UpTrop: A Versatile Python Software for Retrieving Tropospheric Profiles of NO_2 and O_3 from Satellite Observations

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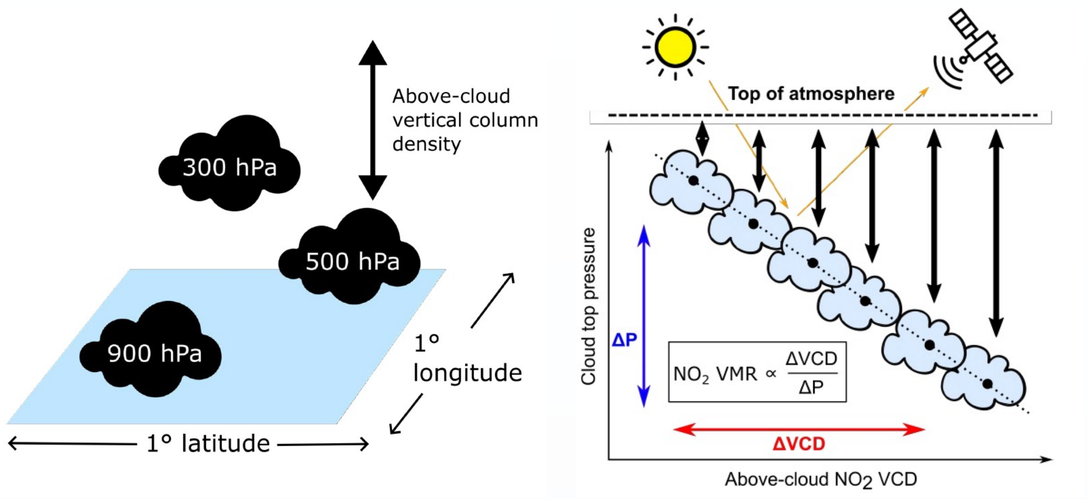
1. Introduction to UpTrop

UpTrop is a Python software to convert satellite observations of total atmospheric column densities of air pollutants to vertical profiles in the global troposphere using the cloud-slicing technique. At present, UpTrop is equipped to utilize total column densities of nitrogen dioxide (NO_2) and ozone (O_3) from the ESA Sentinel-5P TROPOspheric Monitoring Instrument (TROPOMI) positioned in low-Earth orbit, and accompanying cloud data from TROPOMI products. The software can retrieve mixing ratios of NO_2 and O_3 in user-defined atmospheric pressure ranges at spatial resolutions of 1° x 1° to 4° x 5°. The approach has potential to be extended to instruments in geostationary orbit, namely Geostationary Environment Monitoring Spectrometer (GEMS) and the Tropospheric Emissions: Monitoring of Pollution (TEMPO).

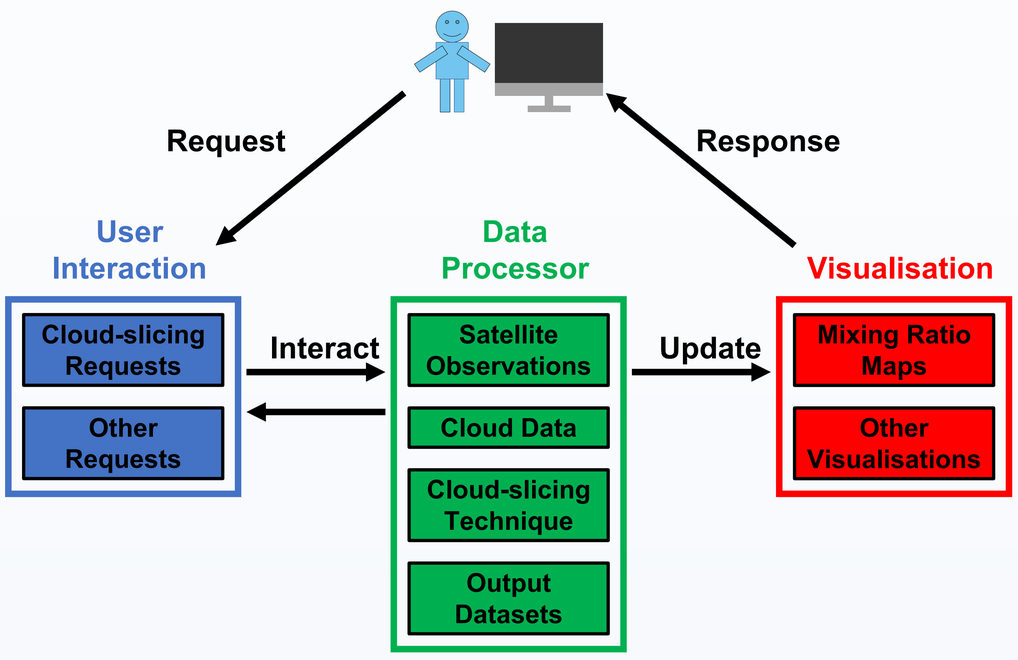
2. Cloud-slicing TROPOMI Columns



Figures created by Rebekah P. Horner, UCL

Cloud-slicing uses optically thick clouds to slice up the troposphere. NO_2 (or O_3) mixing ratios are calculated using the relationship between cloud top pressure and vertical column density.

3. Software Design Framework



The software uses the architecture shown above, known as 'Model-View-Controller (MVC)' in software engineering and so is primed for future expansion to include more species (formaldehyde, bromine monoxide) and satellite instruments (Sentinel-4, Sentinel-5, TEMPO, GEMS).

Python Version: 3.9

Key Dependencies: NumPy, netCDF4, Matplotlib, Cartopy

4. Example Usages

- UpTrop is designed for flexibility and ease-of-use, allowing integration into custom Python scripts or direct operation via terminal-based command-line tools.
- To use UpTrop, users simply input retrieval parameters including target species, product version, retrieval date range, pressure range, etc. Default values are provided for some parameters, such as the grid resolution of 1° × 1°.
- For large-scale operations, a Bash script can be utilized to dispatch multiple retrieval tasks to a computing cluster, eliminating the need to modify the underlying Python code.

Python Programming Application Interface (API)

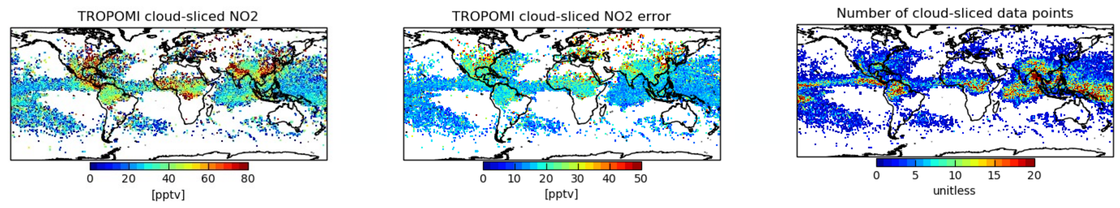
```
cloud_slice_tropomi(
    species="no2",
    product="PAL",
    trop_dir="/lustre/projects/uptrop/tropomi/Data/",
    out_dir="/cloud_slice_output",
    start_date="2019-06-01",
    end_date="2019-08-31",
    cloud_threshold='07',
    pmin=180,
    pmax=450,
    version=1,
    save_data=True,
    save_plot=True
)
```

Command Line Interface (CLI)

```
cloud_slice_tropomi --species "no2" \
                    --product "PAL" \
                    --trop_dir "/lustre/projects/uptrop/tropomi/Data/" \
                    --out_dir "/cloud_slice_output" \
                    --start_date "2019-06-01" \
                    --end_date "2019-08-31" \
                    --cloud_threshold "07" \
                    --pmin 180 \
                    --pmax 450 \
                    --version 1 \
                    --save_data "True" \
                    --save_plot "True"
```

5. Gallery and Output Data

The below visualisations, generated by the software provide insights into the cloud-slicing TROPOMI NO_2 in June-August 2019 at 1° × 1° at 450-180 hPa (~8-12 km).



The data shown are also output as NetCDF files along with gridded mean ceiling and range of cloud top pressures used to cloud-slice TROPOMI NO_2.

6. New Features Under Development

Extended Capabilities (long term):

Expand the software's scope by integrating with more satellite instruments.

Interactive Data Exploration & Code-free Analysis:

Develop a data application that enables users to:

- Zoom in, pan, or hover to get comprehensive details about specific data points. For instance, users could simultaneously view NO_2 mixing ratios, NO_2 error, number of cloud-sliced data point, latitude and longitude all by simply hovering over a particular grid.
- Apply filters on data based on various parameters. For instance, users could filter data by NO_2 mixing ratios and immediately see updated visualisations.
- Perform fundamental data analyses, such as deriving the average NO_2 mixing ratios within a user-defined latitude-longitude range, without the need to write code.
- Extract data from a user-defined area and save it into data frames for easy access.

7. Software Quality, Enhancements and Distributions

Example log file detailing retrieval progress and data retention diagnostics:

```
2023-07-31 13:27 - INFO - Found total of 14 TROPOMI files and 14 Cloud files
2023-07-31 13:27 - INFO - Processing: S5P_PAL__L2__NO2____20200501T013558_20200501T031728_13204_01_020301_20211111T040536.nc
2023-07-31 13:27 - INFO - Processing: S5P_PAL__L2__NO2____20200501T031728_20200501T045858_13205_01_020301_20211111T040600.nc
2023-07-31 13:28 - INFO - Processing: S5P_PAL__L2__NO2____20200501T045858_20200501T064028_13206_01_020301_20211108T022016.nc
2023-07-31 13:29 - INFO - Processing: S5P_PAL__L2__NO2____20200501T064028_20200501T082158_13207_01_020301_20211111T040606.nc
2023-07-31 13:31 - INFO - Processing: S5P_PAL__L2__NO2____20200501T082158_20200501T100329_13208_01_020301_20211111T040608.nc
2023-07-31 13:32 - INFO - Processing: S5P_PAL__L2__NO2____20200501T100329_20200501T114459_13209_01_020301_20211111T040637.nc
2023-07-31 13:32 - INFO - Processing: S5P_PAL__L2__NO2____20200501T114459_20200501T132629_13210_01_020301_20211111T040714.nc
2023-07-31 13:32 - INFO - Processing: S5P_PAL__L2__NO2____20200501T132629_20200501T150759_13211_01_020301_20211111T040904.nc
2023-07-31 13:32 - INFO - Processing: S5P_PAL__L2__NO2____20200501T150759_20200501T164929_13212_01_020301_20211111T040945.nc
2023-07-31 13:33 - INFO - Processing: S5P_PAL__L2__NO2____20200501T164929_20200501T183100_13213_01_020301_20211111T041004.nc
2023-07-31 13:34 - INFO - Processing: S5P_PAL__L2__NO2____20200501T183100_20200501T201230_13214_01_020301_20211111T041031.nc
2023-07-31 13:35 - INFO - Processing: S5P_PAL__L2__NO2____20200501T201230_20200501T215400_13215_01_020301_20211111T041046.nc
2023-07-31 13:35 - INFO - Processing: S5P_PAL__L2__NO2____20200501T215400_20200501T233531_13216_01_020301_20211111T041051.nc
2023-07-31 13:35 - INFO - Processing: S5P_PAL__L2__NO2____20200501T233531_20200502T011701_13217_01_020301_20211111T041059.nc
2023-07-31 13:35 - INFO - Max no. of data points in a gridsquare: 9.0
2023-07-31 13:35 - INFO - (1) Too few points: 3241
2023-07-31 13:35 - INFO - (2) Low cloud height range: 5341
2023-07-31 13:35 - INFO - (3) Low cloud height std dev: 0
2023-07-31 13:35 - INFO - (4) Large error: 0
2023-07-31 13:35 - INFO - (5) Significantly less than zero: 209
2023-07-31 13:35 - INFO - (6) Outlier (NO2 > 200 pptv): 0
2023-07-31 13:35 - INFO - (7) Non-uniform stratosphere: 1819
2023-07-31 13:35 - INFO - (8) Successful retrievals: 1191
2023-07-31 13:35 - INFO - (9) Total possible points: 11801
2023-07-31 13:35 - INFO - Mean % points retained: 2.739262914536996
2023-07-31 13:35 - INFO - Saving data to: tropomi-no2-fresco-wide-0.7-1x1-20200501-20200501-140-480hPa-v1.nc
```

In addition to adding new features, we also plan on improving the following aspects:

- **Performance**: Profile and refine the software to identify bottlenecks, ensuring faster processing, and greater memory efficiency in anticipation of larger file processing from geostationary satellites.
- **CI/CD**: Implement a Continuous Integration & Deployment (CI/CD) pipeline to automate testing, linting, and deployment processes, ensuring rapid and reliable releases.
- **Compatibility**: Ensure UpTrop works seamlessly with a wider range of Python and Dependency versions.
- **Distribution**: Prepare and package UpTrop for release on platforms like PyPI and Conda, facilitating easy installation for users.
- **Documentation**: Enhance and expand documentation to cover new features, usage examples and tutorials.

We also welcome user feedback and contributions from the community.

8. Resources & Contact

TROPOMI Products: https://www.tropomi.eu/

Cloud-slicing Technique: Marais et al., https://doi.org/10.5194/amt-14-2389-2021, 2021

UpTrop GitHub: https://github.com/eamarais/erc-uptrop

UpTrop Documentation: https://erc-uptrop.readthedocs.io/en/latest/

Contact us if interested in using the data or software. Email gongda.lu@ucl.ac.uk

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