

SFIT4 version 1.0

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many others of the NDACC-IRWG

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Changes since 0.9.4.4



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mathias@mini-mp: ~/Vortraege/NDACC_FTIR_2021/sfit4

```
3 43      ! number of isotope separation species (blocks), # VMR's
H2O       ! old name
1 4 2     ! old molec id and isotope id
HDO       ! new name
77 1 19,0 3 1,5 1. ! new molec id, isotope id, mass, mode, tdep, intensity scale
2724,1, 1403,1, 3707,1 ! band center, degen 47 ! number of
H2O       ! old name - Add as second HDO isotope
1 5 2     ! old molec id and isotope id
HDO       ! new name
77 2 21,0 0 1,5 1. ! new molec id, isotope id, mass, mode, tdep, intensity scale
H2O       ! old name - Add as third HDO isotope
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(END)
```



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```
gas.layers = 47
gas.profile.list = CH4
gas.profile.CH4.correlation = T
gas.profile.CH4.correlation.type = 6
gas.profile.CH4.correlation.lambda = 10000.0
gas.profile.CH4.scale = 1.0
gas.profile.CH4.sigma = 1.000000 1.000000 1.000000 1.000000 1.000000 1
1.000000 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000
0 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000
00 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000
000000 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000
0000 1.000000 1.000000 1.000000 1.000000
:|
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- ▶ Error calculation for arbitrary ILS



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Download and installation



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- ▶ <https://wiki.ucar.edu/display/sfit4/> -> SFIT 4 Version 1.0. Release
 - ▶ `sfit-core-code`



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test_cases_NDACC	examples of setups for NDACC retrieval species



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Preferably use provided tools and templates.



The lineshapes



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1. Voigt lineshape (original routine since the beginning of sfit4)



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`fw.linemixing` 1st order Linemixing calculated if line parameters given.



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`create_refprofile` creates a valid reference profile for `sfit4` version 1 from default data and data from the WACCM run. Note some the names and numbers of the molecules have changed in between SFIT4 versions 0.9.4.4 to 1.0.



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`create_testcase` creates a testcases from a running directory. Reads all the files needed for running `hbin` and `sfit4` and packs them into in tarball `release.tgz`. This can be sent to the maintainers along with description of the problem.



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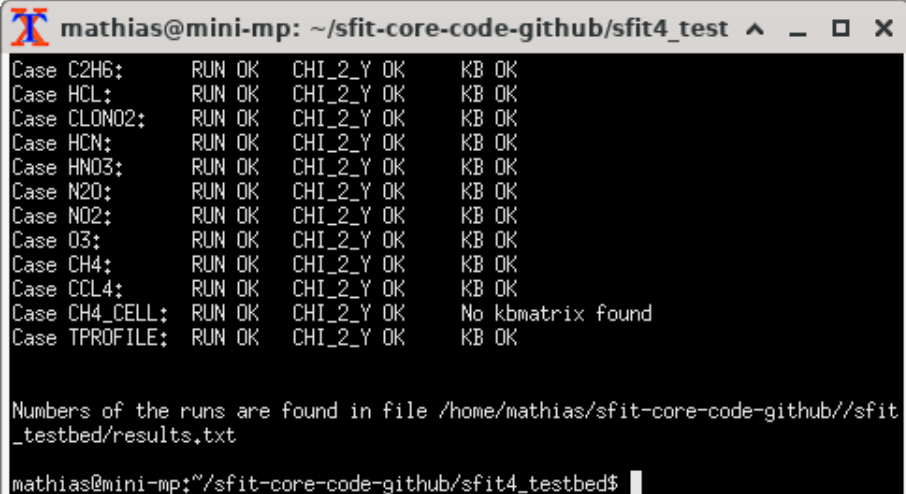
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sfit4 testbed

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A terminal window titled "mathias@mini-mp: ~/sfit-core-code-github/sfit4_test" displays the output of a test suite. The output lists 13 test cases, each with four columns of results: the case name, the execution status (all "RUN OK"), the chemical formula (all "CHI_2_Y OK"), and the basis set (all "KB OK" except for "CH4_CELL" which is "No kbmatrix found"). Below the list, a message states: "Numbers of the runs are found in file /home/mathias/sfit-core-code-github//sfit_testbed/results.txt". The prompt at the bottom is "mathias@mini-mp:~/sfit-core-code-github/sfit4_testbed\$".

```
mathias@mini-mp: ~/sfit-core-code-github/sfit4_test ^ _ □ X
Case C2H6:      RUN OK   CHI_2_Y OK   KB OK
Case HCL:      RUN OK   CHI_2_Y OK   KB OK
Case CLONO2:   RUN OK   CHI_2_Y OK   KB OK
Case HCN:      RUN OK   CHI_2_Y OK   KB OK
Case HNO3:     RUN OK   CHI_2_Y OK   KB OK
Case N2O:      RUN OK   CHI_2_Y OK   KB OK
Case NO2:      RUN OK   CHI_2_Y OK   KB OK
Case O3:       RUN OK   CHI_2_Y OK   KB OK
Case CH4:      RUN OK   CHI_2_Y OK   KB OK
Case CCL4:     RUN OK   CHI_2_Y OK   KB OK
Case CH4_CELL: RUN OK   CHI_2_Y OK   No kbmatrix found
Case TPROFILE: RUN OK   CHI_2_Y OK   KB OK

Numbers of the runs are found in file /home/mathias/sfit-core-code-github//sfit
_testbed/results.txt

mathias@mini-mp:~/sfit-core-code-github/sfit4_testbed$
```

sfit4 testbed

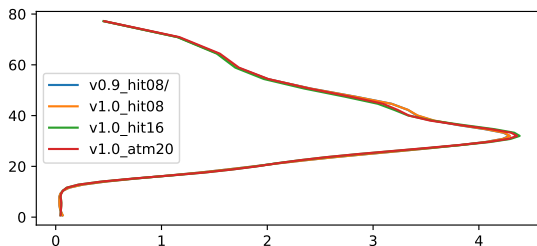
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 - ▶ after upgrade of computer system
 - ▶ if code does not work
 - ▶ after code modifications
- ▶ all output should be ok.
- ▶ More detailed output can be found in results.txt



Comparisons

Ozone

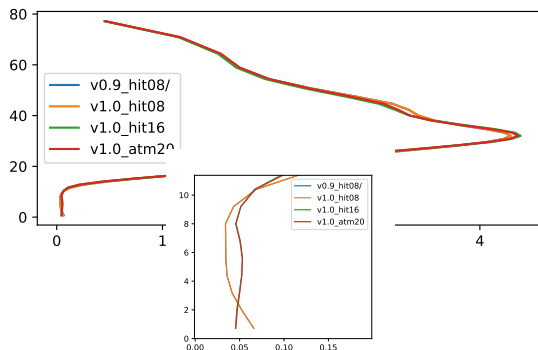
v0.9_hit08	Chi_2: 2.745835	DOFS: 6.316
v1.0_hit08	Chi_2: 2.745693	DOFS: 6.315
v1.0_hit16	Chi_2: 2.561871	DOFS: 6.319
v1.0_atm20	Chi_2: 2.382878	DOFS: 6.32



Comparisons

Ozone

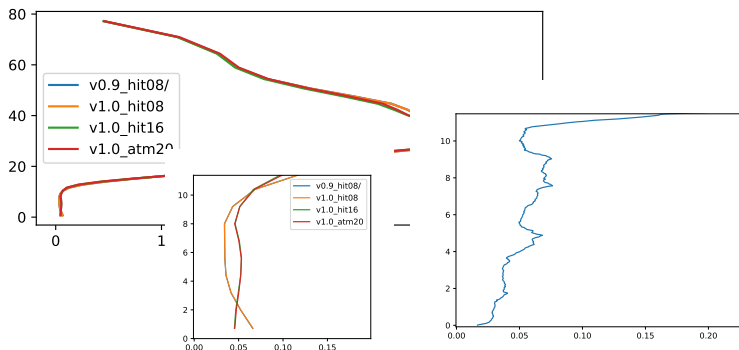
v0.9_hit08	Chi_2: 2.745835	DOFS: 6.316
v1.0_hit08	Chi_2: 2.745693	DOFS: 6.315
v1.0_hit16	Chi_2: 2.561871	DOFS: 6.319
v1.0_atm20	Chi_2: 2.382878	DOFS: 6.32



Comparisons

Ozone

v0.9_hit08	Chi_2: 2.745835	DOFS: 6.316
v1.0_hit08	Chi_2: 2.745693	DOFS: 6.315
v1.0_hit16	Chi_2: 2.561871	DOFS: 6.319
v1.0_atm20	Chi_2: 2.382878	DOFS: 6.32

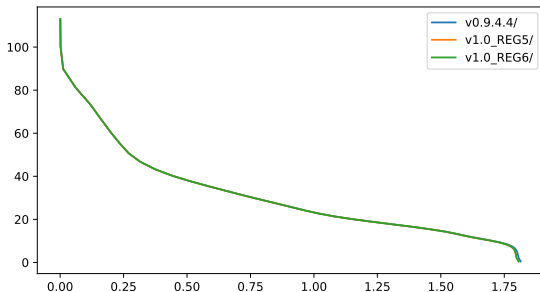


Comparisons

Methan

Comparison of TP regularisation with smoothness constraint internally calculated (profile.gas.regmethod=6) versus input of S_a^{-1} matrix (profile.gas.regmethod=5)

	χ^2	DOFS	COL (10^{19} molec/ cm^2)
v0.9_hit08	0.852044	1.691	3.52770
v1.0_REG5_hit08	0.859529	1.692	3.51423
v1.0_REG6_hit08	0.859537	1.688	3.51424

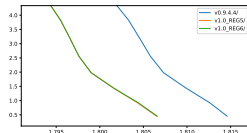
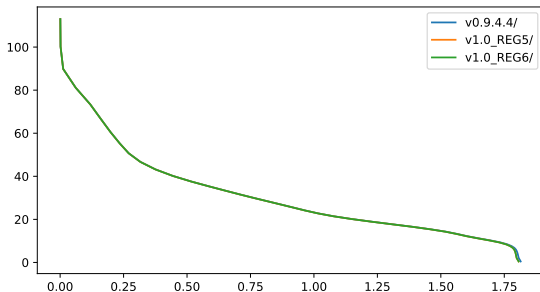


Comparisons

Methan

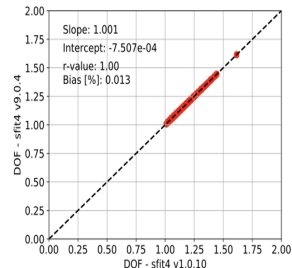
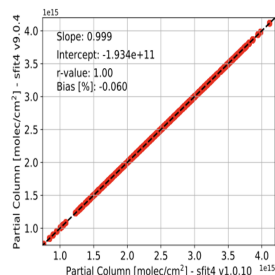
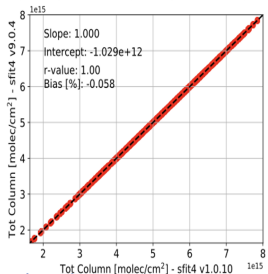
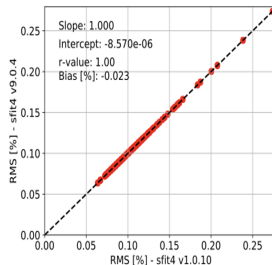
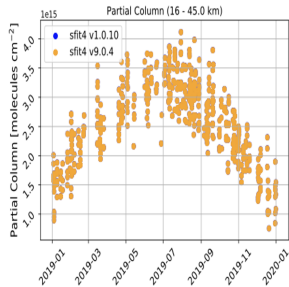
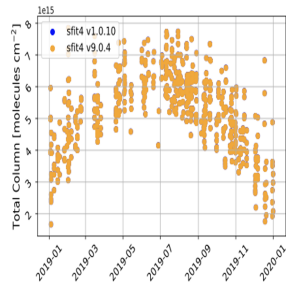
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NO₂

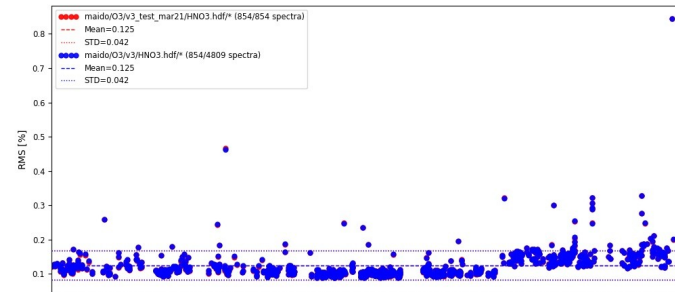
Is there a difference between sfit4 v1.010 and v9.04? No



Case study old vs new HNO_3

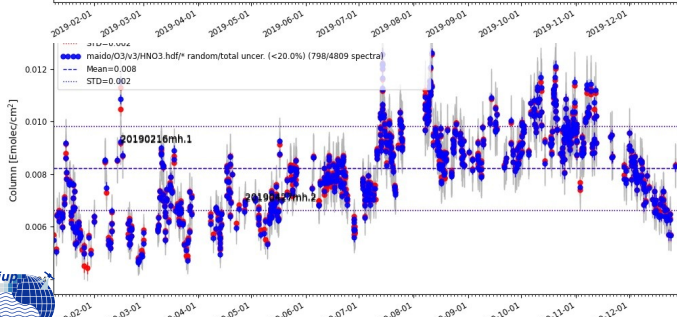
HNO_3 RMS of retrievals

(filter: mtime>=(2019,1,1))



► blue is old
 □ red is new

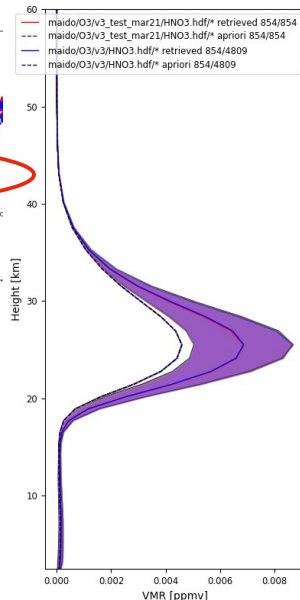
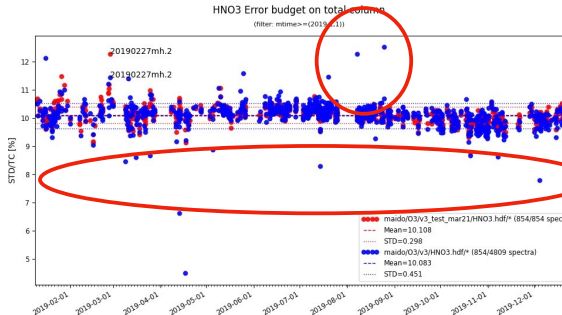
□ red tested with
 a slightly
 stronger
 regularisation





Case study old vs new HNO_3

Mean and STD retrieved HNO_3 profiles



- rms, tc, profiles unchanged
- less scatter in uncertainties (temp fix?)



sfit4 not working?



sfrit4 not working?

- ▶ code is working well? Use `sfrit_testbed` to check again.



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- ▶ Check `sfit4.dtl`



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Miscellaneous and Outlook

- ▶ parallelisation of sfit4 itself not foreseen



Miscellaneous and Outlook

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- ▶ Outlook: inclusion of continua in the thermal infrared



Miscellaneous and Outlook

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- ▶ Outlook: inclusion of continua in the thermal infrared

Thanks for your attention



- [Gal61] Louis Galatry. Simultaneous Effect of Doppler and Foreign Gas Broadening on Spectral Lines. *Phys. Rev.*, 122(4), 1961.
- [TNH13] H. Tran, N.H. Ngo, and J.-M. Hartmann. Efficient computation of some speed-dependent isolated line profiles. *Journal of Quantitative Spectroscopy and Radiative Transfer*, (0):—, 2013.

