ESO SCIENCE DATA PRODUCTS STANDARD

Doc. No. GEN-SPE-ESO-33000-5335, Issue 5

Addendum

Date: 15/07/2015

Integral Field Spectroscopy: 3D Data Cubes

The data format being defined in this section applies to reduced integral field spectroscopy data, in particular to observations using the VLT instruments ERIS, KMOS, MUSE, SINFONI and XSHOOTER in IFU mode.[1]

Herein it is assumed that the data reduction process includes the following steps, though not necessarily in the given sequence: astrometric calibration, calibration of the dispersion axis to physical wavelength scale, removal/correction for instrumental and sky background signal (if applicable), calibration of the detected signal to physical scale (spectral flux density), re-sampling to a regular 3-dimensional grid, signal combination of multiple exposures (if applicable), error propagation in each processing step to obtain a final error estimate for the science data, and propagation of pixel quality information.

The spectral flux density – in physical units as declared in the `BUNIT` keyword – is stored as 3-dimensional FITS image (called "science data cube" hereafter) with the first two array dimensions `NAXIS1/2` representing the projected celestial coordinates and the third dimension `NAXIS3` the spectral coordinate.

Taking into account that science data cubes normally employ the 32- or 64-bit floating-point data format signified by `BITPIX = -32` or `-64`, the use of the `BSCALE` and `BZERO` keywords is not recommended. [2]

Celestial and spectral coordinates are encoded following the FITS WCS conventions [1] and [2], respectively.

The data cube should be stored in a FITS image extension, i.e. the primary HDU shall not contain any data.

The science data cube may be optionally associated with pixel-by-pixel error (ERR) and data quality (DQ) information. Science data and their associated error and DQ information shall be stored in different Header Data Units (HDU) of the same FITS file using the scheme of referencing keywords according to [3].

If the DQ extension is missing the bad pixel status should be encoded as *NaN* values in the data and the error extensions.

Storing several sets of HDU's with associated science data, error and data quality in a single FITS file, though permitted in [3], is not supported by the ESO/SDP standard. Only three HDU's are permitted of which one must be the science data and

[1] Aiming at the production of 3D data cubes in compliance with the format defined herein, the ESO pipeline data reduction software will be updated accordingly, starting off with MUSE and KMOS.
[2] Expressing the pixel values in units which are not physical (e.g. adu, counts, or similar) with the addition of a zeropoint or scale factor to scale the cube to physical units is explicitly not allowed.

the other two are optional, one being ERR and the other DQ, other kind of extensions, except for PROVXTN, are currently not supported.[3]

Reference Documents

1. Representations of celestial coordinates in FITS (Paper II), Calabretta, M. R., and Greisen, E. W., Astronomy & Astrophysics, 395, 1077-1122, 2002.
2. Representations of spectral coordinates in FITS (Paper III), Greisen, E. W., Calabretta, M. R., Valdes, F. G., and Allen, S. L., Astronomy & Astrophysics, 446, 747-771, 2006.
3. FITS format description for pipeline products with data, error and data quality information, Kuemmel, Ballester & Kuntschner, VLT-SPE-ESO-19500-5667, Issue 1.0, 11 July 2012.

Data Types

The science data cube represents the main data type for integral field spectroscopy products. Error and data quality information may be included within the same FITS file. Other types of ancillary data may be optionally associated as separate files.

Data Type `PRODCATG`	**Description**
`SCIENCE.CUBE.IFS`	3-dimensional FITS image with two spatial and one spectral axis. Separate FITS extensions of the same file shall be used to store the science data cube and optional supporting information (error, data quality). The primary HDU should not contain any data (`NAXIS=0`). FITS header keywords according to **Table 1** must be present.

Structure of associated error and data quality information

The main requirements for the encoding of error and data quality information are listed below, more details can be found in [3].

1. SCI, ERR and DQ information shall be stored in different HDUs of the same FITS file.
2. The ERR and DQ units are optional.
3. Each HDU with data must be identified via EXTNAME.
4. The dimensions and WCS of the ERR and DQ units shall be identical to the SCI unit.
5. The primary unit of the FITS file shall not contain data.
6. The order of the extensions (SCI, ERR, DQ) is recommended though any other choice is possible.

[3] The requirement of one unique science data HDU applies to the main science file but not to the associated ancillary files, which may contain multiple data extensions, referring for example to individual instrument arms, dispersion orders, or exposures.

7. The header shall contain a reference to the keyword convention (e.g. ESO DICD version HDU* keywords) and to the HDU type (HDUCLAS* keywords).
8. The headers shall have specific keywords pointing to the complementary information. The values of the SCIDATA, ERRDATA, QUALDATA keywords shall contain the EXTNAME. EXTVER should not be used for unique identification of HDU's.
9. There are 4 different error types: MSE (mean squared), RMSE (root mean square), INVMSE (inverse mean squared), INVRMSE (inverse root mean square).
10. There are 4 different data quality types: MASKZERO, MASKONE, FLAG32BIT (Euro3D-like), FLAG16BIT.

Data Type `ASSOCi`	**Description**
`ANCILLARY.IMAGE`	Broad-band image, also known as "white-light" image (mandatory). 2D image obtained by averaging the data cube along the wavelength axis between WAVELMIN and WAVELMAX. Pixels having data quality issues should be excluded from the average. FITS image with the same dimension and WCS as the science data cube's spatial axes (NAXIS1 and NAXIS2).
`ANCILLARY.CUBE.IFS.STD`	3D data cube of a standard star (optional). FITS data cube with the same dimension as the science data cube.

Data Reprocessing

Intermediate pipeline products may be provided to allow regenerating the final science data cube using customized processing parameters for the respective data reduction recipes. Starting data reprocessing from intermediate products is more convenient than repeating the entire processing chain from the beginning, i.e. by starting from the raw data.

Data Type `ASSOCi`	**Description**
`ANCILLARY. MUSE.PIXTABLE_REDUCED`	Intermediate product compatible with the MUSE data reduction pipeline. `PRO.CATG = PIXTABLE_REDUCED`
`ANCILLARY.KMOS.SCI_RECONSTRUCTED`	Intermediate product compatible with the KMOS data reduction pipeline.

	PRO.CATG = SCI_RECONSTRUCTED

Table 1: Sample FITS header of the 3D data cube based on MUSE

```
SIMPLE  =                    T / file does conform to FITS standard
BITPIX  =                    8 / number of bits per data pixel
NAXIS   =                    0 / number of data axes
EXTEND  =                    T / FITS dataset may contain extensions
DATE    = '2015-05-20T10:20:35' / file creation date (YYYY-MM-DDThh:mm:ss UT)
ORIGIN  = 'ESO-PARANAL'         / European Southern Observatory
TELESCOP= 'ESO-VLT-U4'          / ESO Telescope
INSTRUME= 'MUSE     '           / ESO Instrument name
RA      =            183.46028 / [deg] Image centre (J2000.0)
DEC     =              7.20120 / [deg] Image centre (J2000.0)
EQUINOX =                2000. / Standard FK5
RADECSYS= 'FK5     '            / Coordinate system
EXPTIME =               2520.0 / Total integration time per pixel
TEXPTIME=               2520.0 / Total integration time all exposures
NCOMBINE=                    3 / # of combined raw science data files
MJD-OBS =       57126.04953770 / 2015-04-14T01:11:20.1
MJD-END =       57126.08556889 / 2015-04-14T02:03:13.2
DATE-OBS= '2015-04-14T01:11:20.057' / Observing date
OBJECT  = 'NGC 4191'            / Target designation
OBID1   =              1164690 / Observation block ID
PROG_ID = '095.B-0686(A)'       / ESO programme identification code
PROV1   = 'MUSE.2015-04-14T01:11:20.057.fits' / Original science file
PROV2   = 'MUSE.2015-04-14T01:27:10.371.fits' / Original science file
PROV3   = 'MUSE.2015-04-14T01:49:13.152.fits' / Original science file
OBSTECH = 'IFU     '            / Technique of observation
PRODCATG= 'SCIENCE.CUBE.IFS'    / Data product category
ASSON1  = 'IMAGE_FOV_0001.fits' / Collapsed data cube
ASSOC1  = 'ANCILLARY.IMAGE'     / Category of associated file
WAVELMIN=                475.0 / [nm] Minimum wavelength
WAVELMAX=                843.0 / [nm] Maximum wavelength
SPEC_RES=                 2500 / Spectral resolving power at central wavelength
SKY_RES =                 0.94 / [arcsec] FWHM effective spatial resolution (mea
SKY_RERR=                 0.10 / [arcsec] Error of SKY_RES (estimated)
ABMAGLIM=                 22.5 / 5-sigma magnitude limit for point sources
PIXNOISE=             4.50E-20 / [erg/s/cm**2/Angstrom] pixel-to-pixel noise
FLUXCAL = 'ABSOLUTE'            / Certifies the validity of BUNIT
PROCSOFT= 'muse/1.0.4'          / Data reduction software/version no.
REFERENC= '        '            / Bibliographic reference
```

```
CHECKSUM= 'RGhHRGhGRGhGRGhG'   / HDU checksum updated 2015-07-15T16:27:36
DATASUM = '         0'         / data unit checksum updated 2015-05-20T10:20:48
END
```

Extension 1

```
XTENSION= 'IMAGE   '           / IMAGE extension
BITPIX  =                  -32 / number of bits per data pixel
NAXIS   =                    3 / number of data axes
NAXIS1  =                  329 / length of data axis 1
NAXIS2  =                  317 / length of data axis 2
NAXIS3  =                 3681 / length of data axis 3
NAXIS1  =                  329 / length of data axis 1
NAXIS2  =                  317 / length of data axis 2
NAXIS3  =                 3681 / length of data axis 3
PCOUNT  =                    0 / required keyword; must = 0
GCOUNT  =                    1 / required keyword; must = 1
EXTNAME = 'DATA    '           / This extension contains data values
HDUCLASS= 'ESO     '           / class name (ESO format)
HDUDOC  = 'DICD    '           / document with class description
HDUVERS = 'DICD version 6'     / version number (according to spec v2.5.1)
HDUCLAS1= 'IMAGE   '           / Image data format
HDUCLAS2= 'DATA    '           / this extension contains the data itself
ERRDATA = 'STAT    '           / pointer to the variance extension
OBJECT  = 'NGC 4191 (DATA)'
BUNIT   = '10**(-20)*erg/s/cm**2/Angstrom'
CRPIX1  =     170.061496799859 / Pixel coordinate of reference point
CRPIX2  =     152.429853570976 / Pixel coordinate of reference point
CD1_1   = -5.55555555555556E-05 / Coordinate transformation matrix element
CD1_2   =                   0. / Coordinate transformation matrix element
CD2_1   =                   0. / Coordinate transformation matrix element
CD2_2   = 5.55555555555556E-05 / Coordinate transformation matrix element
CUNIT1  = 'deg     '           / Units of coordinate increment and value
CUNIT2  = 'deg     '           / Units of coordinate increment and value
CTYPE1  = 'RA---TAN'           / Right ascension, gnomonic projection
CTYPE2  = 'DEC--TAN'           / Declination, gnomonic projection
CSYER1  =    1.66499066997E-05 / [deg] Systematic error in coordinate
CSYER2  =    6.60827614552E-06 / [deg] Systematic error in coordinate
CRVAL1  =               183.46
CRVAL2  =              7.20083
CTYPE3  = 'AWAV    '
CUNIT3  = 'Angstrom'
CD3_3   =                 1.25
CRPIX3  =                   1.
CRVAL3  =        4749.81640625
```

```
CD1_3   =                   0.
CD2_3   =                   0.
CD3_1   =                   0.
CD3_2   =                   0.
CRDER3  =                0.026 / [Angstrom] Random error in spectral coordinate
CHECKSUM= 'ZUJFZS9DZSGDZS9D'   / HDU checksum updated 2015-07-15T16:27:36
DATASUM = '39318882'           / data unit checksum updated 2015-05-20T10:20:54
END
```

Extension 2

```
XTENSION= 'IMAGE   '           / IMAGE extension
BITPIX  =                  -32 / number of bits per data pixel
NAXIS   =                    3 / number of data axes
NAXIS1  =                  329 / length of data axis 1
NAXIS2  =                  317 / length of data axis 2
NAXIS3  =                 3681 / length of data axis 3
NAXIS1  =                  329 / length of data axis 1
NAXIS2  =                  317 / length of data axis 2
NAXIS3  =                 3681 / length of data axis 3
PCOUNT  =                    0 / required keyword; must = 0
GCOUNT  =                    1 / required keyword; must = 1
EXTNAME = 'STAT    '           / This extension contains data variance
HDUCLASS= 'ESO     '           / class name (ESO format)
HDUDOC  = 'DICD    '           / document with class description
HDUVERS = 'DICD version 6'     / version number (according to spec v2.5.1)
HDUCLAS1= 'IMAGE   '           / Image data format
HDUCLAS2= 'ERROR   '           / this extension contains variance
HDUCLAS3= 'MSE     '           / the extension contains variances (sigma**2)
SCIDATA = 'DATA    '           / pointer to the data extension
OBJECT  = 'NGC 4191 (STAT)'
BUNIT   = '(10**(-20)*erg/s/cm**2/Angstrom)**2'
CRPIX1  =     170.061496799859 / Pixel coordinate of reference point
CRPIX2  =     152.429853570976 / Pixel coordinate of reference point
CD1_1   = -5.55555555555556E-05 / Coordinate transformation matrix element
CD1_2   =                   0. / Coordinate transformation matrix element
CD2_1   =                   0. / Coordinate transformation matrix element
CD2_2   = 5.55555555555556E-05 / Coordinate transformation matrix element
CUNIT1  = 'deg     '           / Units of coordinate increment and value
CUNIT2  = 'deg     '           / Units of coordinate increment and value
CTYPE1  = 'RA---TAN'           / Right ascension, gnomonic projection
CTYPE2  = 'DEC--TAN'           / Declination, gnomonic projection
CSYER1  =    1.66499066997E-05 / [deg] Systematic error in coordinate
CSYER2  =    6.60827614552E-06 / [deg] Systematic error in coordinate
CRVAL1  =               183.46
```

```
CRVAL2  =              7.20083
CTYPE3  = 'AWAV    '
CUNIT3  = 'Angstrom'
CD3_3   =                 1.25
CRPIX3  =                   1.
CRVAL3  =        4749.81640625
CD1_3   =                   0.
CD2_3   =                   0.
CD3_1   =                   0.
CD3_2   =                   0.
CHECKSUM= 'JfcaJeZYJeaaJeYW'   / HDU checksum updated 2015-05-20T10:20:55
DATASUM = '2131780454'         / data unit checksum updated 2015-05-20T10:20:55
END
```

FITS Keyword Definitions

Type	Keyword	Description
(S)	`INSTRUME`	Instrument name as defined in the original raw FITS file. The VLT instruments *GIRAFFE, KMOS, MUSE, SINFONI, VIMOS, and XSHOOTER* support IFU observations.
(R)	`WAVELMIN` `WAVELMAX`	Electromagnetic wave band coverage in terms of the wavelength interval in units of nanometers (nm). `WAVELMIN` and `WAVELMAX` correspond to the physical wavelength of the first and the last plane of the science data cube, respectively.
(S)	`BUNIT`	Physical unit of array values. *Example for the IFS data cube:* `BUNIT   = '10**(-20)*erg/s/cm**2/Angstrom'`

Type	Keyword	Description
(R)	ABMAGLIM	5-sigma limiting AB magnitude[4] in terms of the total flux of an unresolved source (i.e. point source). ABMAGLIM quantifies the noise level of the image outside of astronomical sources i.e. due to the combined effect of instrumental, atmospheric and diffuse sky background emission. In the case of SCIENCE.IMAGE, the limiting AB magnitude refers to the passband defined by FILTER. In the case of SCIENCE.CUBE.IFS the limiting AB magnitude refers to the associated broad-band image (type ANCILLARY.IMAGE) as defined on page 3 with wavelength interval between WAVELMIN and WAVELMAX.[5] Note: In case of non-uniform magnitude limit across the field of view, e.g. due to the combination of several offset exposures, ABMAGLIM refers to the median, i.e. the level reached in at least 50% of the mapped area.
(R)	PIXNOISE	Median background pixel-to-pixel noise of the 3D data cube in units of erg/s/cm**2/Angstrom. "Background" here means the noise outside of objects, i.e. the estimate does not include the Poissonian noise contributed by objects (e.g. mode of the error cube).
(R)	SPEC_RES	Spectral resolving power (lambda / Δ lambda) at the central wavelength of the data (WAVELMIN+WAVELMAX)/2. In case of data combination from different IFU's, slices, exposures (e.g. MUSE) the average spectral resolving power should be assigned to SPEC_RES.
(R)	SKY_RES	Effective spatial resolution of the data in terms of the FWHM of the profile of unresolved sources (arcsec).[6,7] In case of SCIENCE.CUBE.IFS, unless the effective spatial resolution varies strongly with wavelength, SKY_RES refers to the broad-band image (type ANCILLARY.IMAGE) as defined on page 3.
(R)	SKY_RERR	Error of SKY_RES (arcsec), specifies the overall uncertainty in the RMS sense including random and systematic effects.

[4] Oke, J. B., & Gunn, J. E. 1983, ApJ, 266, 713
[5] The 5σ noise shall be estimated within an image area that corresponds to the broad-band PSF. Then, the measured noise is converted to AB magnitudes assuming a flat spectrum (f_ν=const.)
[6] In case of multiple suitable point sources SKY_RES shall be obtained by averaging over individual measurement.
[7] If the image quality cannot be measured directly from the data (normally due to the lack of suitable sources within the FOV), then SKY_RES shall be estimated appropriately, e.g. based on the DIMM seeing, and SKY_RERR must indicate the typically expected deviation with respect to the actual resolution (in the RMS sense).

Type	Keyword	Description
(S)	`PROVi`	List of original science files, which were processed to generate this data product. Original **raw** files must be referenced in terms of the ESO/SAF identifier recorded as `ARCFILE` in the FITS header, also known as “DP.ID” in the SAF query forms. References to raw files in terms of `ORIGFILE` must be converted to the corresponding `ARCFILE` name prior to Phase 3 data submission.[8]

Inapplicable Keywords

- The `FILTER` keyword is inapplicable in the context of IFU cubes. If `FILTER` exists in the raw data it should be propagated as `OFILTER`.

[8] In case of very large sets of PROVi keywords it is possible to use the Phase 3 provenance extension instead. See GEN-SPE-ESO-33000-5335, Issue 5, §2.4.2, for further details.