



PROFFAST 2.0 and PROFFASTpylot

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www.kit.edu



Outline

- PROFFAST v 2.0 (Frank Hase)
- PROFFASTpylot (Lena Feld and Benedikt Herkommer)
 - Motivation
 New features
 - How to install How to run
- Closing words and time for questions



Motivation

- Simplified Usage
 - One combined input file
 - Start PROFFASTpylot once and run all parts of PROFFAST automatically
- Benefits
 - Avoid careless mistakes
 - Reduce workload when processing data

New Features

- Support of GGG2020 map files
- Select start- and end date of processing
- Identifies days with corrupt interferograms
- ILS values are read automatically
- Usable with Windows and Linux

User friendly additions



- Paths for input data and results can be chosen freely
- Merged result file with local time and UTC
- Possibility to store frequently occurring coordinates in file
- Option to start with spectra
- Source code can be extended to read different pressure input files

Installation: Where to find PROFFASTpylot



Available at https://gitlab.eudat.eu/coccon-kit/proffastpylot



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Install with Git (recommended)



1) If you do not have Git. Download and more information: https://git-scm.com/

- 2) Navigate to a folder where you want to install PROFFASTpylot
- 3) Open Git-Bash
- 4) Enter "git clone https://gitlab.eudat.eu/coccon-kit/proffastpylot.git"



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Collaborative Carbon Column Observing Network



Installation: Download PROFFAST v 2.0



- Go to https://www.imk-asf.kit.edu/english/3225.php
- Download PROFFASTv2.0
- Extract zip file and rename folder to prf
- Move it to \proffastpylot\ such that the path to e.g. invers20.exe is \proffastpylot\prf\invers20.exe

Installation: Download PROFFAST v 2.0



The processing and analysis of the FTIR measurements requires firstly a preprocessing of the raw interferograms for the generation of spectra and secondly the quantitative analysis of the absorption spectra for the determination of the desired trace gas abundances. For the latter task, a radiative transfer code and an inversion scheme is applied which fits synthetic spectra to the measurements. For this purpose, the KT offers source-open tools for both the preprocessing PREPROCESS and the subsequent quantitative trace gas analysis named PROFFAST. PREPROCESS has been developed in the framework of the COCCON-PROCEEDS project supported by ESA_PROFFAST has been developed at KTT coffra user-friendly application for the trace gas analysis with an optimized performance. PROFFAST accepts *.mod files as used in TCCON for ensuring identical choices for the temperature and water vapor profiles, and the a-priori vertical profiles of the target gases.

IMPORTANT, PLEASE NOTE:

The species order in the state vector has been changed. See new input files!!!

TECHNICAL NOTE:







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Create a python virtual environment



- We strongly recommend to use a virtual environment (venv) to run the PROFFASTpylot
- A venv is an isolated python environment
 - \rightarrow No interference with other python packages
- For creation:
 - Open a PowerShell/cmd
 - Navigate to the folder "proffastpylot"
 - Execute "python -m venv prf_venv"



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Installation of PROFFASTpylot



Open a console and navigate to the proffastpylot folder

- Activate the virtual environment
- Execute pip install -e .



| Mindows PowerShell | |
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| Using cached pandas-1.3.5-cp38-cp38-win_amd64.whl (10.2 MB) | |
| LI I Collecting PyYAML | hstitute of Technology |
| Using cached PyYAML-6.0-cp38-cp38-win_amd64.wh1 (155 KB) | |
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| Collecting numpy>=1.17.3; platform_machine != "aarch64" and platform_machine != "arm64" and | |
| python_version < "3.10" | |
| Using cached numpy-1.22.1-cp38-cp38-win_amd64.wh1 (14.7 MB) | |
| Collecting six>=1.5 | |
| Using cached six-1.16.0-py2.py3-none-any.whl (11 kB) | |
| Using legacy setup py install for fortranformat, since package 'wheel' is not installed. | |
| Installing collected packages: wheel, six, python-dateutil, numpy, pytz, pandas, PyYAML, tim | |
| ezonefinder, fortranformat, prfPylot | |
| Running setup.py install for fortranformat done | |
| Running setup.py develop for prfpylot | |
| Successfully installed PyYAML-6.0 fortranformat-1.1.1 numpy-1.22.1 pandas-1.3.5 pripylot pyt | |
| non-dateutii-2.8.2 pytz-2021.3 six-1.16.0 timezonefinder-5.2.0 wheel-0.37.1 | |
| WARNING: You are using pip version 20.1.1; nowever, version 21.3.1 is available. | |
| You should consider upgrading via the e:\proffastpylot_telecon_installation\proffastpylot\p | |
| <pre>//rt_venv\scripts\python.exe -m pip installupgrade pip command. /rnf.venv\ DS_E.\preffectpulet telecep installetion\preffectpulet.</pre> | |
| (prit_venv) PS E: protrastpylot_telecon_installation protrastpylot | |
| | |

Test of the Installation: Execute the Sodankyla-Example



- The PROFFASTpylot comes with an out-of-the-box example which can be used for testing.
- It can be executed by running run.py in proffastpylot\example
 - Downloads the example interferograms and input data automatically
 - Automatically generates an input file with the required settings
 - Automatically generates folders for the output data
- Do not forget to activate your virtual environment

Test of Installation: Execute Sodankyla-Example



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🔁 Windows PowerShell

PS E:\proffastpylot_telecon_installation\proffastpylot> .\prf_venv\Scripts\Activate.ps1 (prf_venv) PS E:\proffastpylot_telecon_installation\proffastpylot> cd .\example\ (prf_venv) PS E:\proffastpylot_telecon_installation\proffastpylot\example> python run.py Example data where not found on disk. Do you like to download them? This will download 104 MB of data to your disk. Enter 'yes' to download the data or 'no' to abort:

Test of Installation: Execute Sodankyla-Example



Test of Installation: Execute Sodankyla-Example



How to Run: Sodankyla Example





Three different data folders:

- 1) input_data: contains e.g. interferograms
- 2) analysis: contains spectra generated by preprocess
- 3) result_data: contains the results and logs

For each site and spectrometer one input file is needed, containing ALL settings and information about the side. To run a site one single python script is needed

run.py

Only 17 lines of code to execute the whole example!

Only needed in Example: Download the interferograms and input data

Input file generator: Here in the special use case of generating the example input-file. It also provides a interactive wizard to generate input files.

Pylot class:

- Working horse of PROFFASTpylot
- input_file contains the path to sondankyla_example_input.yml
- run method does all the work for a standard evaluation of EM27/SUN data (supporting multiprocessing!)



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input_sodankyla_example.yml



Contains all information and settings to one site and one spectrometer
 3 Blocks:

- Site and Instrument
- Behavior of PROFFASTpylot
- Path



| | × E | <u>File Edit Selection View Go Run Terminal Help</u> • input_sodankyla_example.yml - proffastpylot - Visual Studio Code | – 🗆 X | |
|-----------|-------|---|---|-----------------------------------|
| | L) | ! input_sodankyla_example.yml ● | th 🛛 … | |
| | | example > ! input_sodankyla_example.yml | | |
| | Q | 44 #################################### | 121822/17757Aurona and a second | |
| Innuttile | | 45 # BEHAVIOUR # | | |
| npatine | പ്പ | 46 ############# 47 | | Karlsruhe Institute of Technology |
| | | 48 # Start the processing chain with already available spectra. | | |
| | å | 49 # The directory to the spectra is given as the 'analysis_path'. | United With the second se | |
| | | 50 # NOTE: | | |
| | HC | 51 # In this case the folder this path points to must have a | CORE International Control of Con | |
| | ш | 52 # Substructure like analysis/sitewame_instrumenthumber/fimebb. | | |
| | | 53 # set to Internate. | | |
| | ΓŌ | 55 | | |
| | | 56 # Process only dates in a specific time range | | |
| | Д | 57 # date format: YYYY-MM-DD. | | |
| | | 58 # Leave empty to process all dates in the data folder | | |
| | | 59 start date: | | |
| | | 60 end date: | | |
| | | 61 | | |
| | | 62 # Optional comment included in bin-files by PREPROCESS | | |
| | | 63 # Leave empty for adding no comment | | |
| | | 64 note: | | |
| | | | | |
| | | 66 # Delete the abscos.bin files? (True/False) | | |
| | | 67 # The abscos.bin file contains the simulation of the atmosphere which is | | |
| | | 68 # the result of the 'pcxs' program part of PROFFAST. | | |
| | | 69 delete_abscosbin_files: True | | |
| | | | | |
| | | 71 # Delete PROFFAST input files? (True/False) Default: False | | |
| | | 72 # If False: Files will be moved to results folder | | |
| | | 73 delete_input_files: False | | |
| | | | | |
| | | 75 # The pressure_type defines the format of the pressure file | | |
| | | 76 # Uptions: | | |
| | | 77 # Origina: | | |
| | | 70 # praining of the files should be (site abbrevs (vurgendd) inp | | |
| | Q | 80 # log. | | |
| | 0 | 81 # the 'MTRA-datalogger' format as used by KIT | | |
| | stry. | 82 # (It is possible to define own pressure types) | | |
| | 523 | 83 pressure type: log | | na Climate Research |
| | × 3 | P master ↔ Python 3.8.5 64-bit ('prf venv'; venv) ⊗ 0 △ 0 ↔ Git Graph | TF-8 CRLF YAML & ロ | n Observing Network |



P master ↔ Python 3.8.5 64-bit ('prf_venv': venv) ⊗ 0 🛆 0 🏚 Git Graph

How to Run: Sodankyla Example





Three different data folders:

- 1) input_data: contains e.g. interferograms
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For each site and spectrometer one input file is needed, containing ALL settings and information about the side. To run a site one single python script is needed



For the input file of an arbitrary site:

- Modify the example manually
- Use the InputfileGenerator



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赵 Windows PowerShell

(prf_venv) PS E:\proffastpylot_telecon_installation\proffastpylot> cd .\prfpylot\ (prf_venv) PS E:\proffastpylot_telecon_installation\proffastpylot\prfpylot> ls

Directory: E:\proffastpylot_telecon_installation\proffastpylot\prfpylot

| Node | LastWriteTime | Length Name | |
|------|--------------------|--------------------------|----|
| | | | |
| d | 1/19/2022 5:31 PM | templates | |
| d | 1/20/2022 8:14 AM | pycache | |
| -a | 1/19/2022 12:42 PM | 15753 create_inputfile.p | уy |
| -a | 1/19/2022 5:31 PM | 2533 download_example.p | уy |
| -a | 1/19/2022 5:31 PM | 9470 filemover.py | |
| -a | 1/19/2022 12:42 PM | 5846 ILSList.csv | |
| -a | 1/19/2022 12:42 PM | 25559 prepare.py | |
| -a | 1/19/2022 12:42 PM | 2966 pressure.py | |
| -a | 1/19/2022 5:31 PM | 15886 pylot.py | |
| | 1/10/2022 12.42 DM | 0 init nv | |

(prf_venv) PS E:\proffastpylot_telecon_installation\proffastpylot\prfpylot> python .\create_inputfile.py_

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🔁 Windows PowerShell



files can be shared among various intruments at the same site.

Please give the path to the PROFFAST executable. In this folder the PROFFAST executable have to be located. As the automatic detected default value the following path is used: E:\proffastpylot_telecon_installation\proffastpylot\prf To use this path do not enter anything and press enter:

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How to run: General usage of PROFFASTpylot

For the input file of an arbitrary site:

- Modify the example manually
- Use the InputfileGenerator



Run PROFFASTpylot

- Execute the run() method of the Pylot class
- Or: Execute the single steps separately

```
run karlsruhe.py - proffastpylot - Visual Studio Code
   File Edit Selection View Go Run Terminal Help
Ð
      🔮 run_karlsruhe.py 🗙
      example > 🗣 run karlsruhe.py > ...
             from prfpylot.pylot import Pylot
Ω
                                                                                                                          Karlsruhe Institute of Technology
             if name == " main ":
۶°
                 input file = r"E:\karslruhe PROFASTpylot settingfiles\ka SN037 default.yml"
                 # create prfPylot and run PROFFAST using the prfPylot
                 # we set logginglevel to 'debug' to get more information of the run
                 # run the processing with 8 processes in parallel
                 processes = 8
Ģ
                 MyPylot = Pylot(input file, logginglevel="debug")
                      # Use try block to ensure that in case something goes wrong
                      MyPylot.run preprocess(n processes=processes)
                      MyPylot.run pcxs(n processes=processes)
                      MyPylot.run_inv(n_processes=processes)
                      MyPylot.combine results()
\otimes
                      MyPylot.clean_files()
                                                                                                                         d Climate Research
                                                                                                                          Observing Network
```

Ln 1, Col 1 Spaces: 4 UTF-8 CRLF Python 🔊 🔾



For an arbitrary side Input file:

- Modify the example manually
- Use the InputfileGenerator

Run PROFFASTpylot

- Execute the `run` method of Pylot
- Execute the single steps separately



How to run: File structure



- Your interferograms must be saved in folders named YYMMDD
- We recommend using the following structure interferograms_<site>\<instrument_number>\YYMMDD



How to run: Starting from spectra

- PROFFASTpylot gives the possibility to process spectra directly
- The analysis path must have a structure as shown on the right hand side:

analysis\<site>_<instrument_number>\YYMMDD\
cal

In 'normal' processing mode PROFFASTpylot automatically generates this structure of the analysis folder





How to run: Add custom pressure type



| > | | | | | | | | al <u>H</u> el | | -08_00 | | | | | | | | | × |
|------------|--------|---------|---------------------------|---------------|----------------------|---------------|---------------------|----------------|------------------------|---------|-----------------------|------|-------------------|----------------|---------|------|-----|----|--------|
| Ð | 5 2 | | | | | | | | | | | | | | | | | | |
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| 0 | | | 111111111 | | | | | | 7.3000e+0 | 0 -3. | 4028e+38 | | | 2 + 2 . | 6630e+0 | | | | |
| J L C | | | 111111111 | | | | | | 7.5000e+0 | 0 -3. | 4028e+38 | | | | 6630e+0 | | | | |
| | | | 111111111 | | | | | | 7.4000e+0 | 0 -3. | 4028e+38 | | 912e+0 | 2 + 2 . | 6630e+0 | | | | |
| | | | 111111111 | | | | | | 7.5000e+0 | 0 -3. | 4028e+38 | | 912e+0 | | 6630e+0 | | | | |
| æ | | | 111111111 | | | | | | 7.7000e+0 | 0 -3. | 4028e+38 | | 912e+0 | 2 +2 . | 6630e+0 | | | | |
| | | | 111111111 | | | | | | 7.7000e+0 | 0 -3. | 4028e+38 | | | | 6630e+0 | | | | |
| Ш | | | 111111111 | | | | | | 3.0000e+0 | 0 -3. | 4028e+38 | | 912e+0 | 2 + 2 . | 6630e+0 | | | | |
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| | | | 111111111 | | 111e+1 | | 1.11116 | | 1.5700e+0 | 1 -3. | 4028e+38 | +9.9 | 912e+0 | 2 +2. | 6630e+0 | 1 +6 | | | |
| | | | 111111111 | | 111e+1 | | 1.11114 | | 1.5900e+0 | 1 -3. | 4028e+38 | | 912e+0 | 2 +2. | 6630e+0 | | | | |
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| 0 | | | 111111111 | | 111e+1 | | 1.11114 | ≥+11 +1 | 1.6500e+0 | 1 -3. | 4028e+38 | +9.9 | 902e+0 | 2 +2 . | 6630e+0 | 1 +6 | | | |
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| - | | | | | - and (b) | | | | and on a | · · · · | | | | | | | | | |

Beyond the scope of this presentation

Procedure will be changed

Explained in docs/pressure_input.md

Prerequisites on Hardware



Free space on Hard-drive: Per day approximately 2,4 GB

- 2 GB of Interferograms
- 100 MB of spectra
- 300 MB of `abscos.bin`-file
- RAM: pcxs20.exe needs the most memory: Approximately 700 MB per instance.

Closing words



First operational Version



Closing words



First operational Version

- If you have ideas or suggestions or you find a bug please contact us (benedikt.herkommer@kit.edu, lena.feld@kit.edu)!
- We can offer an installation workshop

Disclaimer

Preliminary correction factors \rightarrow not use for publications yet.



Backup

| 🤟 GitLab 🗏 Menu | | Sea | arch GitLab Q 📿 🗸 Sign i |
|---|---|--|---|
| P PROFFASTpylot | 📢 Dear GitLab Users, due to maintance w | ble for a few minutes between 20:00-20:30 CET on 20.01.2022. Wi ence. | |
| Project information Repository | coccon-kit > PROFFASTpylot | | |
| Issues In Merge requests | P PROFFASTpylo | 🛱 Star 🛛 0 | |
| Deployments Monitor Packages & Registries | - 🏕 184 Commits 🛛 🖓 2 Branches 🔗 | 🕈 O Tags 🗈 1.5 MB Files 🕞 1.5 MB Storage | |
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Available at https://gitlab.eudat.eu/coccon-kit/proffastpylot

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| | 🔒 LICENCE | 27 | | |
| | README.md | 28 | | |
| | 🗢 setup.pv | 29 | } | |
| | | | | |
| 0 | | 31 | <pre>def get_filename(self, pressure_type, date):</pre> | |
| \diamond | | 32 | """Return merged filename of pressure_type.""" | |
| ~~~ | | 33 | <pre>params = self.filename_parameters[pressure_type]</pre> | |
| ጚ፝ዸ፞፞ | | 34 | filename = "".join(| Research |
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| | × E | ile <u>E</u> dit <u>S</u> election <u>V</u> iew <u>G</u> o | <u>R</u> un <u>T</u> ermina | l <u>H</u> elp | pressure.py - proffastpylot - Visual | Studio Code | | × |
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| | ſЪ | EXPLORER ···· | 🥏 pressure. | ру 9+, М > | < | | ⊳~ \$] | |
| 1 | | V PROFFASTPYLOT | prfpylot > 4 | 🕹 pressure | .py > 😫 PressureParameters | | | |
| | Q | > docs > example | 11 12 | filenam | e_parameters = { | | | uhe Institute of Technology |
| | 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 | > prf > prf_venv ∨ prfpvlot ● | 13 14 15 | "lo | g": { "basename": "", "time_format": "%Y-%m-%d", | <u>R</u> un <u>T</u> erminal <u>H</u> e | elp HI | D_p_file_2022-01-01.csv - proffastpylot |
| | ₽ B | > _pycache_ > templates � _initpy | 16 17 18 19 | }, "НС | "ending": "*.dat" -style-pressure": { "basename": "HD_p_file_", | Pressure.py 9+ example > ■ HD 1 datetim | , M ■ D_p_file_202 me,pressur | □ HD_p_file_2022-01-01.csv X 2-01-01.csv re |
| | - - | create_inputfile.py download_example.py filemover.py | 20 21 22 23 | } | "time_format": "%Y-%m-%d", "ending": "*.csv" | 2 2022-01 3 2022-01 4 2022-01 5 | L-01T10:00 L-01T10:01 L-01T10:02 | 2:00,1024.00 2:00,1024.34 2:00,1024.15 |
| | A | ILSList.csv repare.py repare.py to pressure.pv reput | 24 25 26 | datafra | me_parameters = { g"• { | | | |
| | | protocology prfPylot.pg > prfPylot.egg-info > .gitignore £ LICENCE BEADMEmd | 27 28 29 30 31 | | "key_pressure": "BaroTHB40", "key_time": "UTCtime", "fmt_time": "%H:%M:%S", "csv_kwargs": { sep": "\t" | | | |
| | 8 | setup.py | 32 33 34 35 36 37 38 | "нс | }, -style-pressure": { "key_pressure": "pressure", "key_time": "datetime", "fmt_time": "%Y-%m-%dT%H:%M:%S "csv_kwargs": [] sep": ",] | 5 . . | | |
| | ŝ | > OUTLINE | 40 41 | | U | | | imate Research |
| | <u>۲</u> | 2 master* 😚 Python 385 64-bit (| nrf venv' venv) | ⊗ 25 A 3 | Git Graph In 38 Col 26 Sr | naces: 4 LITE-8 CRLE | F Python | serving Network |