

RadSim v3.1 Test Log - Appendix to RadSim v3 Test Plan (NWPSAF-MO-TV-047)

This document summarises the results of testing performed on the RadSim v3.1 code. The test scenarios are described in the RadSim v3 Test Plan. A summary is given here with some additional details about test configurations:

0.a Portability testing:

RadSim is compiled with ifort (on Intel and Cray), gfortran and pgfortran. This includes both OpenMP-enabled (optimised), non-OpenMP (optimised), and debugging compiler flags. It is expected that users will compile with optimised compiler flags, and usually with OpenMP support. The ifort OpenMP build was against RTTOV v13.0 while all other builds were against RTTOV v13.1.

0.b Run *radsim_check_install*:

Users should run this script after compilation to test their installation. It runs RadSim for a single instrument and compares the output to a reference file included in the package. This is run for all compilers tested.

The following tests correspond to the test scenarios listed in the Test Plan.

1. General validation test

The tests run as part of this test scenario involve the following sensors: SNPP ATMS (microwave), MSG-4 SEVIRI (visible/infrared) and Metop-2 IASI (hyperspectral infrared). The following tests are configured:

Clear-sky tests (on full grid and with obs data file except for NWP SAF profile datasets):

- ATMS clear-sky, including CLW absorption, direct and Jacobian model outputs
- SEVIRI visible+IR clear-sky, including ozone, modified background CO₂, solar radiation, direct and Jacobian model outputs

Clear-sky tests with computed geostationary satellite zenith and azimuth angles (on full grid and with obs file):

- SEVIRI visible+IR clear-sky, including ozone, modified background CO₂, solar radiation, direct model outputs

Cloud simulation tests (with obs data file except for NWP SAF profile datasets):

- ATMS cloudy, direct model outputs
- SEVIRI visible+IR channels cloudy using DOM (visible)/Chou-scaling (IR), including ozone, solar radiation, direct model outputs
- SEVIRI visible channels cloudy using MFASIS with OPAC cloud liquid water properties, direct model outputs
- SEVIRI visible channels cloudy using MFASIS with Deff cloud liquid water properties, direct model outputs
- SEVIRI visible+IR channels cloudy using DOM (visible)/Chou-scaling (IR), including ozone, solar radiation, direct model outputs, ingest of liquid/ice Deff fields (ICON only)
- SEVIRI visible channels cloudy using MFASIS with Deff cloud liquid water properties, direct model outputs, ingest of liquid/ice Deff fields (ICON only)

Footprint simulation tests:

- Same as the cloud tests, but with footprints enabled.

CAMS aerosol tests (with obs data file):

- SEVIRI visible+IR channels aerosol only using DOM (visible)/Chou-scaling (IR), including ozone, solar radiation, direct model outputs
- SEVIRI visible+IR channels aerosol+cloud using DOM (visible)/Chou-scaling (IR), including ozone, solar radiation, direct model outputs

Hyperspectral sounder/PC model tests (with obs data file except for NWP SAF profile datasets):

- IASI (subset of 302 channels) including ozone, modified background CO₂, direct and Jacobian model outputs, CADS height assignments
- IASI (subset of 302 channels) using PC-RTTOV including ozone, modified background CO₂, direct and Jacobian model outputs
- IASI (subset of 302 channels) using HTFRTC including ozone, modified background CO₂, direct and Jacobian model outputs

The following input data are tested:

- NWP SAF 60L profiles (clear-sky and cloud tests, IASI tests for direct model only)
- NWP SAF 91L profiles (clear-sky and cloud tests, IASI tests for direct model only)
- NWP SAF 137L profiles (clear-sky and cloud tests, IASI tests for direct model only)
- ECMWF GRIB data (all tests including temporal interpolation with obs data files, excluding aerosol tests)
- ECMWF netCDF data (all tests including temporal interpolation with obs data files, excluding aerosol tests)
- ECMWF CAMS GRIB data including aerosol fields (aerosol and aerosol+cloud tests only)
- ICON GRIB data (all tests including temporal interpolation with obs data files, excluding aerosol tests and computed geo sat angle tests)
- HARMONIE GRIB data (all tests, excluding aerosol tests and computed geo sat angle tests)
- JMA NWP GRIB data (clear-sky (direct model only on full grid, no CLW for MW) and IASI tests)
- JMA JRA-55 GRIB data (clear-sky (direct model only on full grid, no CLW for MW) and IASI tests)
- UM PP file, (clear-sky for obs data file only and IASI tests, no ozone)
- UM fieldsfile, (clear-sky and IASI tests including temporal interpolation, no ozone)

For clear-sky tests with solar radiation, the full grid simulations are run using fixed solar angles and then again allowing RadSim to compute the solar angles. Similarly, for clear-sky solar tests using an observation file, two obs files are used, one with explicit solar angles, and the other with obs date/time so that RadSim computes the solar angles. For cloudy solar tests, the solar angles are always computed by RadSim. Emissivity and BRDF atlases are used with all NWP model inputs except for the NWP SAF profile datasets.

Together, these tests cover the majority of RadSim functionality including all input model data types and all simulation types. As described in the Test Plan, where possible the outputs are compared with results from external RTTOV simulations to ensure RadSim is performing simulations as expected. Small differences are expected: these result primarily from RadSim using single precision to store certain types of data. It is not possible to do these comparisons for footprint simulations: these are validated in test scenario 3 below. It is not possible to do these comparisons for internal RadSim geostationary satellite zenith and azimuth angle calculations: these are validated in test scenario 4 below. It is also not currently possible to do the external RTTOV validation in the same way for PC-RTTOV and HTFRTC simulations. For these, the RadSim results for IASI are compared with those for PC-RTTOV and HTFRTC to ensure the differences are within expected tolerances, though they are certainly not expected to be identical in this case.

NB At the time of testing RadSim there are known problems with the RTTOV v13.x HTFRTC simulations which are under investigation (HTFRTC coefficients have not yet been made available on the RTTOV v13 website so users cannot run HTFRTC simulations in RTTOV v13). As such the RadSim testing performed here verified that the HFRTC simulations ran, but the outputs cannot yet be validated.

This test is performed for all compilers. This includes a single-threaded run (gfortran v8.1 optimised non-OpenMP builds of RTTOV and RadSim). Other runs use multiple threads for RTTOV (via OpenMP) and for non-debug flags, multiple threads for RadSim (only relevant for footprint simulations). The outputs from all compilers are cross compared to

ensure any differences are within expected tolerances. This therefore covers test scenario 2 below (OpenMP test).

2. OpenMP test

This falls under test scenario 1 above: the general validation test script is run for multiple compilers for both single-threaded (gfortran v8.1 optimised) and OpenMP (gfortran v8.1 optimised OpenMP) cases, and the results are compared as part of the validation of test scenario 1.

3. Footprints test

This test scenario involves running RadSim in various configurations and comparing the outputs (as described in the Test Plan) to validate the footprint simulation capability. This is run for a gfortran v8.1 build with OpenMP and success is indicated by any reported differences being within expected tolerances.

4. Satellite and solar angles validation

As described in the Test Plan this scenario compares the RadSim calculations for satellite and solar zenith and azimuth angles with those from the Met Office operational Satellite Processing System. This is run for a gfortran v8.1 build with OpenMP and success is indicated by reported/plotted differences being within expected tolerances.

5. Misc options test

This tests other RadSim capabilities not tested elsewhere. Currently two features are tested:

- the *use_all_atlas_months* option
- specification of SSU PMC CO2 cell pressures

This is run for a gfortran v8.1 build with OpenMP and the test script reports success or failure for each feature tested.

6. Comparison to RadSim v3.0

RadSim v3.1/RTTOV v13.1 should replicate results from RadSim v3.0/RTTOV v13.0 for all simulation types/configurations supported by both RadSim versions.

The general validation test (test scenario 1) is used. Results are compared for all simulation types/configurations supported by both RadSim versions (this is a subset of those supported by v3.1).

This is run for gfortran v8.1 builds with OpenMP.

7. Batching test

This test scenario compares output from a run with no batching to that from the same run with artificially small batch thresholds to ensure that outputs are identical. This is run for a gfortran v8.1 build with OpenMP.

8. Heavy load test

This test scenario involves running RadSim for two cases which involve large amounts of data to see whether RadSim copes. The first is for clear-sky SEVIRI simulations (all channels) with around 10^7 observations (corresponding to a full disc scan): this is a large number of input observations. The second is for clear-sky IASI simulations (all channels) on a global model grid at 0.5 degree lat/lon resolution (around 2.6×10^5 grid points) with emissivity output enabled: this test involves a very large amount of output data. Success is indicated by the RadSim runs completing successfully. The test is run for a gfortran v8.1 build with OpenMP.

9. Valgrind/memcheck test

In this test scenario the general validation test (test scenario 1) is run for a gfortran v8.1 optimised, non-OpenMP build with the Valgrind memcheck tool. Output is examined to ensure there are no memory leaks or other issues. NB Valgrind reports a large number of allocations that are “still reachable” for calls to the ecCodes library for tests involving ingest of GRIB data: these are not related to RadSim and are not necessarily considered problematic (see the Valgrind documentation).

10. Timing tests

These tests are run using a gfortran v8.1 build with optimised non-OpenMP flags. The model grid here comprises ~250000 profiles, and the observation data files define ~126000 profiles. These results give an indication of the run-times one can expect from RadSim. The run-times are broadly comparable between RadSim v3.0 and v3.1, though for the model grid simulations (tests 1-3) there is an indication that RadSim v3.0/RTTOV v13.0 is around 3-6% faster than RadSim v3.1/RTTOV v13.1. This is unexpected because RTTOV itself takes the bulk of the run-time and there was not any significant change in RTTOV performance between v13.0 and v13.1 (see the RTTOV v13.1 Performance Test Log available on the RTTOV web pages). Test 6 also runs about 3% faster in RadSim v3.0, but this may be because the footprint data were stored and written out in v3.1 which involves a small amount of extra processing. The footprint simulations take significantly longer than the equivalent clear-sky interpolated observations. This can be mitigated by compiling with OpenMP flags and using multiple threads, and where applicable in v3.1, by writing out and subsequently re-reading the footprint data as shown in the difference in run-times for tests 6 and 7 for RadSim v3.1. Note that for cloudy simulations which are significantly more expensive than clear-sky simulations, the time taken for footprint calculations will be a smaller proportion of the total run-time.

Test	Date	Platform	Compiler	Compiler flags	Pass/fail	Notes
0.a Compilation	17/01/22	x86_64 GNU/Linux	ifort v17.0.1	ifort (with OpenMP)	Pass	HDF5 v1.8.8 NetCDF v4.1.1 ecCodes v2.24.0 RTTOV v13.0
	17/01/22	x86_64 GNU/Linux	ifort v17.0.1	ifort (debugging flags)	Pass	HDF5 v1.8.8 NetCDF v4.1.1 ecCodes v2.24.0
	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	HDF5 v1.8.8 NetCDF v4.1.1 ecCodes v2.24.0
	18/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (optimised flags without OpenMP)	Pass	HDF5 v1.8.8 NetCDF v4.1.1 ecCodes v2.24.0
	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (debugging flags)	Pass	HDF5 v1.8.8 NetCDF v4.1.1 ecCodes v2.24.0
	18/01/22	x86_64 GNU/Linux	gfortran v11.2.0	gfortran (with OpenMP)	Pass	HDF5 v1.8.8 NetCDF v4.1.1 ecCodes v2.24.0
	17/01/22	x86_64 GNU/Linux	pgf90 v18.7-0	pgf90 (with OpenMP)	Pass	HDF5 v1.8.8 NetCDF v4.1.1 ecCodes v2.24.0
	17/01/22	Cray	cray-ifort v15.0.0	cray-ifort	Pass	HDF5 v1.8.13 NetCDF v4.3.2 ecCodes v2.6.0
0.b radsim_check_install	17/01/22	x86_64 GNU/Linux	ifort v17.0.1	ifort (with OpenMP)	Pass	
	17/01/22	x86_64 GNU/Linux	ifort v17.0.1	ifort (debugging flags)	Pass	
	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	
	18/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (optimised flags without OpenMP)	Pass	
	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (debugging flags)	Pass	
	18/01/22	x86_64 GNU/Linux	gfortran v11.2.0	gfortran (with OpenMP)	Pass	

	17/01/22	x86_64 GNU/Linux	pgf90 v18.7-0	pgf90 (with OpenMP)	Pass	
	17/01/22	Cray	cray-ifort v15.0.0	cray-ifort	Pass	

Test scenario	Date	Platform	Compiler	Compiler flags	Pass/fail	Notes
1. General validation test	17/01/22	x86_64 GNU/Linux	ifort v17.0.1	ifort (with OpenMP)	Pass	MFASIS simulations did not run because the <i>radsim_test.sh</i> script uses the new RTTOV v13.1 MFASIS files which are not compatible with v13.0. Separate tests show MFASIS simulations with the v13.0 MFASIS files work with RadSim v3.1/RTTOV v13.0 as expected.
	17/01/22	x86_64 GNU/Linux	ifort v17.0.1	ifort (debugging flags)	Pass	
	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	
	18/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (optimised flags without OpenMP)	Pass	
	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (debugging flags)	Pass	
	18/01/22	x86_64 GNU/Linux	gfortran v11.2.0	gfortran (with OpenMP)	Pass	
	17/01/22	x86_64 GNU/Linux	pgf90 v18.7-0	pgf90 (with OpenMP)	Pass	
	17/01/22	Cray	cray-ifort v15.0.0	cray-ifort	Fail	The ICON tests with cloud liquid and ice Deff fields failed as the ecCodes library is too old so the fields are not recognised in the GRIB file (noted in section 2.2 of the user guide). Since ifort builds on Linux are OK there is no reason to suspect they would not work on Cray with a newer ecCodes version. All other tests passed.
2. OpenMP test	18/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (optimised flags with/without OpenMP)	Pass	
3. Footprints test	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	

4. Satellite and solar angles	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	
5. Misc options test	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	
6. Comparison to RadSim v3.0	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	Discovered bug in v3.1 related to modifications related to pressure level calculations for GRIB data affecting JMA files only: the pressure coefficients from the file were not being used when present due to a logic error in the code. This was fixed and the tests all passed.
7. Batching test	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	
8. Heavy load test	17/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (with OpenMP)	Pass	
9. Valgrind/memcheck test	18/01/22	x86_64 GNU/Linux	gfortran v8.1.0	gfortran (optimised flags without OpenMP)	Pass	

Test scenario 10 - Timing test

Test	RadSim v3.0 time (s)	RadSim v3.1 time (s)
1. ATMS clear-sky grid	184	191
2. ATMS cloudy grid	426	440
3. SEVIRI IR channels cloudy grid	705	750
4. SEVIRI IR channels cloudy obs	424	415
5. SEVIRI VIS/IR channels clear-sky obs	46	46
6. SEVIRI VIS/IR channels clear-sky obs with footprints (writing footprint data file in v3.1 only)	1023	1053
7. SEVIRI VIS/IR channels clear-sky obs with footprints reading footprint data file, v3.1 only	N/A	502