# NWP SAF

# NWPSAF 1D-Var v1.2 Release Note

Version 1.2

21st May 2020

# NWP SAF 1D-Var Release Note

This documentation was developed within the context of the EUMETSAT Satellite Application Facility on Numerical Weather Prediction (NWP SAF), under the Cooperation Agreement dated 7 December 2016, between EUMETSAT and the Met Office, UK, by one or more partners within the NWP SAF. The partners in the NWP SAF are the Met Office, ECMWF, DWD and Meteo France.



| Change record | | | |
|---|---|---|---|
| Version | Date | Author/changed by | Remarks |
| 0.1 | 17/02/14 | P. Weston | First version, based on Met Office 1D-Var v3.5 release note |
| 0.2 | 21/05/14 | P. Weston | Modified after testing of NWPSAF 1D-Var v1.0 beta |
| 0.3 | 29/05/14 | P. Weston | Updated with new header, new document ID, new copyright statement and changed font following comments from B. Conway |
| 1.0 | 22/08/14 | P. Weston | Version valid for NWPSAF 1D-Var v1.0 |
| 1.1 | 21/02/17 | F. Smith | Version valid for NWPSAF 1D-Var v1.1 |
| 1.1.1 | 22/06/18 | S. Havemann | Version valid for NWPSAF 1D-Var v1.1.1. Updated following a bug fix in the liquid water path calculation and further updated following comments from Simon Keogh (moved the changes from 1.0 to 1.1 into a new section 4 to contain a change history). |
| 1.2 | 21/05/20 | S.Havemann | Version valid for NWPSAF 1D-Var v1.2 Updated following the addition of functionality to retrieve surface emissivity. |

**NWPSAF software made available to registered users via the "software downloads" section of the NWP web site (linked from the top bar of http://nwp-saf.eumetsat.int or https://www.nwpsaf.eu/site/). To use this software, users need to have registered for 1D-Var v.1.2 with the NWP SAF, and to have agreed to the terms of the license agreement.**

## 1. Files provided with this release

The NWPSAF 1D-Var code is distributed in the tar file
`NWPSAF_1DVar_v1.2.tar.gz`

This file contains two subdirectories. The program and the files required by it are contained in the `1DVar/` folder. The documentation (including this document) is contained in the `docs/` folder.

Additional background information on the package may be found in
`docs/nwpsaf-mo-ds-026_top_level_design.pdf` and
`docs/nwpsaf-mo-ds-025_product_specification.pdf`.

The main user manual is
`docs/nwpsaf-mo-ud-032_NWPSAF_1DVar_Manual.html`
also supplied as
`docs/nwpsaf-mo-ud-032_NWPSAF_1DVar_Manual.pdf`

Important information and instructions for installation are also in `1DVar/readme.txt` .

## 2. What has changed at this release (version 1.2.)

**Version 1.2 of the NWPSAF 1D-Var package adds the new capability to retrieve surface emissivity for the first time. The surface emissivity is represented by principal components in the retrieval state vector. This allows a compact representation of the surface emissivity and keeps the number of additional state vector elements low. The new capability is applied to IASI.**

**An example case of the surface emissivity retrieval has been constructed and all the required files to run this case are part of the package. The example case has also been used in extensive compiler testing and the output files from those test runs are included in the package as well. All the details of the example case and the testing are presented in an Appendix and the end of this document.**

The following files have been added at version 1.2:

```
1DVar/IASI_COEFFS_DIR/:
ChannelChoice_surf_emiss.dat Rmatrix_surf_emiss

1DVar/Sample_Namelists/:
Retrieval_IASI_SURFEMISS_54L.NL
1DVar/Sample_ObsFiles/:
```

```
ObsFile_IASI_SURFEMISS.dat

1DVar/Sample_Output_Surfemiss/:
IASI_SURFEMISS_54L_gfortran485/ IASI_SURFEMISS_54L_gfortran64/ IASI_SURFEMISS_54L_gfortran73/
IASI_SURFEMISS_54L_gfortran81/  IASI_SURFEMISS_54L_ifort16/    IASI_SURFEMISS_54L_ifort17/
IASI_SURFEMISS_54L_ifort18/     IASI_SURFEMISS_54L_ifort19/    IASI_SURFEMISS_54L_nagfor61/
IASI_SURFEMISS_54L_nagfor62/    IASI_SURFEMISS_54L_pgf9016/    IASI_SUREFMISS_54L_pgf9018/
The above directories all contain:
A-matrix.out  AveragingKernel.out  Minimisation.log    ProfileQC.dat   Retrieved_BTs.dat
Am-matrix.out BgJacobian.out       Minimisation_BT.log RetJacobian.out Retrieved_Profiles.dat

1DVar/WorkDir/:
Run_1DVar_SurfEmiss.ksh

1DVar/Sample_Surfemiss/:
EmisEigenVec, EmisPCAtlas

1DVar/include/:
NWPSAF_Read_EmisEigenVec.interface, NWPSAF_Read_EmisPCAtlas.interface


1DVar/src/main/:
NWPSAF_Read_EmisEigenVec.f90, NWPSAF_Read_EmisPCAtlas.f90
```

## The following files have been changed at version 1.2:

```
1DVar/:
readme.txt


docs:

NWPSAF_1DVar_User_Manual.pdf, nwpsaf-mo-ds-025_product_specification.pdf, nwpsaf-mo-ds-
026_top_level_design.pdf, nwpsaf-mo-ud-031_release_note.pdf, nwpsaf-mo-ud-
032_NWPSAF_1DVar_Manual.html

1DVar/src/main/:
NWPSAFMod_ObsInfo.f90, NWPSAFMod_Params.f90, NWPSAFMod_RTmodel.f90, NWPSAF_Pr1DVar_Driver.f90,
NWPSAF_CheckIteration.f90, NWPSAF_DeAllocate.f90, NWPSAF_InitBmatrix.f90, NWPSAF_ProcessData.f90,
NWPSAF_RTTOV11_GetHMatrix.f90, NWPSAF_RTTOV_Interface.f90, NWPSAF_RTTOV12_GetHMatrix.f90,
NWPSAF_RTTOV12_Interface.f90, NWPSAF_RTTOV_Initialise.f90, NWPSAF_Read_Background.f90,
NWPSAF_SetUpBackground.f90, NWPSAF_SetUpRetrievals.f90, NWPSAF_TranslateDataIn.f90,
NWPSAF_TranslateDataOut.f90
```

Previous versions contained a `Release_Information.txt` file. Such a file has been omitted at this release as the same information is contained in `nwpsaf-mo-ud-031_release_note.pdf`

## The version 1.2 has been tested with the following compilers:

```
ifort 16.0.1
ifort 17.0.1
ifort 18.0.3
ifort 19.0.3
gfortran 4.8.5
gfortran 6.4.0
gfortran 7.3.0
gfortran 8.1.0
nagfor 6.1
nagfor 6.2
pgf90 16.10
pgf90 18.7

An issue has been found with the Portlsnd Fortran Compiler, versions 16.10
and 18.7. The code compiles without problems, but at runtime the arrays
profiles and profiles_k_pc in the routines NWPSAF_RTTOV11_Interface.f90
and NWPSAF_RTTOV12_Interface.f90 are not dimensioned correctly.
This reason for this does not seem to be erroneous source code.
```

```
To support users of the Portland Fortran Compiler, modified versions
of the two interface routines have been added to the package which
work fine with the Portland Fortran Compiler. These routines are
NWPSAF_RTTOV11_Interface_change_for_pgf90.f90 and
NWPSAF_RTTOV11_Interface_change_for_pgf90.f90, respectively.
```

## 3. Full package listing

```
.:
1DVar/  docs/

1DVar/:
AIRS_COEFFS_DIR/          IASI_COEFFS_DIR_RAD/                Sample_Output_RTTOV12/
ATMS_COEFFS_DIR/                                              WorkDir/
ATOVS_CLOUDY_COEFFS_DIR/  SSMIS_COEFFS_DIR/                   build/
ATOVS_COEFFS_DIR/         Sample_Background/                  include/
CrIS_COEFFS_DIR/          Sample_Bmatrices/                   output/
IASI_COEFFS_DIR/          Sample_Namelists/                   readme.txt
IASI_COEFFS_DIR_BT/       Sample_ObsFiles/                    src/
IASI_COEFFS_DIR_PC/       Sample_Output_RTTOV11/

The following directories contain files of the same name:
1DVar/AIRS_COEFFS_DIR/
1DVar/ATMS_COEFFS_DIR/
1DVar/ATOVS_CLOUDY_COEFFS_DIR/
1DVar/ATOVS_COEFFS_DIR/
1DVar/CrIS_COEFFS_DIR/
1DVar/SSMIS_COEFFS_DIR/
Each contains:
ChannelChoice_orig.dat   Rmatrix_orig

1DVar/IASI_COEFFS_DIR:
ChannelChoice_orig.dat ChannelChoice_surf_emiss.dat Rmatrix_orig Rmatrix_surf_emiss

1DVar/IASI_COEFFS_DIR_BT/:
Rmatrix_8461_instPCRTTOV_plusRT.out  meto1dvar_ch8461
Rmatrix_8461_instnoise_PCRTTOV.out   meto1dvar_ch8461_314

1DVar/IASI_COEFFS_DIR_PC/:
ChannelChoice_200.dat  Rmatrix_identity_200.dat
ChannelChoice_400.dat  Rmatrix_identity_400.dat

1DVar/IASI_COEFFS_DIR_RAD/:
Rmatrix_8461_instnoise_PCRTTOV.out  meto1dvar_ch8461  meto1dvar_ch8461_314
Sample_Background/:
BACKGROUND_43L.dat  BACKGROUND_54L.dat   BACKGROUND_with_CLW.dat  truth_51L.dat      truth_70L.dat
BACKGROUND_51L.dat  BACKGROUND_70L.dat   truth_43L.dat            truth_54L.dat

1DVar/Sample_Bmatrices/:
Bmatrix_43L  Bmatrix_51L  Bmatrix_54L  Bmatrix_70L

1DVar/Sample_Namelists/:
ControlData_AIRS.NL           Retrieval_AIRS_43L.NL           Retrieval_CrIS_43L.NL
ControlData_ATMS.NL           Retrieval_AIRS_51L.NL           Retrieval_CrIS_51L.NL
ControlData_ATOVS.NL          Retrieval_AIRS_54L.NL           Retrieval_CrIS_54L.NL
ControlData_ATOVS_CLOUDY.NL   Retrieval_ATMS_43L.NL           Retrieval_IASI_43L.NL
ControlData_CrIS.NL           Retrieval_ATMS_51L.NL           Retrieval_IASI_51L.NL
ControlData_IASI.NL           Retrieval_ATMS_54L.NL           Retrieval_IASI_54L.NL
ControlData_IASI_CLOUDY.NL    Retrieval_ATOVS_43L.NL          Retrieval_IASI_CLOUDY_43L.NL
ControlData_IASI_RAD.NL       Retrieval_ATOVS_51L.NL          Retrieval_IASI_CLOUDY_51L.NL
ControlData_PC.NL             Retrieval_ATOVS_54L.NL          Retrieval_IASI_CLOUDY_54L.NL
ControlData_SSMIS.NL          Retrieval_ATOVS_CLOUDY_43L.NL   Retrievel_IASI_SURFEMISS_54L.NL
ControlData_emis_IASI.NL      Retrieval_ATOVS_CLOUDY_51L.NL    Retrieval_SSMIS_43L.NL
Retrieval_70L_nosurf.NL       Retrieval_ATOVS_CLOUDY_54L.NL

1DVar/Sample_ObsFiles/:
ObsFile_AIRS.dat  ObsFile_ATOVS.dat          ObsFile_CrIS.dat  ObsFile_SSMIS.dat
ObsFile_ATMS.dat  ObsFile_ATOVS_CLOUDY.dat   ObsFile_IASI.dat  ObsFile_IASI_SURFEMISS.dat
Sim_RTTOV11/      Sim_RTTOV12/
```

```
1DVar/Sample_ObsFiles/Sim_RTTOV11/ and 1DVar/Sample_ObsFiles/Sim_RTTOV11/:
70L_200_PC.dat              70L_8461_RAD.dat              70L_8461_RRFromPCFromRR_truth.dat
70L_200_PCFromBT.dat        70L_8461_RBT.dat              70L_8461_RR_truth.dat
70L_200_PCFromRR_truth.dat  70L_8461_RBTFromPCFromBT.dat
70L_8461_BT.dat             70L_8461_RR.dat

1DVar/Sample_Output_RTTOV11/ and 1DVar/Sample_Output_RTTOV12/:
gfortran_4.4.7/   ifort_12.0/

1DVar/Sample_Output_RTTOVxx/gfortran_4.4.7/ and 1DVar/Sample_Output_RTTOVxx/ifort_12.0/:
AIRS_43L/  ATMS_54L/   ATOVS_CLOUDY_43L/  CrIS_54L/  IASI_70L_PC/      SSMIS_43L/
AIRS_54L/  ATOVS_43L/  ATOVS_CLOUDY_54L/  IASI_43L/  IASI_CLOUDY_43L/
ATMS_43L/  ATOVS_54L/  CrIS_43L/          IASI_54L/  IASI_CLOUDY_54L/
The above directories all contain:
Minimisation.log     ProfileQC.dat          Retrieved_Profiles.dat
Minimisation_BT.log  Retrieved_BTs.dat

1DVar/Sample_Output_Surfemiss/:
IASI_SURFEMISS_54L_gfortran485/ IASI_SURFEMISS_54L_gfortran64/ IASI_SURFEMISS_54L_gfortran73/
IASI_SURFEMISS_54L_gfortran81/  IASI_SURFEMISS_54L_ifort16/    IASI_SURFEMISS_54L_ifort17/
IASI_SURFEMISS_54L_ifort18/     IASI_SURFEMISS_54L_ifort19/    IASI_SURFEMISS_54L_nagfor61/
IASI_SURFEMISS_54L_nagfor62/    IASI_SURFEMISS_54L_pgf9016/    IASI_SUREFMISS_54L_pgf9018/
The above directories all contain:
A-matrix.out  AveragingKernel.out  Minimisation.log    ProfileQC.dat   Retrieved_BTs.dat
Am-matrix.out BgJacobian.out       Minimisation_BT.log RetJacobian.out Retrieved_Profiles.dat

1DVar/Sample_Surfemiss/:
EmisEigenVec         EmisPCAtlas

1DVar/WorkDir/:
Run_1DVar.ksh      Run_1DVar_Rad.ksh        Run_Convert.ksh
Run_1DVar_PC.ksh   Run_1DVar_test.ksh       Run_SimSpec.ksh
Run_1DVar_SurfEmiss.ksh

1DVar/build:/
makefile

1DVar/include:/
NWPSAF_1DVar.interface                        NWPSAF_OpenFile.interface
NWPSAF_AdditionalCost_Cloud.interface         NWPSAF_ProcessData.interface
NWPSAF_BandInverse.interface                  NWPSAF_QSAT.interface
NWPSAF_BandMultiply.interface                 NWPSAF_Qtot_to_q_ql.interface
NWPSAF_CO2Slice.interface                     NWPSAF_RMatrix_ChanSelect.interface
NWPSAF_Calculate_Cost_Function.interface      NWPSAF_RTTOV11_Allocate.interface
NWPSAF_Channellist.interface                  NWPSAF_RTTOV11_GetHMatrix.interface
NWPSAF_CheckIteration.interface               NWPSAF_RTTOV11_Interface.interface
NWPSAF_Check_Temperatures.interface           NWPSAF_RTTOV12_Allocate.interface
NWPSAF_Cholesky.interface                     NWPSAF_RTTOV12_GetHMatrix.interface
NWPSAF_CloudCost.interface                    NWPSAF_RTTOV12_Interface.interface
NWPSAF_CloudStructure.interface               NWPSAF_RTTOV_Initialise.interface
NWPSAF_CloudyOrNot.interface                  NWPSAF_ReadHeaders.interface
NWPSAF_DeAllocate.interface                   NWPSAF_Read_Background.interface
NWPSAF_Fastmodel_Interface.interface          NWPSAF_Read_ControlData.interface
NWPSAF_FreeUnit.interface                     NWPSAF_Read_Observations.interface
NWPSAF_GetUnit.interface                      NWPSAF_Report.interface
NWPSAF_InitBmatrix.interface                  NWPSAF_SatMatInv.interface
NWPSAF_InitRmatrix.interface                  NWPSAF_SetUpBackground.interface
NWPSAF_Initialise.interface                   NWPSAF_SetUpRetrievals.interface
NWPSAF_IntegerSort.interface                  NWPSAF_StratosExtrap.interface
NWPSAF_Minimize.interface                     NWPSAF_TranslateDataIn.interface
NWPSAF_Minimize_100.interface                 NWPSAF_TranslateDataOut.interface
NWPSAF_Minimize_100ML.interface               NWPSAF_svp.interface
NWPSAF_Minimize_101.interface                 NWPSAF_svp_deriv.interface
NWPSAF_Read_EmisEigenVec.interface            NWPSAF_Read_EmisPCAtlas.interface

1DVar/src/:
main/  sim_spec/
1DVar/src/main/:
NWPSAFMod_Channellist.f90                     NWPSAF_IntegerSort.f90
NWPSAFMod_Constants.f90                       NWPSAF_Minimize.f90
```

```
NWPSAFMod_CovarianceMatrices.f90              NWPSAF_Minimize_100.f90
NWPSAFMod_LiquidWater.f90                     NWPSAF_Minimize_100ML.f90
NWPSAFMod_ObsInfo.f90                         NWPSAF_Minimize_101.f90
NWPSAFMod_Params.f90                          NWPSAF_OpenFile.f90
NWPSAFMod_RTmodel.f90                         NWPSAF_ProcessData.f90
NWPSAF_1DVar.f90                              NWPSAF_QSAT.f90
NWPSAF_1DVar_Driver.f90                       NWPSAF_Qtot_to_q_ql.f90
NWPSAF_AdditionalCost_Cloud.f90               NWPSAF_RMatrix_ChanSelect.f90
NWPSAF_BandInverse.f90                        NWPSAF_RTTOV11_Allocate.f90
NWPSAF_BandMultiply.f90                       NWPSAF_RTTOV11_GetHMatrix.f90
NWPSAF_CO2Slice.f90                           NWPSAF_RTTOV11_Interface.f90
NWPSAF_Calculate_Cost_Function.f90            NWPSAF_RTTOV12_Allocate.f90
NWPSAF_Channellist.f90                        NWPSAF_RTTOV12_GetHMatrix.f90
NWPSAF_CheckIteration.f90                     NWPSAF_RTTOV12_Interface.f90
NWPSAF_Check_Temperatures.f90                 NWPSAF_RTTOV_Initialise.f90
NWPSAF_Cholesky.f90                           NWPSAF_ReadHeaders.f90
NWPSAF_CloudCost.f90                          NWPSAF_Read_Background.f90
NWPSAF_CloudStructure.f90                     NWPSAF_Read_ControlData.f90
NWPSAF_CloudyOrNot.f90                        NWPSAF_Read_Observations.f90
NWPSAF_DeAllocate.f90                         NWPSAF_Report.f90
NWPSAF_Fastmodel_Interface.f90                NWPSAF_SatMatInv.f90
NWPSAF_FreeUnit.f90                           NWPSAF_SetUpBackground.f90
NWPSAF_GetUnit.f90                            NWPSAF_SetUpRetrievals.f90
NWPSAF_InitBmatrix.f90                        NWPSAF_StratosExtrap.f90
NWPSAF_InitRmatrix.f90                        NWPSAF_TranslateDataIn.f90
NWPSAF_Initialise.f90                         NWPSAF_TranslateDataOut.f90
NWPSAF_Read_EmisEigenVec.f90                  NWPSAF_Read_EmisPCAtlas.f90

1DVar/src/sim_spec/:
pc_to_spec.f90      sim_spec_rttov11.f90  sim_spec_rttov12.f90  spec_to_pc.f90

docs:
AppendixB.html          Eqn1.gif                      img18.gif
AppendixB.pdf           Eqn2a.gif                     nwpsaf-mo-ds-025_product_specification.pdf
AppendixC.html          Eqn2b.gif                     nwpsaf-mo-ds-026_top_level_design.pdf
AppendixC.pdf           Eqn3.gif                      nwpsaf-mo-tv-033_test_plan.pdf
AppendixD.html          NWPSAF_1DVar_User_Manual.pdf  nwpsaf-mo-tv-034_portability.pdf
AppendixD.pdf           Trans.gif                     nwpsaf-mo-ud-031_release_note.pdf
AppendixE.html          delyx.gif                     nwpsaf-mo-ud-032_NWPSAF_1DVar_Manual.html
AppendixE.pdf           img16.gif
Cost_Gradient.gif       img17.gif
```

## 4. What has changed at previous releases

```
Changes for version 1.1.1 (June 2018)

A bug was found in the NWPSAF 1D-Var package (version 1.1)
which has been fixed in this minor release (version 1.1.1).

It affected the microwave retrievals that included the liquid water path.
In the 1DVar source code file NWPSAFMod_LiquidWater.f90
the order of the arguments to the function Layers_to_LWP was incorrect.

The sample test data for SSMIS (for RTTOV11 / RTTOV12 and ifort / gfortran )
were affected by the bug. New corrected sample test data are provided with version 1.1.1.

There are no changes to the structure of the package.


Changes for version 1.1 (February 2017)

Version 1.1 was a major release. The substantial changes from version 1.0 to 1.1 are described in
the following.

Contents:
---------
 - 1DVar/build/makefile
 - New features of 1D-Var v 1.1
```

```
 - More info on the test script
 - More info on Sample Output
 - Compilers tested

Note in particular that the structure of the makefile and the compilation of the code was completely
reorganized for version 1.1.

1DVar/build/makefile:
---------------------

The directory structure has been tidied up for this release: the
fortran files are in the 'src' directory, but the interface files are now
in 'include'. The makefile is now in 'build', and the compiled
executable, along with object, mod, and any other byproducts of compilation (e.g.
*_genmod.f90 files), will also appear in the 'build' directory.

The makefile has been significantly improved from the previous release. You no
longer have to comment out and uncomment sections of the makefile, or use
"dummy" routines to control which version of the RT model you are using. All you
should need to do is edit the top section of the file to set the relevant
options for how you wish to use the 1D-Var at the top, and the makefile should
automatically link in the relevant libraries. The comments in the makefile
should make it clear what you need for each option, but you will certainly need
to change a few:

COMPILER CHOICE:
The makefile is set up for the Intel Fortran Compiler (ifort) by default. The Top
section of the makefile can be used to select a different compiler by setting
the FC variable. Compilers that are provided for are ifort, nagfor, pgf90,
gfortran and xlf95_r. xlf95_r has not been tested for this release but is
provided as a convenient starting point.

The compiling options in the make file are for Linux machines. Replace these
with the relevant options for your own compiler if necessary, noting that you
may need to adjust CPPFLAGS and LFLAGS as well as FFLAGS.

For ifort and gfortran, two sets of FFLAGS are provided: normal compiling and
debug compiling. The normal compiling flags are used by default, but if you
encounter any problems, you could try switching to the debug FFLAGS instead (you
may want to compile RTTOV with debug options as well before recompiling 1D-Var).
Feel free to edit the FFLAGS to add whatever compiling options you want for your
compiler. Note that the FFLAGS are set below the line that says
"No Editing below this line should be necessary"!

RT MODEL LOCATION:
Edit the variables in the next section to point to your installation of RTTOV,
and also to set up the compiler options, depending on whether you compiled RTTOV
with HDF or NetCDF options, and whether you're using the emissivity atlas.

OPTIONS FOR COMPILATION:
This is the area of the makefile where you specify the location of HDF/NetCDF
libraries, and whether you want to run with the emissivity atlas or not.


New Features of 1DVar v1.1:
---------------------------
The main new features of this release are:

ENHANCED RT:
 - Code upgraded to support RTTOV-11.3 (note, will no longer run with RTTOV11.1
   as there are a few differences in the interface to RTTOV between the two
   versions).
 - Support for RTTOV-12, enabling the most up-to-date RT capabilities
 - Ability to use PC-RTTOV to simulate PC scores from hyperspectral sounders,
   for use with PC score observations. This mode is for experimentation and has
   not been extensively tested.
 - Support for calculation and use in the 1D-Var of radiance observations as
   well as brightness temperatures and PC scores.
- The code will now fail if an input file is not there, rather than just
   reporting a warning and hanging.
```

```
For ifort and gfortran, two sets of FFLAGS are provided: normal compiling and
debug compiling. The normal compiling flags are used by default, but if you
encounter any problems, you could try switching to the debug FFLAGS instead (you
may want to compile RTTOV with debug options as well before recompiling 1D-Var).
Feel free to edit the FFLAGS to add whatever compiling options you want for your
compiler. Note that the FFLAGS are set below the line that says
"No Editing below this line should be necessary"!

RT MODEL LOCATION:
Edit the variables in the next section to point to your installation of RTTOV,
and also to set up the compiler options, depending on whether you compiled RTTOV
with HDF or NetCDF options, and whether you're using the emissivity atlas.

OPTIONS FOR COMPILATION:
This is the area of the makefile where you specify the location of HDF/NetCDF
libraries, and whether you want to run with the emissivity atlas or not.

DIRECTORY STRUCTURE TIDIED:
 - A new 'include' directory has been introduced. The *.interface files now
   reside here.
 - A new 'build' directory has been introduced. The makefile now resides here,
   and compilation should be done from within that directory. All compiled
   object files etc will be placed in this directory.
 - The 'src' directory now contains only code.
 - The 'Sample_Scripts' directory has been replaced by the directory 'WorkDir'.

NEW CALLING SCRIPT:
 - 'WorkDir' contains a script, Run_1DVar_test.ksh that will run through the
   installation test configurations. All required files will be linked into
   WorkDir. This avoids cluttering the top directory with files.
 - Output from the installation tests will be put into a directory called
   'testoutput', and you can compare this output with that in the
   'Sample_Output_RTTOV11' or 'Sample_Output_RTTOV12' directory to test your
   installation. Information about the coefficient files used to produce this
   output is included below.
 - There is also a very similar script for one ob type, Run_1DVar.ksh that is
   easy for users to modify for their own application. WorkDir can be copied
   multiple times; just set different values for outputdir and myoutputdir
   in each copy, and the user can then run multiple instances of the 1D-Var
   at once.
  -Two directory locations, which in previous releases were set in the
   ControlData.NL file, are now set via environment variables. These are:
    * COEFFS_DIR
    * OUTPUT_DIR
   These variables should be set and exported before calling the 1D-Var.

CHANGES TO OUTPUT:
 - The RTTOV11 interface code now sets profiles(1) % gas_units = 2 by default
   If you wish to replicate results with the previous version of the
   NWPSAF_1DVar, set gas_units=0 in the Control.NL file.
   Please see RTTOV documentation for more information.
 - Most of the Sample_output files were run with a mode Legacy_Settings in the
   Control.NL file. There are two settings (apart from gas_units) that massively
   alter the output of RTTOV: use_q2m and interpolation_mode=5. For
   compatibility with the older test files, Legacy_settings was set up to set
   these to the older settings. By default, the code will run with the newer
   recommended settings and may thus produce different results from the previous
   release even with the same RTTOV coefficient files..

ADDITIONAL UTILITIES:
 - See Appendix E of the documentation for more information.
 - Code provided to simulate observation files, in either radiance, brightness
   temperature, or PC Score units, for IASI. This code can be adapted for other
   instruments. Simulated noise is added to the observations based on provision
   of a diagonal R-matrix file in the standard format required for 1D-Var.
 - Code provided to convert observation input files from brightness temperature
   or radiance to principal component scores, and back again.
 - The new utilities are also compiled using the same makefile as the 1D-Var.
 - Calling scripts have been added to WorkDir to run these utilities.

More info on the test script
```

```
---------------------------

The test script should be run in the WorkDir directory, or a copy of it, rather
than in the top installation directory as previously. You will need to link the
necessary RTTOV coefficient files into this directory. There are no longer any
coefficient files on 43 levels but the code will still run a retrieval on 43
levels, with coefficients on any number of levels, as the RTTOV internal
interpolation will be called automatically. Look through the script and read the
readme.txt file for more info on what changes you need to make to the script
before you run it.

Run_1DVar_test.ksh will copy sample input files in to the top 1DVar directory
and copies one of the two B matrices in to the relevant coeffs directory.
The sample script is set up to run using 54 levels by default for everything
except SSMIS (there is only a 43 level test profile containing cloud liquid
water provided). If you want to run the test retrievals on 43 levels, change the
line where the number of levels is specified (line 36).

More information on Sample Output
---------------------------------

Sample_Output_RTTOV* directory. Sample output is provided for both RTTOV11 and
RTTOV12. The sample output was generated using code compiled with
 - ifort-12.0.4
 - gfortran-4.7.7
on a DELL T3500 running RHEL-6.8.

The following RTTOV-11 coefficients were used to generate the sample output for
retrievals on 54 and 43 levels (except SSMIS, run on 43L only) using RTTOV11.3.
HDF coefficient files for all instruments where available.
 - IASI:  rtcoef_metop_2_iasi.H5:   RTTOV-9 Predictors / LBLRTM / 101L
 - AIRS:  rtcoef_eos_2_airs.dat:    RTTOV-7 Predictors / LBLRTM / 54L
 - ATOVS: rtcoef_noaa_15_hirs.dat:  RTTOV-7 Predictors / LBLRTM / 54L
          rtcoef_noaa_15_amsua.dat: RTTOV-7 Predictors / LIEBE-MPM / 54L
          rtcoef_noaa_15_amsub.dat: RTTOV-7 Predictors / LIEBE-MPM / 54L
 - ATMS:  rtcoef_jpss_0_atms.dat:   RTTOV-7 Predictors / LIEBE-MPM / 54L
 - CrIS:  rtcoef_jpss_0_cris.dat:   RTTOV-7 Predictors / LBLRTM / 54L
 - SSMIS: rtcoef_dmsp_16_ssmis.dat: RTTOV-7 Predictors / LIEBE-MPM / 54L
This output is in Sample_Output_RTTOV11.

The following RTTOV-12 coefficients were used to generate the sample output for
retrievals on 54 and 43 levels (except SSMIS, run on 43L only) using RTTOV12.
HDF coefficient files for all instruments where available.
 - IASI:  rtcoef_metop_2_iasi_pcrttov_compat.H5: RTTOV-9 Predictors / LBLRTM / 101L
 - AIRS:  rtcoef_eos_2_airs.dat:    RTTOV-7 Predictors / LBLRTM / 54L
 - ATOVS: rtcoef_noaa_15_hirs.dat:  RTTOV-7 Predictors / LBLRTM / 54L
          rtcoef_noaa_15_amsua.dat: RTTOV-7 Predictors / LIEBE-MPM / 54L
          rtcoef_noaa_15_amsub.dat: RTTOV-7 Predictors / LIEBE-MPM / 54L
 - ATMS:  rtcoef_jpss_0_atms.dat:   RTTOV-7 Predictors / LIEBE-MPM / 54L
 - CrIS:  rtcoef_jpss_0_cris.dat:   RTTOV-7 Predictors / LBLRTM / 54L
 - SSMIS: rtcoef_dmsp_16_ssmis.dat: RTTOV-7 Predictors / LIEBE-MPM / 54L
This output is in Sample_Output_RTTOV12.

For RTTOV12, additionally, the following were used to generate PC Score and
Radiance output for IASI:
rtcoef_metop_2_iasi_pcrttov_compat.H5: RTTOV-9 predictors / LBLRTM / 101L
pccoef_metop_2_iasi_landsea_nlte.H5

For RTTOV11, additionally, the following were used to generate PC Score output
for IASI:
rtcoef_metop_2_iasi.H5: RTTOV-9 predictors / LBLRTM / 101L
pccoef_metop_2_iasi.H5

The output from RTTOV11 and RTTOV12 is near identical: there are differences to
a few thousandths of a K in one or two channels for each instrument (more
channels for SSMIS); and some differences in the retrieved profiles, notably to
the surface water vapour (s2m % q) retrieval.

Compilers tested
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The code has been compiled, and the test scripts run for both RTTOV11 and
```

RTTOV12 with the following compilers:
ifort 12.0.4
gfortran 4.4.7
gfortran 6.2.0
nagfor 5.2
pgf90 11.7
pgf90 14.6
pgf90 15.1
It has also been compiled with ifort 17.0.

# Appendix: Details of the testing carried out for 1D-Var version 1.2

The new version of the code was tested with a number of different versions of the Fortran compilers from Intel, GNU, NAG and Portland. In order to test the new functionality a suitable surface emissivity retrieval case was constructed. For this case a simulated observation was generated. The simulation used the US Standard Atmosphere for the definition of the profile and was complemented with a surface emissivity spectrum from the emissivity atlas that has been included in the distribution of version 1.2. The spectrum is for the 30$^{th}$ September and for a grid point in the London area (51.5N, 0.0E). Intentionally a rather different surface emissivity was chosen for the background surface, which was taken from a grid point in the Algerian Saharan desert at (30.0N,0.0E) again for the 30$^{th}$ September. The result of the retrieval is a surface which resembles the emissivity spectrum that went into the simulated observation quite closely which demonstrates the skill of the surface emissivity retrieval. The different emissivity spectra relevant for the retrieval case have been plotted in Figure 1.

Any retrieval involving surface emissivity needs access to the two files in the `Sample_SurfEmiss` directory: `EmisPCAtlas` and `EmisEigenVec`. The setup of the retrieval test case requires a number of additional files which are specific to the test case. To run the test case, a special shell has been constructed: `WorkDir/Run_1DVar_SurfEmiss.ksh`. The simulated observation is contained in `Sample_ObsFiles/ObsFile_IASI_SURFEMISS.dat` and the quantities in the retrieval state vector to be retrieved (which include the surface emissivity principal components) are controlled by `Sample_Namelists/Retrieval_IASI_SURFEMISS_54L.NL`. The files specific to the test case in the `IASI_COEFFS_DIR` directory are `ChannelChoice_surf_emiss.dat` and `Rmatrix_surf_emiss` which are specifically designed for the 314 IASI channels involved.

Table 1 gives an overview of the different versions of the Fortran compilers from Intel, GNU, NAG and Portland that were used to build RTTOV and the 1D-Var version 1.2. The test case was then run using each of these builds. For each compiler tested, a subdirectory with the output files can be found under `Sample_Output_Surfemiss/`. The Portland Fortran compiler required a source code modification to the RTTOV interface routines. The Fortran code of these routines represents correct Fortran. For this reason the default source code in the distribution was not modified. To support users of the Portland Fortran compiler, modified source code routines are provided for use with this line of compiler. More details can be found in the result section of Table 1.

| Test | Performed by | Date | Result |
|---|---|---|---|
| | | | |
| 1D-Var v1.2<br>(RTTOV12.3 linked) | | | |
| | | | |
| Compiler: Intel Fortran ifort16.0.1build | Stephan Havemann (SH) | 13/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_ifort16<br>The files in this folder are:<br>Retrieved_Profiles.dat,<br>Retrieved_BTs.dat,<br>ProfileQC.dat,<br>Minimisation.log,<br>Minimisation_BT.log,<br>A-matrix.out,<br>Am-matrix.out,<br>BgJacobian.out,<br>RetJacobian.out,<br>AveragingKernel.out |
| Compiler: Intel Fortran ifort17.0.1build | SH | 13/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_ifort17<br>The list of files in this folder is identical to those of the test with ifort16 above and the same list of files applies to all the following tests with other compilers. |

| | | | |
|---|---|---|---|
| Compiler: Intel Fortran ifort18.0.3 build | SH | 13/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_ifort18 |
| Compiler: Intel Fortran ifort19.0.3 build | SH | 13/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_ifort19 |
| | | | |
| Compiler: GNU Fortran gfortran4.8.5 build | SH | 12/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_gfortran485 |
| Compiler: GNU Fortran gfortran6.4.0 build | SH | 15/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_gfortran64 |
| Compiler: GNU Fortran gfortran7.3.0 build | SH | 15/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_gfortran73 |
| Compiler: GNU Fortran gfortran8.1.0 build | SH | 15/05/2020 | Pass;<br><br>The folder containing the files with the |

| | | | |
|---|---|---|---|
| | | | test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_gfortran81 |
| | | | |
| Compiler: NAG Fortran nagfor6.1 | SH | 15/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_nagfor61 |
| Compiler: NAG Fortran nagfor6.2 | SH | 15/05/2020 | Pass;<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_nagfor62 |
| | | | |
| Compiler Portland Fortran pgf16.10-0 | SH | 18/05/2020 | Pass;<br>But note that while the code compiles successfully with Portland Fortran, to successfully run the code with any Portland Fortran compiler, a change to the source code routine src/NWPSAF_RTTOV12_Interface.f90 is required (even though it represents correct Fortran).<br>The failure to correctly dimension the arrays Profiles and Profiles_K_PC can be rectified by making these arrays allocatable and allocating and deallocating them appropriately.<br>This has been done in the routine src/NWPSAF_RTTOV12_Interface_portland.f90 which has been included in the distribution for users of the Portland Fortran compiler.<br>The same issue applies to |

| | | | |
|---|---|---|---|
| | | | src/NWPSAF_RTTOV11_Interface.f90<br>for which there is<br>src/NWPSAF_RTTOV11_Interface_portland.f90<br>provided as the alternative for use with Portland Fortran compilers.<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_pgf9016 |
| Compiler: Portran Fortran pgf18.7-0 | SH | 17/05/2020 | Pass;<br>But note that the same issue arises as with the older Portland compiler version pgf16.10-0.<br><br>The folder containing the files with the test results:<br>Sample_Output_Surfemiss/<br>IASI_SURFEMISS_54L_pgf9018 |
| | | | |

Table 1: The different Fortran compiler version from Intel, GNU, NAG and Portland that have been used to build RTTOV and the 1D-Var version 1.2. The results of the runs of the test cases using these builds including the location of the output files from the test runs.

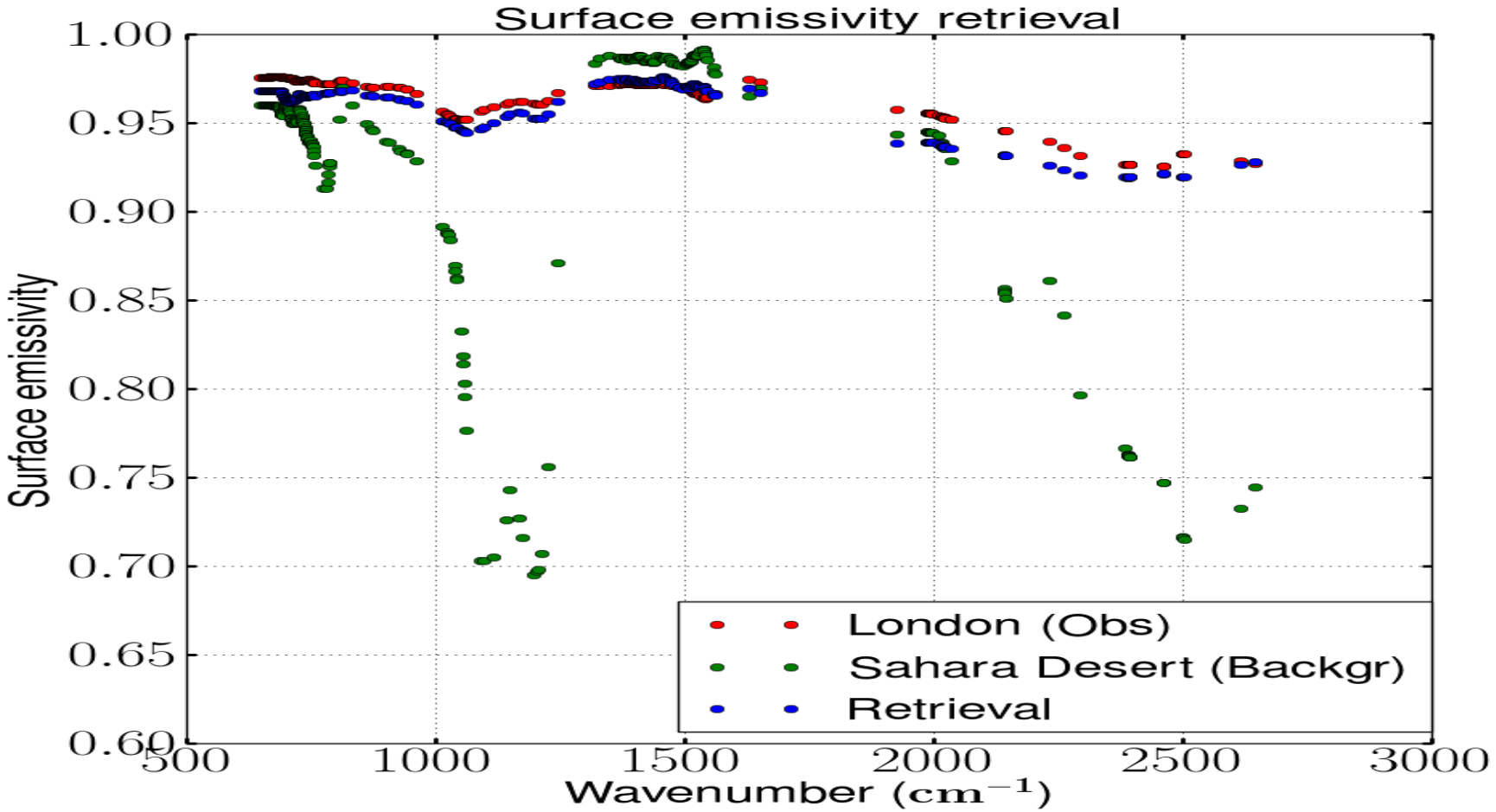


Figure 1: Surface emissivity retrieval test case. The simulated observation assumes the US Standard Atmosphere together with the surface emissivity spectrum for a point of the emissivity atlas for the 30$^{th}$ September in London (51.5N, 0.0E). As a background a point for the same day in the Algerian Sahara Desert (30.0N,0.0E) is chosen. The retrieved surface emissivity spectrum is again close to that of London which was used for the simulated observation.