections. This file is normally associated with a CBF handle using the `cbf_read_template` call and provides a framework into which images and other experiment-specific data may be entered.

Fig. 5.6.4.1 is a sample template for an ADSC Quantum 4 detector (ADSC, 1997) with a $\kappa$-geometry diffractometer at Stanford Synchrotron Radiation Laboratory (SSRL) beamline 1-5.

The template for a MAR345 image plate detector (MAR Research, 1997) is almost identical. The major differences are in the size of the array (2300 × 2300 *versus* 2304 × 2304), the parameters for the CCD elements and the geometry of the elements. Therefore a few of the values in the AXIS, ARRAY_STRUCTURE_LIST, ARRAY_STRUCTURE_LIST_AXIS and ARRAY_INTENSITIES categories are different, as listed in Fig. 5.6.4.2.

```
###CBF: VERSION 1.1

data_image_1

# category DIFFRN
loop_
_diffrn.id
_diffrn.crystal_id
 DIFFRN_ID DIFFRN_CRYSTAL_ID

# category DIFFRN_SOURCE
loop_
_diffrn_source.diffrn_id
_diffrn_source.source
_diffrn_source.current
_diffrn_source.type
 DIFFRN_ID synchrotron 100.0 'SSRL beamline 1-5'

# category DIFFRN_DETECTOR_ELEMENT
loop_
_diffrn_detector_element.id
_diffrn_detector_element.detector_id
 ELEMENT1 ADSCQ4

# category DIFFRN_RADIATION
loop_
_diffrn_radiation.diffrn_id
_diffrn_radiation.wavelength_id
_diffrn_radiation.probe
_diffrn_radiation.monochromator
_diffrn_radiation.polarizn_source_ratio
_diffrn_radiation.polarizn_source_norm
_diffrn_radiation.div_x_source
_diffrn_radiation.div_y_source
_diffrn_radiation.div_x_y_source
_diffrn_radiation.collimation
 DIFFRN_ID WAVELENGTH1 x-ray 'Si 111' 0.8 0.0 0.08
    0.01 0.00 '0.20 mm x 0.20 mm'

# category DIFFRN_RADIATION_WAVELENGTH
loop_
_diffrn_radiation_wavelength.id
_diffrn_radiation_wavelength.wavelength
_diffrn_radiation_wavelength.wt
 WAVELENGTH1 0.98 1.0

# category DIFFRN_DETECTOR
loop_
_diffrn_detector.diffrn_id
_diffrn_detector.id
_diffrn_detector.type
_diffrn_detector.details
_diffrn_detector.number_of_axes
 DIFFRN_ID ADSCQ4 'ADSC QUANTUM4' 'slow mode' 4

 # category DIFFRN_DETECTOR_AXIS
loop_
_diffrn_detector_axis.detector_id
_diffrn_detector_axis.axis_id
 ADSCQ4 DETECTOR_X
 ADSCQ4 DETECTOR_Y
 ADSCQ4 DETECTOR_Z
 ADSCQ4 DETECTOR_PITCH

# category DIFFRN_DATA_FRAME
loop_
_diffrn_data_frame.id
_diffrn_data_frame.detector_element_id
_diffrn_data_frame.array_id
_diffrn_data_frame.binary_id
 FRAME1 ELEMENT1 ARRAY1 1
```

Fig. 5.6.4.1. Template imgCIF for use with an ADSC Quantum 4 detector.

```
# category DIFFRN_MEASUREMENT
loop_
_diffrn_measurement.diffrn_id
_diffrn_measurement.id
_diffrn_measurement.number_of_axes
_diffrn_measurement.method
_diffrn_measurement.details
 DIFFRN_ID GONIOMETER 3 rotation
; i0=1.000 i1=1.000 i2=1.000 ib=1.000 beamstop=20 mm
  0% attenuation
;


# category DIFFRN_MEASUREMENT_AXIS
loop_
_diffrn_measurement_axis.measurement_id
_diffrn_measurement_axis.axis_id
 GONIOMETER GONIOMETER_PHI
 GONIOMETER GONIOMETER_KAPPA
 GONIOMETER GONIOMETER_OMEGA


# category DIFFRN_SCAN
loop_
_diffrn_scan.id
_diffrn_scan.frame_id_start
_diffrn_scan.frame_id_end
_diffrn_scan.frames
 SCAN1 FRAME1 FRAME1 1


# category DIFFRN_SCAN_AXIS
loop_
_diffrn_scan_axis.scan_id
_diffrn_scan_axis.axis_id
_diffrn_scan_axis.angle_start
_diffrn_scan_axis.angle_range
_diffrn_scan_axis.angle_increment
_diffrn_scan_axis.displacement_start
_diffrn_scan_axis.displacement_range
_diffrn_scan_axis.displacement_increment
 SCAN1 GONIOMETER_OMEGA 0.0 0.0 0.0 0.0 0.0 0.0
 SCAN1 GONIOMETER_KAPPA 0.0 0.0 0.0 0.0 0.0 0.0
 SCAN1 GONIOMETER_PHI   0.0 0.0 0.0 0.0 0.0 0.0
 SCAN1 DETECTOR_Z       0.0 0.0 0.0 0.0 0.0 0.0
 SCAN1 DETECTOR_Y       0.0 0.0 0.0 0.0 0.0 0.0
 SCAN1 DETECTOR_X       0.0 0.0 0.0 0.0 0.0 0.0
 SCAN1 DETECTOR_PITCH   0.0 0.0 0.0 0.0 0.0 0.0

# category DIFFRN_SCAN_FRAME
loop_
_diffrn_scan_frame.frame_id
_diffrn_scan_frame.frame_number
_diffrn_scan_frame.integration_time
_diffrn_scan_frame.scan_id
_diffrn_scan_frame.date
 FRAME1 1 0.0 SCAN1 1997-12-04T10:23:48

# category DIFFRN_SCAN_FRAME_AXIS
loop_
_diffrn_scan_frame_axis.frame_id
_diffrn_scan_frame_axis.axis_id
_diffrn_scan_frame_axis.angle
_diffrn_scan_frame_axis.displacement
 FRAME1 GONIOMETER_OMEGA 0.0 0.0
 FRAME1 GONIOMETER_KAPPA 0.0 0.0
 FRAME1 GONIOMETER_PHI   0.0 0.0
 FRAME1 DETECTOR_Z       0.0 0.0
 FRAME1 DETECTOR_Y       0.0 0.0
 FRAME1 DETECTOR_X       0.0 0.0
 FRAME1 DETECTOR_PITCH   0.0 0.0
```

Fig. 5.6.4.1. (*cont.*)

```
# category AXIS
loop_
_axis.id
_axis.type
_axis.equipment
_axis.depends_on
_axis.vector[1] _axis.vector[2] _axis.vector[3]
_axis.offset[1] _axis.offset[2] _axis.offset[3]
 GONIOMETER_OMEGA rotation    goniometer
   . 1 0 0 . . .
 GONIOMETER_KAPPA rotation    goniometer
   GONIOMETER_OMEGA 0.64279 0 0.76604 . . .
 GONIOMETER_PHI   rotation    goniometer
   GONIOMETER_KAPPA 1 0 0 . . .
 SOURCE           general     source   . 0 0 1 . . .
 GRAVITY          general     gravity  . 0 -1 0 . . .
 DETECTOR_Z       translation detector
   . 0 0 -1 0 0 0
 DETECTOR_Y       translation detector
   DETECTOR_Z 0 1 0 0 0 0
 DETECTOR_X       translation detector
   DETECTOR_Y 1 0 0 0 0 0
 DETECTOR_PITCH   rotation    detector
   DETECTOR_X 0 1 0 0 0 0
 ELEMENT_X        translation detector
   DETECTOR_PITCH 1 0 0 -94.0032 94.0032 0
 ELEMENT_Y        translation detector
   ELEMENT_X 0 1 0 0 0 0

# category ARRAY_STRUCTURE_LIST
loop_
_array_structure_list.array_id
_array_structure_list.index
_array_structure_list.dimension
_array_structure_list.precedence
_array_structure_list.direction
_array_structure_list.axis_set_id
 ARRAY1 1 2304 1 increasing ELEMENT_X
 ARRAY1 2 2304 2 increasing ELEMENT_Y

# category ARRAY_STRUCTURE_LIST_AXIS
loop_
_array_structure_list_axis.axis_set_id
_array_structure_list_axis.axis_id
_array_structure_list_axis.displacement
_array_structure_list_axis.displacement_increment
 ELEMENT_X ELEMENT_X 0.0408 0.0816
 ELEMENT_Y ELEMENT_Y -0.0408 -0.0816

# category ARRAY_INTENSITIES
loop_
_array_intensities.array_id
_array_intensities.binary_id
_array_intensities.linearity
_array_intensities.gain
_array_intensities.gain_esd
_array_intensities.overload
_array_intensities.undefined_value
 ARRAY1 1 linear 0.23 0.03 65000 0


 # category ARRAY_STRUCTURE
loop_
_array_structure.id
_array_structure.encoding_type
_array_structure.compression_type
_array_structure.byte_order
 ARRAY1 "signed 32-bit integer" packed little_endian
```

Fig. 5.6.4.1. (*cont.*)

```
# category ARRAY_DATA
loop_
_array_data.array_id
_array_data.binary_id
_array_data.data
 ARRAY1 1 ?
```

Fig. 5.6.4.1. (*cont.*)

```
loop_
_axis.id
_axis.type
_axis.equipment
_axis.depends_on
_axis.vector[1] _axis.vector[2] _axis.vector[3]
_axis.offset[1] _axis.offset[2] _axis.offset[3]
 GONIOMETER_OMEGA rotation    goniometer
   . 1 0 0 . . .
 GONIOMETER_KAPPA rotation    goniometer
   GONIOMETER_OMEGA 0.64279 0 0.76604 . . .
 GONIOMETER_PHI   rotation    goniometer
   GONIOMETER_KAPPA 1 0 0 . . .
 SOURCE           general     source
   . 0 0 1 . . .
 GRAVITY          general     gravity
   . 0 -1 0 . . .
 DETECTOR_Z       translation detector
   . 0 0 -1 0 0 0
 DETECTOR_Y       translation detector
   DETECTOR_Z 0 1 0 0 0 0
 DETECTOR_X       translation detector
   DETECTOR_Y 1 0 0 0 0 0
 DETECTOR_PITCH   rotation    detector
   DETECTOR_X 0 1 0 0 0 0
 ELEMENT_X        translation detector
   DETECTOR_PITCH 1 0 0 -172.5 172.5 0
 ELEMENT_Y        translation detector
   ELEMENT_X 0 1 0 0 0 0

loop_
_array_structure_list.array_id
_array_structure_list.index
_array_structure_list.precedence
_array_structure_list.direction
_array_structure_list.axis_set_id
 ARRAY1 1 2300 1 increasing ELEMENT_X
 ARRAY1 2 2300 2 increasing ELEMENT_Y

 loop_
_array_structure_list_axis.axis_set_id
_array_structure_list_axis.axis_id
_array_structure_list_axis.displacement
_array_structure_list_axis.displacement_increment
 ELEMENT_X ELEMENT_X 0.075 0.150
 ELEMENT_Y ELEMENT_Y -0.075 -0.150

 loop_
_array_intensities.array_id
_array_intensities.binary_id
_array_intensities.linearity
_array_intensities.gain
_array_intensities.gain_esd
_array_intensities.overload
_array_intensities.undefined_value
 ARRAY1 1 linear 1.15 0.2 240000 0
```

Fig. 5.6.4.2. Part of the template file for a MAR345 detector. Values that differ from those in Fig. 5.6.4.1 are underlined.



references