DFMS PDS L3 enhancement documentation

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Introduction

This document describes the software written to enhance the mass scale of the DFMS Planetary Data Systems (PDS) processing level 3 (L3) data produced by the DFMS PDS L2-to-L3 Data Processing software.

The DFMS PDS L3 enhancement software is complementary to the DFMS PDS L2-to-L3 data processing software; its use is mandatory to obtain DFMS PDS L3 products with an accurate mass scale.

1. Code installation and environment setup

The software has been developed in C and consists in one file named `ROSINA_DFMS_L3_ENHANCEMENT.c`.

It has been successfully compiled and tested under Windows 10 with gcc version 3.4.2 (Thread model: win32) using the following command line:

```
gcc -O2 -Wall -o ROSINA_DFMS_L3_ENHANCEMENT.exe ROSINA_DFMS_L3_ENHANCEMENT.c
```

2. Process description

2.1. Input

The inputs of the DFMS PDS L3 enhancement software are:

- the DFMS PDS L2 products,
- the DFMS PDS L3 products generated by the DFMS PDS L2-to-L3 data processing software.

The software requires the inputs to have the following folder architecture:

[DFMS PDS L2 path]
> MTP2
> > DFMS
> > > CE
> > > MC

> MTP3
> > DFMS
> > > CE
> > > MC

> MTP4
> > > …

[DFMS PDS L3 path]
> MTP2
> > DFMS
> > > CE
> > > MC

> MTP3
> > DFMS
> > > CE
> > > MC

> MTP4
> > > …

2.2. Output

The produced output consists in PDS compliant files, with the same format as the input, and with a corrected & enhanced mass scale. The file tree architecture is the same as for the DFMS PDS L3 data input.

2.3. Software parameters

The DFMS PDS L3 enhancement software requires the following entries to be set correctly in the first section of the **`ROSINA_DFMS_L3_ENHANCEMENT.c`** file:

- Paths (need to be written with double **`\\`** for compatibility with Windows)
  - **`DFMS_L2_path`** – the path to the DFMS PDS L2 data (top folder)
  - **`DFMS_L3_path`** – the path to the DFMS PDS L3 data generated by the DFMS PDS L2-to-L3 data processing software (top folder)
  - **`DFMS_L3_output_path`** – the path where the enhanced DFMS PDS L2 products will be saved (top folder)
  - **`p0_list`** – path to the files in which the pix0 values will be saved
  - **`p0_skipped`** – path to the files in which the skipped pix0 values will be saved

- Parameters
  - **`process_p0`** – defines whether the pix0 values are computed from the DFMS PDS L2 data (value 1), or read from a previously created pix0 list (value 0)
  - **`delivery`** – defines the number of digits of the mass columns of the output; if equal to 0, all masses will have 4 digits after the decimal point; if equal to 1, only the selected minor species (masses 16, 17, 18, 27, 28, 30, 32, 34, 44, 46, 60, 76) will have 4 digits after the decimal point, the other masses will have 2 digits
  - **`MTP_START`** – defines the first MTP to be processed (first MTP with DFMS spectra = MTP2)
  - **`MTP_STOP`** – defines the last MTP to be processed (last MTP with DFMS spectra = MTP35)

2.4. CEM process description

No mass scale enhancement of the CEM data is foreseen, therefore the CEM data are simply copied to the output folder.

2.5. MCP process description

2.5.1. pix0 calculation

The p0 values used as references for the calculation of the mass scales are calculated using the DFMS PDS L2 products. For more information about the p0 definition, please refer to the DFMS PDS L2-to-L3 data processing documentation.

2.5.1.1. Processed files

In the calculation of the pix0 values, some modes are skipped by the software and are listed below:

- M0600
- M0601
- M0602
- M0620
- M0621
- M0622
- M0630
- M0631
- M0632
- M9999

For each DFMS L2 PDS file with a mode number different from the ones listed above, the software checks the commanded mass (stored in the header in the `ROSINA_DFMS_SCI_MASS` value). Only the spectra with a science masse of 16, 18, 28, 44, 60, or 76 are read entirely and undergo the processing steps detailed in the next sections.

2.5.1.2. Peak finding

The files meeting the requirements mentioned above are read entirely to find the highest value in the spectrum for rowA and rowB. For the specific masses studied, the highest peaks are known to correspond to specific molecules, listed below:

Mass	Main molecule
15.99436604	O
18.01001610	H_2O
27.99436604	N_2
43.98928066	CO_2
59.96643721	OCS
75.94359377	CS_2

2.5.1.3. Calculations

For each row, the pix0 value can be calculated using the following formula:

pix0 = max_value_position – (D · z · log(mass/m0))/25

with:

- *max_value_position* the pixel value of the highest point in the ongoing spectrum,
- *D* the dispersion value (equal to 127'000 for low resolution modes and for high resolution modes with m0 > 70, or equal to 382'200 · $m0^{-0.34}$ otherwise),
- *z* the zoom factor (equal to 6.4 for the high resolution modes, or 1 otherwise),
- *mass* the exact mass of the expected molecule (see table above),
- and *m0* the commanded mass (integer).

Some outlying pix0 values possibly originating from temporary unstable voltages are automatically skipped and stored in the software folder in an ASCII file named `p0_L2_skipped.DAT`. The other (correctly) calculated p0 values are stored in the software folder in an ASCII file named `p0_L2.DAT`.

The skipping criteria is reached when the pix0 value exceeds a specific range, which is depending on the acquisition time of the spectra:

m0	until September 2015		from September 2015 to 26 January 2016 included		from 27 January 2016	
16	200 < rowA < 305	200 < rowB < 305	264 < rowA < 309	264 < rowB < 311	200 < rowA < 230	200 < rowB < 231
18	150 < rowA < 300	150 < rowB < 300	150 < rowA < 309	150 < rowB < 309	200 < rowA < 230	200 < rowB < 230
28	150 < rowA < 320	150 < rowB < 320	150 < rowA < 320	150 < rowB < 320	200 < rowA < 320	200 < rowB < 320
44	150 < rowA < 300	150 < rowB < 300	150 < rowA < 304	150 < rowB < 306	200 < rowA < 230	200 < rowB < 230
60	265 < rowA < 297	265 < rowB < 297	264 < rowA < 304	264 < rowB < 311	200 < rowA < 230	200 < rowB < 230
76	200 < rowA < 304	200 < rowB < 304	200 < rowA < 315	200 < rowB < 315	200 < rowA < 260	200 < rowB < 260

The format of both the files `p0_L2.DAT` and `p0_L2_skipped.DAT` is as follows:

```
"YYYY-MM-DDTHH:MM:SS"  XXX  XXX  X  XX
1                      2    3    4  5
```

with:

1 – the acquisition time associated to the pix0 value

2 – the pix0 value for rowA

3 – the pix0 value for rowB

4 – a value indicating the resolution (0 = LR, 1 = HR)

5 – the commanded mass m0

Figure 1 shows the pix0 values for mass 18 (rowA) calculated during the conversion of the DFMS PDS L3 products (version 2.0).

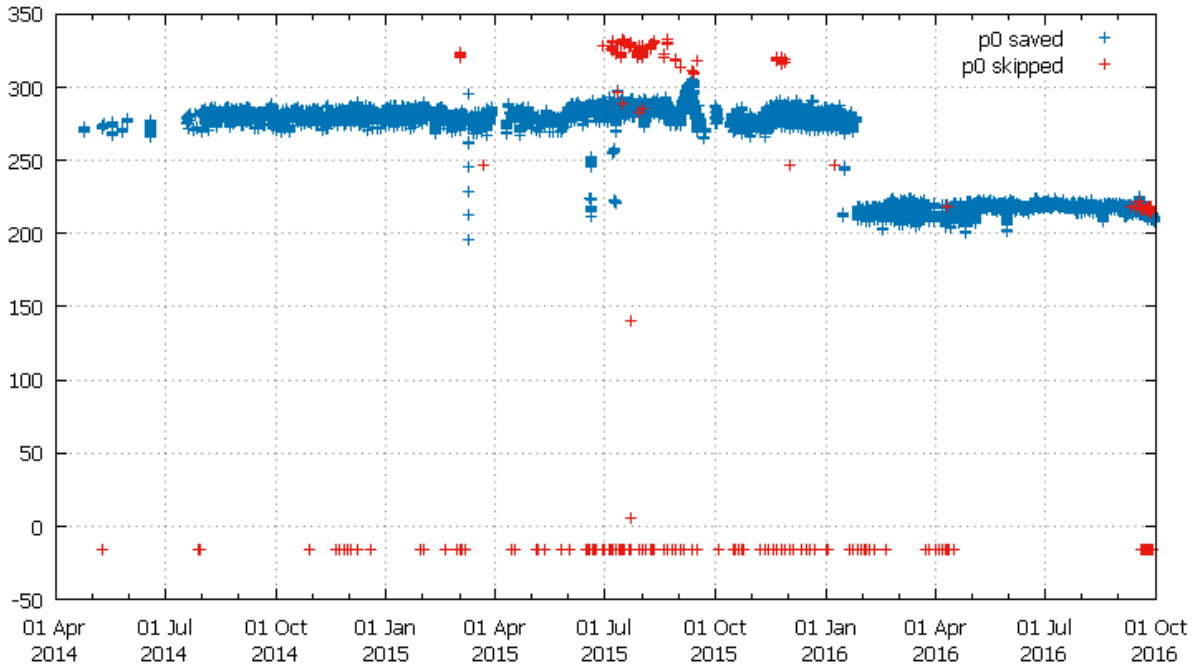

Figure 1: pix0 values calculated for mass 18 (rowA). The points in red are skipped pix0 values.

2.5.2. pix0 interpolation

Once the reference pix0 values are computed after the reading of all the DFMS PDS L2 data, the DFMS PDS L3 products generated by the DFMS PDS L2-to-L3 data processing software are read, and according to their commanded mass (read in the header, in `ROSINA_DFMS_SCI_MASS`), the pix0 value is either interpolated or extrapolated using the following equation:

$$pix0\ (m0) = pix0\_a + (m0 - m\_a) \cdot (pix0\_b - pix0\_a) / (m\_b - m\_a)$$

Commanded mass range	Parameter values			
	m_a	pix0_a	m_b	pix0_b
m0 ≤ 18	16	pix0 (18) + 1.17* + 3.55**	18	pix0 (18)
18 ≤ m0 ≤ 28	18	pix0 (18)	28	pix0 (28)
28 ≤ m0 ≤ 44	28	pix0 (28)	44	pix0 (44)
44 ≤ m0 ≤ 70	44	pix0 (44)	60	pix0 (18) + 0.04* + 2.37**
70 ≤ m0	70	pix0 (18) + 12.79* + 32.83**	–	–

* if date of acquisition is before 2016-01-27 ** if date of acquisition is after 2016-01-27 (included)

2.5.3. DFMS PDS L3 output

Each DFMS PDS L3 enhanced file is written in the **`[DFMS_L3_output_path]`** path defined in section 2.3, following the same file tree architecture as for the DFMS PDS L3 data given in input.

The header of the output files is the same as the one of the input files, except for the following lines which are updated with the appropriate values:

- `ROSINA_DFMS_SCI_SELF_PIXEL0_A`
- `ROSINA_DFMS_SCI_SELF_PIXEL0_UNC`
- `ROSINA_DFMS_SCI_SELF_PIXEL0_B`
- `ROSINA_DFMS_SCI_SELF_PIXEL0_UNC`

Due to mass scale calibration complexities with high-resolution modes the pix0 uncertainty for all high-resolution modes is fixed at 10.0 pixels.

The lines after the header are read from the input files, and then written back in the output files with the corrected / enhanced mass scale, with a number of digits as defined in the parameter **`delivery`** (see section 2.3).