SPEXone Level 1A to 1C Processor Release Notes

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Contents

1 Introduction

The SPEXone data processor consists of three parts: the L1A-L1B processor, the L1B-L1C processor, and a calibration key data (CKD) generator. The CKD generator uses dedicated on-ground calibration measurements to acquire the CKD. The L1A-L1B processor uses flight L1A data together with the CKD to generate L1B data. The L1B-L1C data collocates L1B data to a common geolocation grid for a predefined reference height.
The L1A-L1B processor and the CKD generator are algorithmically interlinked to ensure full consistency of the derived CKD and the calibration of the L1A data. Therefore, it has been decided to include both elements in the same software package even though the CKD generator is not required for processing flight data.

2 New features

2.1 OpenMP

The processor now uses OpenMP instead of MPI for parallelization. It is expected to run slightly faster due to a lower communication overhead between threads.

2.2 Better memory management

When running an L1A-L1B process, there is now an option to read the entire DEM file to memory as opposed to reading it step by step as the calculation progresses. The constant I/O due to reading of the DEM file by different MPI processes incurred considerable overhead and was made even worse in the OpenMP implementation. Reading the DEM file in one go significantly reduces the computational time.
Similarly, there is an option to read in all raw L1A detector images before the L1A-L1B process starts. The overhead of reading each image separately is much less than in the case of the DEM file but a small reduction in computational time is possible.

2.3 Build system updates

It is now possible to only compile source files necessary for the L1B or L1C processes (see `L1BC_ONLY` in the example CMake initial cache file). This also reduces the number of dependencies as the following are no longer required:

- GADfit — a nonlinear optimization package that is used for some processes when generating the CKD but not in L1B/L1C.
- Catch2 — a testing framework.

This reduces the compilation time, the likelihood of compiler errors during compilation, and the effort of maintaining a larger number of dependencies.

3 Installation and running

3.1 Dependencies

- GNU C++ compiler version 11
- CMake version 3.18
- NetCDF C and C++ libraries
- HDF libraries
- Linear algebra library (e.g. blas and lapack or Intel MKL)

3.2 Data

This delivery includes a simulated orbit (L1A product) that is partially populated with data from high-accuracy simulations. Realistic flight data spans the extent of 3 L1C granules (about 15 minutes). The rest of the orbit is a measured dark signal as seen in Fig. 1.

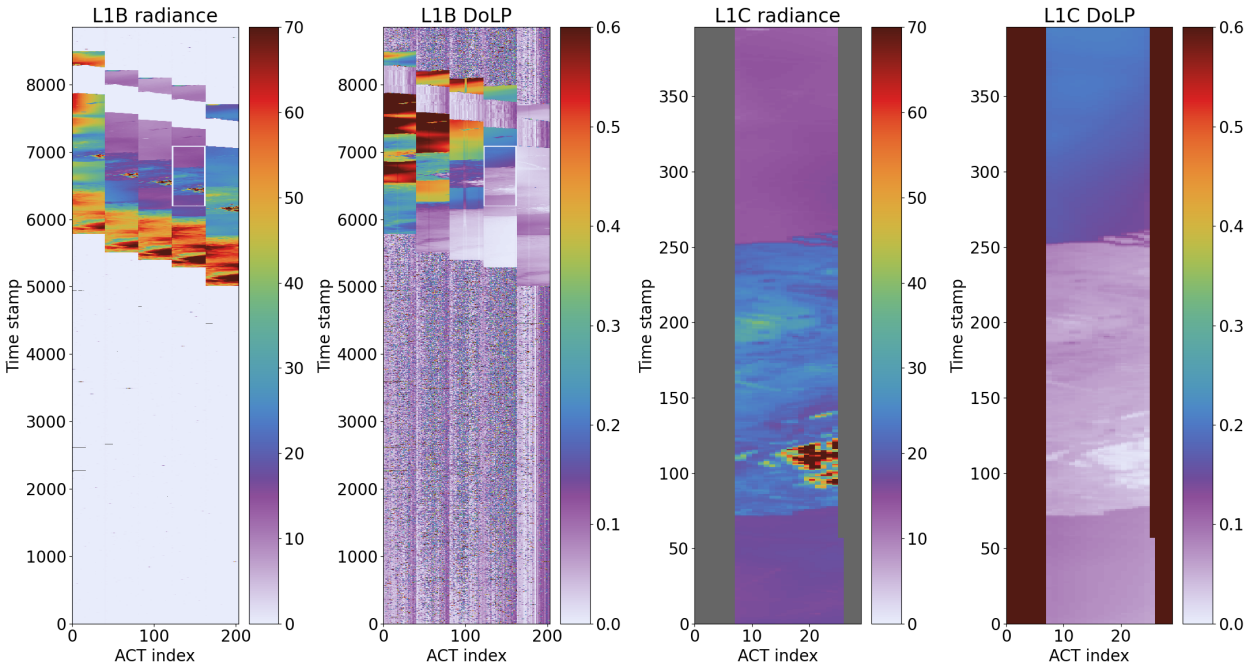

Figure 1: Radiance and DoLP generated from the L1A product as a function of across track index and the timestamp index. Data is shown for all five viewports for a fixed wavelength of 556.1 nm. Left: radiance and DoLP from the generated L1B product. Right: radiance and DoLP from on of the generated L1C products (rectangle on the left shows the location of the L1C granule on the L1B product).

3.3 Building

Make a copy of the initial CMake cache file

```
cp initial_cache.cmake.example initial_cache.cmake
```

found in the root source directory and edit it to reflect your environment. Next, create a build directory for configuring and building the SPEXone executable. From the root directory the procedure could look like this:

```
mkdir build && cd build
cmake -C ../initial_cache.cmake -D CMAKE_BUILD_TYPE=release ..
make -j
```

Notice the `L1BC_ONLY` flag in the example cache file which is enabled by default.

3.4 Running

Start by calibrating the L1A product:

```
export OMP_NUM_THREADS=16
<spexone> l1b.yaml
```

where <spexone> is the SPEXone processor executable. The DEM file and the raw L1A detector images are read into memory by default. On the author's machine the memory consumption with these settings was about 23.3 GB. You can change that by opening l1b.yaml and editing the following lines:

```
l1a_in_memory: yes
dem_in_memory: yes
```

Change to "no" to disable. However, changing the DEM file setting could noticeably slow down the calculation. The generated L1B product may be compared with the reference ones:

```
h5diff l1b.nc l1b_ref.nc
```

Next, generate L1C products using three L1C grid files:

```
<spexone> l1c_20220321T115708.yaml
<spexone> l1c_20220321T120208.yaml
<spexone> l1c_20220321T120708.yaml
```

Compare the results with reference files:

```
h5diff l1c_20220321T115708.nc l1c_20220321T115708_ref.nc
h5diff l1c_20220321T120208.nc l1c_20220321T120208_ref.nc
h5diff l1c_20220321T120708.nc l1c_20220321T120708_ref.nc
```

4 Files

The delivery is accessible at `https://public.spider.surfsara.nl/project/spexone/PACE/L1A-L1C/2023_10_01/`.

- `spexone_cal.tar.gz` — source code. Unpack and compile according to instructions in Sec. 3.3.
- `l1a.nc` — L1A product (input for the first simulation)
- `l1b.yaml` — Configuration file for generating an L1B product from `l1a.nc`
- `l1b_ref.nc` — Reference L1B product. Should be identical to that produced by running `l1b.yaml`
- `l1c_*.yaml` — Configuration files for generating L1C products using either `l1b.nc` or `l1b_ref.nc` and the L1C grid files as input
- `l1c_*_ref.nc` — Reference L1C files. Should be identical to those produced by the `l1c_*.yaml` configuration files.
- `PACE_SPEX.*.L1C.nc` — L1C grid files used for the L1B-L1C runs.
- `ckd.nc` — calibration key data required for the L1A-L1B run
- `gebco_ocssw_v2020_reduced.nc` — reduced elevation map required for geolocation. It's like the original DEM file but uncompressed and the variables `height`, `water_surface_height`, and `watermask` have been preprocessed and reduced to a single variable (`height`). You can also use the original DEM file (in previous releases called `gebco_ocssw_v2020.nc`) but then the L1B startup time is about 20-30 seconds longer.
- `SPX1_CKD_BIN_TBL_20210304T124000_001.nc` — binning table
- `binned_fs_hybrid_reference_spectrum_c2022-11-30_with_unc.nc` — solar spectrum. This will be stored in L1B and L1C products after convolving with the ISRF.
- `l1b.log` — an example log file of the L1A-L1B process so that you would know what to expect.