

SFIT4 version 1.0

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many others of the NDACC-IRWG

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NDACC (Online), June 2021



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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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```
mathias@mini-mp: ~/Vortraege/NDACC_FTIR_2021/sfit4
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 1.000000 1.000000 1.000000
1.000000 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 1.000000
00 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000 1.000000
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- ▶ Error calculation for arbitrary ILS



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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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 - `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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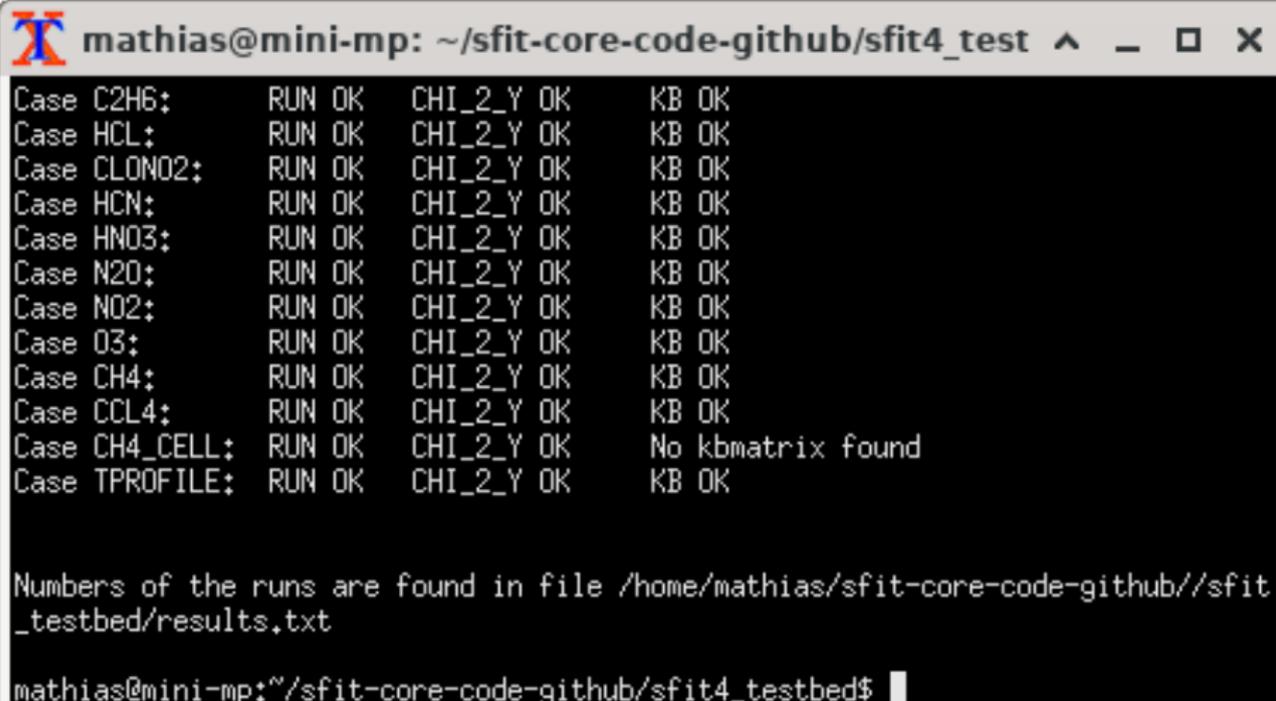
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sfit4 testbed

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```
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

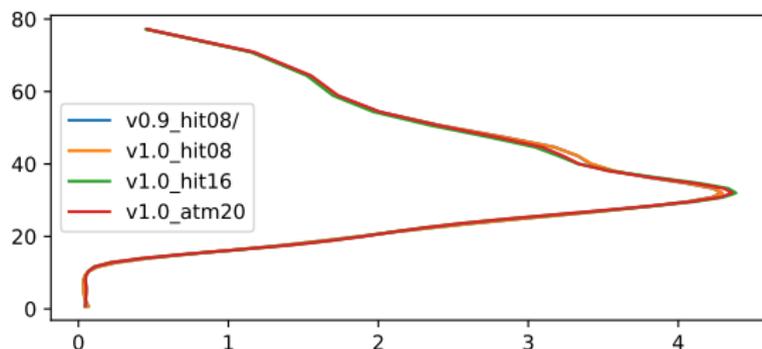
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 - ▶ after upgrade of computer system
 - ▶ if code does not work
 - ▶ after code modifications
- ▶ all output should be ok.
- ▶ More detailed output can be found in results.txt



Comparisons

Ozone

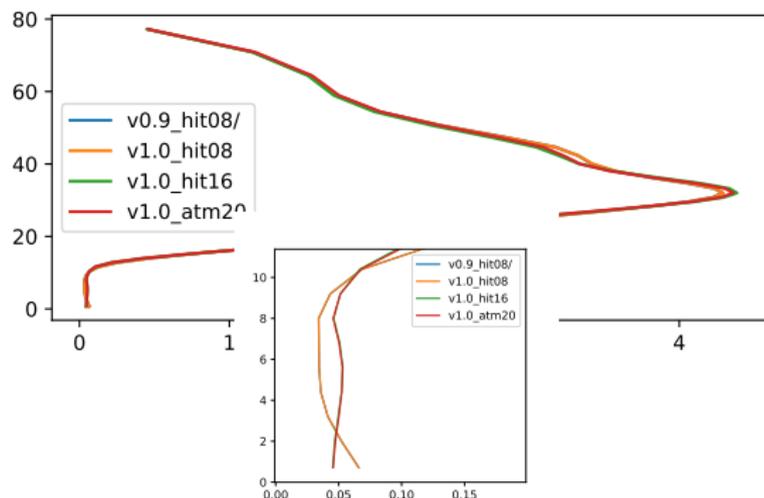
v0.9_hit08	Chi_2: 2.745835	DOFS: 6.316
v1.0_hit08	Chi_2: 2.745693	DOFS: 6.315
v1.0_hit16	Chi_2: 2.561871	DOFS: 6.319
v1.0_atm20	Chi_2: 2.382878	DOFS: 6.32



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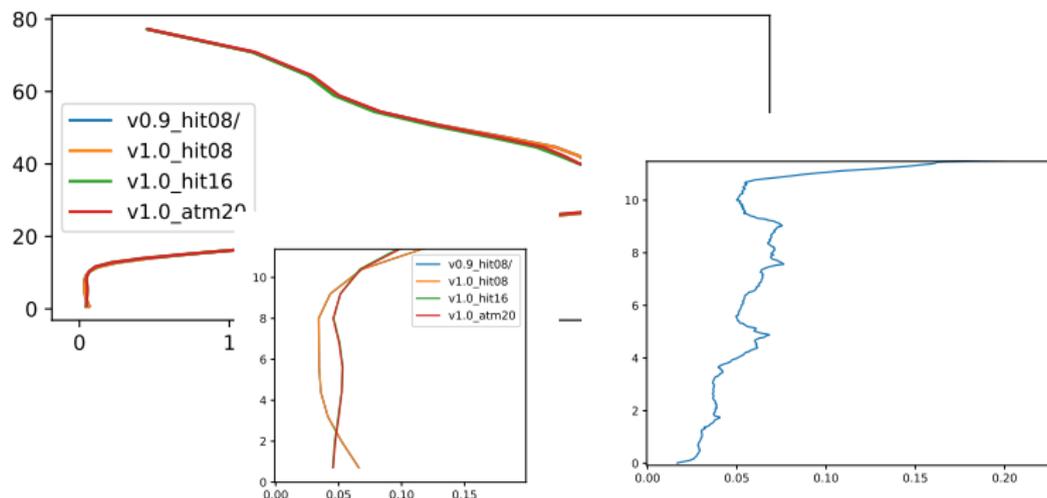
v0.9_hit08	Chi_2: 2.745835	DOFS: 6.316
v1.0_hit08	Chi_2: 2.745693	DOFS: 6.315
v1.0_hit16	Chi_2: 2.561871	DOFS: 6.319
v1.0_atm20	Chi_2: 2.382878	DOFS: 6.32



Comparisons

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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

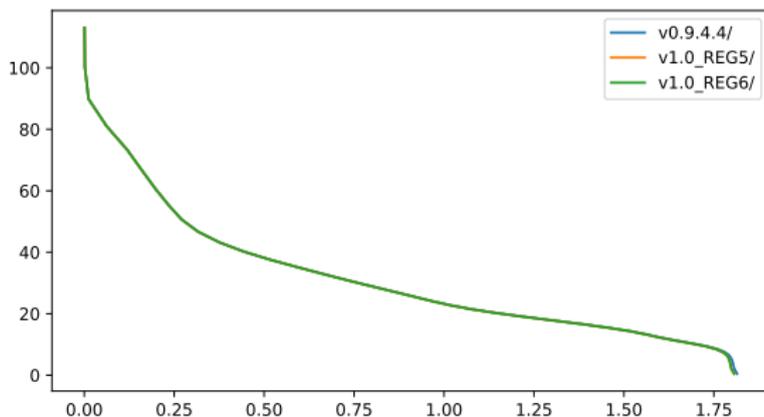


Comparisons

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

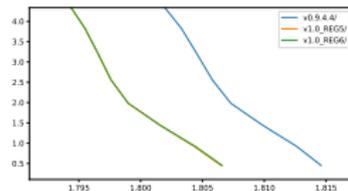
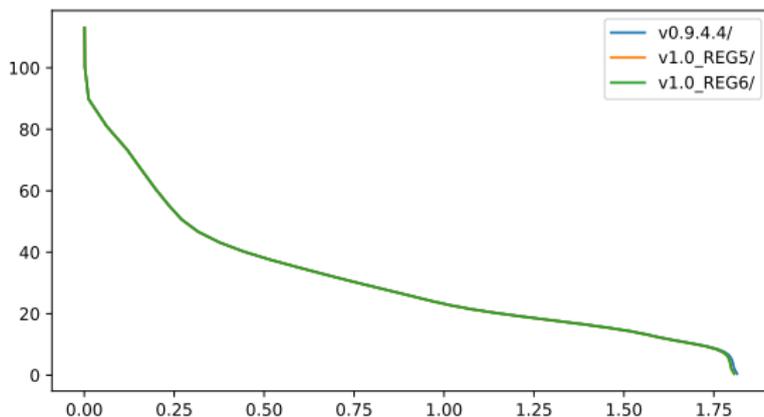


Comparisons

Methan

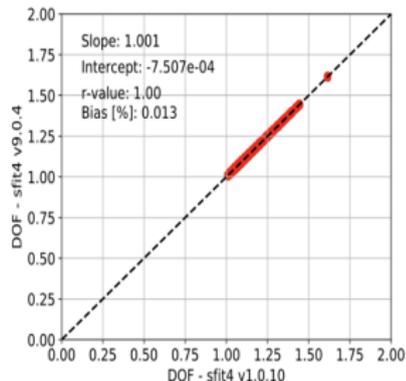
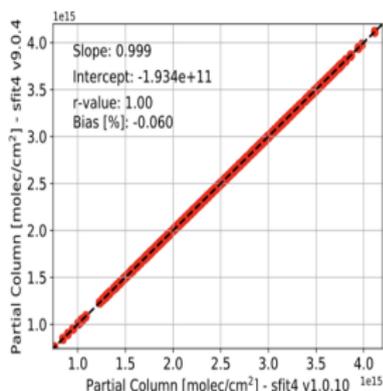
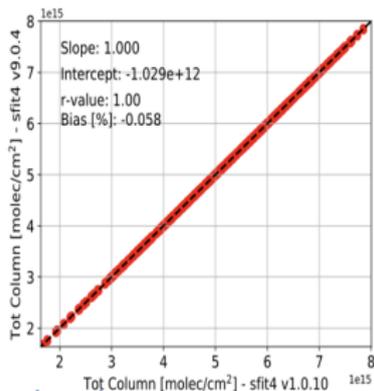
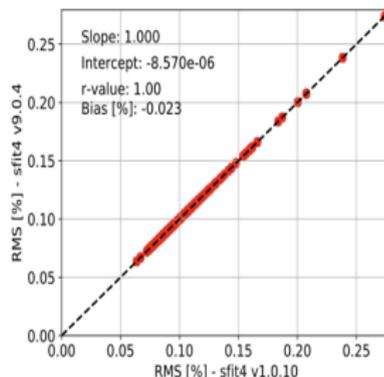
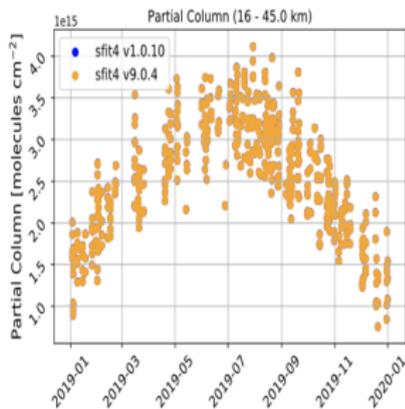
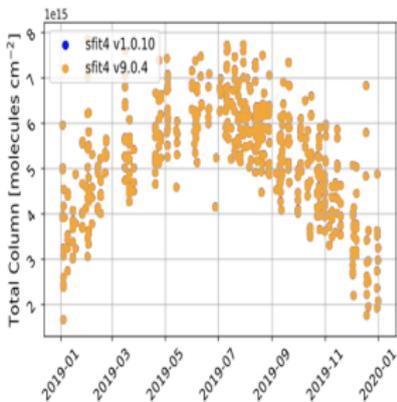
Comparison of TP regularisation with smoothness constraint internally calculated (profile.gas.regmethod=6) versus input of S_a^{-1} matrix (profile.gas.regmethod=5)

	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



NO₂

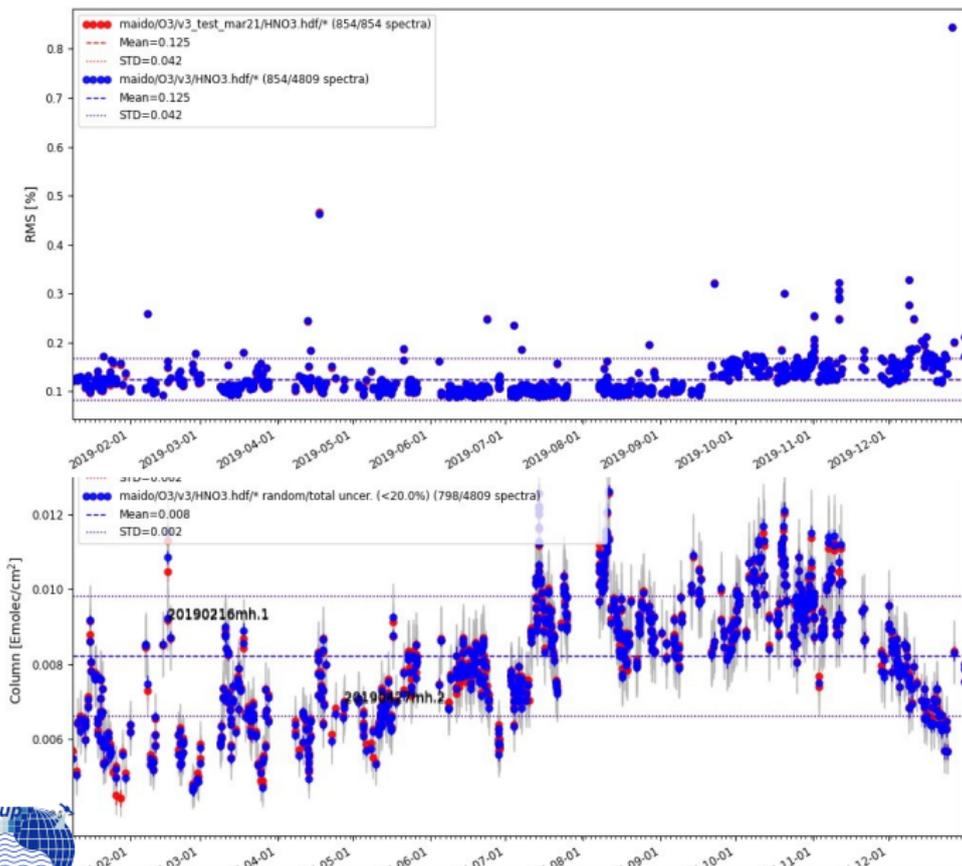
Is there a difference between sfit4 v1.010 and v9.04? No



Case study old vs new HNO₃

HNO₃ RMS of retrievals

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



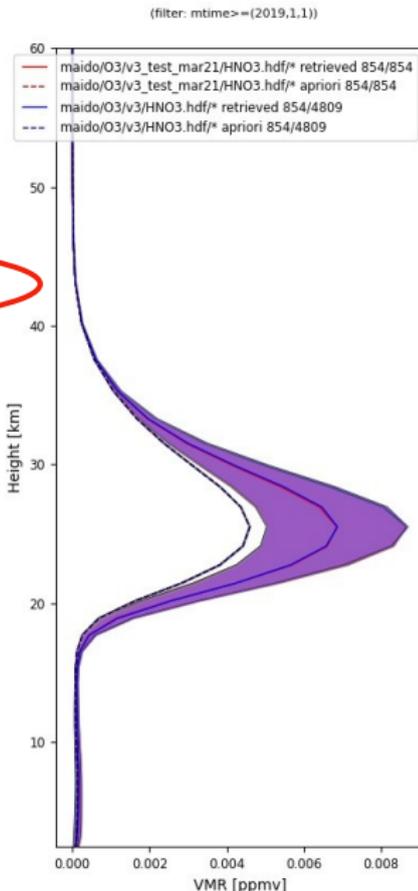
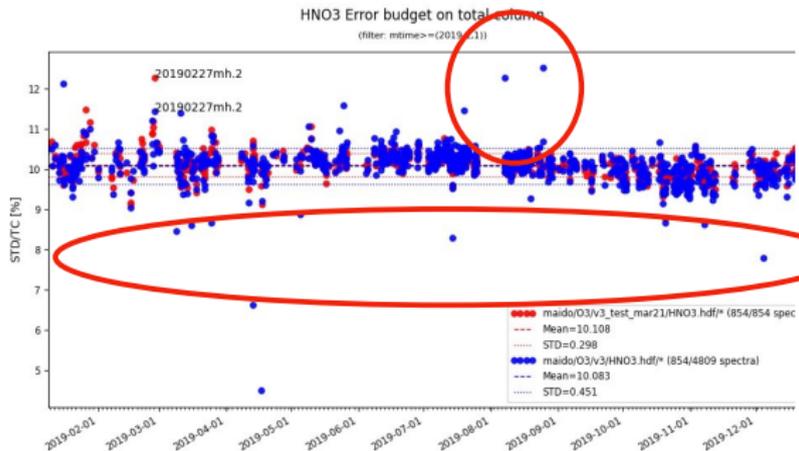
► blue is old
 □ red is new

□ red tested with a slightly stronger regularisation



Case study old vs new HNO₃

Mean and STD retrieved HNO₃ profiles



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



sfit4 not working?



sfit4 not working?

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



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- ▶ Check `sfit4.dtl`



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- ▶ Check the input files



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- ▶ Create a testcase using python3
`tools/create_testcase/Create_testcase_repository.py`



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Miscellaneous and Outlook

- ▶ parallelisation of sfit4 itself not foreseen



Miscellaneous and Outlook

- ▶ parallelisation of sfit4 itself not foreseen
- ▶ 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.

