RTTOV v14.0 Performance Test Log - Appendix to RTTOV v14 Test Plan (NWPSAF-MO-TV-050)

This document describes the tests performed to compare the performance of RTTOV v14.0 with that of RTTOV v13.2. This includes comparisons of execution speed and peak memory usage.

Equivalent profiles have been created for RTTOV v13 and v14. The number of pressure levels in the RTTOV v13 profiles is one less than the number of pressure half-levels in the v14 profiles. The number of levels given below is always the number of pressure half-levels in v14.

RTTOV v14 requires that the internal RTTOV interpolator is used for all practical simulations, so no comparisons are done without interpolation.

In the tests below, "IR" indicates only thermal IR channels (wavelengths above 3 microns) and "VIS" indicates only pure-solar channels (wavelengths below 3 microns). Profiles of all variable gases allowed by each coefficient file are present in each profile unless otherwise specified.

The direct, TL, AD and K models were run separately for the following test cases:

1. MW clear-sky (ATMS, v13pred no variable gas), 70L profile
2. MW clear-sky (ICI, v13pred O3-only), 70L profile
3. MW clear-sky (ATMS, v13pred no variable gas) with CLW absorption, 70L profile
4. IR clear-sky (FCI, v13pred O3+CO2), 70L profile
5. VIS clear-sky (FCI, v13pred O3+CO2), 70L profile
6. Hi-res IR clear-sky (IASI, v13pred 7gas), 70L profile
7. Hi-res IR clear-sky (IASI, v9pred 7gas), 70L profile
8. Hi-res IR clear-sky (IASI, v13pred 7gas), no optional variable gas profiles, 70L profile
9. IR aerosol (FCI, v13pred O3+CO2), Chou-scaling solver, 62L profile
10. IR hydrometeor (FCI, v13pred O3+CO2), Chou-scaling solver, 62L profile
11. IR aerosol (FCI, v13pred O3+CO2), DOM solver, 62L profile
12. IR hydrometeor (FCI, v13pred O3+CO2), DOM solver, 62L profile
13. VIS aerosol (FCI, v13pred O3+CO2), DOM solver, 62L profile
14. VIS hydrometeor (FCI, v13pred O3+CO2), DOM solver, 62L profile
15. VIS aerosol+hydrometeor (FCI, v13pred O3+CO2), DOM solver with Rayleigh multiple scattering, 62L profile
16. VIS hydrometeor (FCI, v13pred O3+CO2), MFASIS-NN solver, 62L profile
17. MW hydrometeor (ATMS, v13pred no variable gas), delta-Eddington solver, 62L profile
18. PC-RTTOV simulation (IASI), O3 profiles only, PCscores only, 70L profile
19. PC-RTTOV simulation (IASI), O3 profiles only with reconstructed radiances, 70L profile
20. PC-RTTOV simulation (IASI), 6gas profiles, PCscores only, 70L profile
21. PC-RTTOV simulation (IASI), 6gas profiles with reconstructed radiances, 70L profile

Coefficients based on v13 predictors are used in all cases except the v9 predictor IASI clear-sky test case, and the RTTOV v13 PC-RTTOV simulations for which v9 predictors must be used. The ATMS, ICI, and FCI coefficients are on 54L and the IASI coefficients are on 101L. In each case the profile surface type was set to sea with *calc_emis*, *calc_brdf*, and *calc_diffuse_refl* set to true for all channels. The following options/inputs were used:

- Interpolation mode 4.
- FASTEM6 for MW sea surface emissivity.
- IREMIS for IR sea surface emissivity.
- Elfouhaily et al option for solar sea surface BRDF.
- MW CLW simulations used Rosenkranz water permittivity parameterisation.
- 7gas implies all variable gases supported by RTTOV.
- 6gas implies all variable gases supported by RTTOV excluding SO_2.
- VIS/IR hydrometeor used the CLW Deff and Baran 2018 ice optical properties.
- VIS/IR aerosol used the OPAC optical properties.
- DOM simulations used 8 streams.
- MFASIS simulations used the CLW Deff and Baum ice optical properties with the Wyser Deff parameterisation.
- Input units for hydrometeors/aerosol profiles were kg/kg.
- MW hydrometeor simulations use only rain, snow, clw and ciw.

- The ATMS and ICI simulations were run for all channels.
- The FCI IR simulations were run for channels 9-16.
- The FCI VIS simulations were run for channels 1-8.
- The FCI MFASIS-NN simulations were run for channels 1, 2, 3, 4, 7.
- The IASI clear-sky simulations were run for 183 channels.
- PC-RTTOV simulations used the v13 NLTE+trace gas enabled PC coefficient file.
- PC-RTTOV was run with 300 predictor channels and 300 PC scores.
- PC-RTTOV reconstructed radiances were calculated for 300 channels.

RTTOV v14 defaults are used for all options where otherwise unspecified.

1. Speed comparisons

Tests were performed on an Intel compute cluster (Haswell) using gfortran v11.2.0 and ifort v17.0.1, a Cray XC-40 (Ivy Bridge) using the Cray Fortran compiler v8.3.4.

The tests were run for a large number of profiles, shown in Table 1.

Test case	Model(s)	Number of profiles
1 (MW clear, no gas)	direct/TL/AD K	500000 250000
2 (MW clear, O3)	direct/TL/AD K	500000 250000
3 (MW clear, CLW)	direct/TL/AD K	250000 200000
4 (IR clear, O3+CO2)	direct/TL/AD K	750000 500000
5 (VIS clear, O3+CO2)	direct/TL/AD K	500000 250000
6 (Hi-res clear, v13pred, 7gas)	direct/TL/AD K	50000 10000
7 (Hi-res clear, v9pred, 7gas)	direct/TL/AD K	50000 10000
8 (Hi-res clear, v13pred, no gas)	direct/TL/AD K	50000 10000
9 (IR aer, Chou)	direct/TL/AD/K	500000
10 (IR hydro, Chou)	direct/TL/AD/K	100000
11 (IR aer, DOM)	direct TL AD/K	100000 50000 5000
12 (IR hydro, DOM)	direct TL AD/K	5000 2000 100
13 (VIS aer, DOM)	direct TL AD/K	100000 50000 10000
14 (VIS hydro, DOM)	direct TL AD/K	5000 2000 500
15 (VIS aer+hydro+Ray, DOM)	direct TL AD/K	2500 1000 50
16 (VIS hydro, MFASIS-NN)	direct TL AD/K	100000 50000 20000
17 (MW hydro, delta-Edd)	direct TL/AD/K	100000 50000
18 (PC-RTTOV, O3, noRR)	direct/TL/AD K	50000 2000

19 (PC-RTTOV, O3, RR)	direct/TL/AD K	50000 2000
20 (PC-RTTOV, 6gas, no RR)	direct/TL/AD K	50000 2000
21 (PC-RTTOV, 6gas, RR)	direct/TL/AD K	50000 2000

Table 1: Number of profiles used for each timing test.

All tests were run with one profile passed to RTTOV per call and the results are shown in Table 2. All tests were repeated with 50 profiles passed to RTTOV per call and the results are shown in Table 3. The tests were run again with one profile per call and allocation of the trajectory structures outside RTTOV: Table 4 shows the comparison of RTTOV v14.0 and v13.2, and Table 5 compares RTTOV v14.0 without and with the external allocation. Some additional tests were run (described below) and those results are shown in Table 6.

Timings are taken from the test suite (“real” time, which includes system calls) and the timing results are shown as *ms per profile.* The colour-coding is as follows:

- green => v14.0 more than 10% faster than v13.2
- blue => v14.0 5-10% faster than v13.2
- white => v14.0 run-time within +/-5% that of v13.2
- orange => v14.0 5-10% slower than v13.2
- red => v14.0 more than 10% slower than v13.2

Note the following known/expected impact of specific code changes in RTTOV v14.0 on the timing results:

1. By default, RTTOV allocates a lot of memory in so-called “trajectory” structures internally at run-time. These are used for internal calculation results. Memory allocations can be expensive, though the cost is compiler/system-dependent: this is particularly notable for gfortran. Modifications were made to the way some data structures are allocated to improve the speed of the code. This affects all simulation types, but the impact is most obvious for clear-sky cases where the overall simulation time is smallest and so the time taken by the memory allocations is a significant fraction of the overall run-time. It also benefits cases with more calls to RTTOV so the impact is seen more in single-profile calls to RTTOV (Table 2 below) than in the case with multiple calls to RTTOV (Table 3) because in both cases the same total number of simulations are performed, but the latter achieves this in fewer calls to RTTOV.

2. RTTOV v13 and earlier allow the user to pre-allocate one of these trajectory structures outside RTTOV and pass it in as an argument (note however that RTTOV-SCATT in v13 and earlier do *not* allow this for MW scattering simulations). This can be more efficient (again system/compiler-dependent, and gfortran seems to benefit substantially, but other compilers also see benefits - Table 5) as these allocations are done once for many calls to RTTOV rather than within each call. RTTOV v14.0 allows all three internal trajectory structures to be pre-allocated and so doing this external allocation should offer additional benefits in v14.0 over that in v13.2 (Table 4). Note that by doing this external allocation, the benefits described in note 1 above are not relevant as the allocations only happen once for any number of calls to RTTOV. In general, RTTOV cannot run slower with the external allocation because the memory is allocated internally if not allocated externally by the user. However, for hydrometeor simulations using the maximum/random cloud overlap scheme (typically VIS/IR rather than MW), the external allocation must allocate a maximal amount of memory as the number of cloud columns is not known a priori. This larger memory footprint, combined with an associated reduction in data locality, could conceivably result in a slowdown in certain situations.

3. To unify the scattering simulations in RTTOV v14.0, the code that interpolates the optical property tables for aerosols and hydrometeors was rewritten so that all optical properties can be interpolated in a general way for any solver. This is not as efficient as in RTTOV v13.2, especially for aerosols and for the hydrometeors for microwave sensors, because the code in v13.2 was much more specific to each application which allowed an efficient implementation but was not generally applicable to multiple solvers. For the aerosols, this is particularly obvious in the Chou-scaling simulations which are very fast (so the optical property interpolation is a significant fraction of total run-time), and it affects all models (direct/TL/AD/K). It is less obvious for VIS/IR hydrometeor simulations because the optical property interpolation takes a smaller fraction of overall run-time due to the radiance calculations required for multiple cloud columns. The DOM solver is much more expensive than the Chou-scaling

solver, and as such the optical property interpolation takes a much smaller fraction of the total run-time and so this should not have a significant impact on those cases. For the MW hydrometeors, the impact is most particularly seen in the TL model, but it can be seen from the results below that the AD/K models run significantly faster for MW scattering in RTTOV v14.0 compared to v13.2 so for NWP applications the overall impact on run-time is likely to be broadly neutral. It is planned to re-visit the optical property interpolation code with a view to improving its performance in a future release.

4. MFASIS-NN has undergone optimisation in v14.0, but this is particularly focussed on the case where multiple profiles are simulated per call (Table 3), rather than the single-profile case (Table 2).

5. PC-RTTOV runs standard RTTOV simulations and uses the resulting radiances as predictors to compute the PC scores. In RTTOV v13.2 the standard RTTOV simulations are based on v9 predictors, while in v14.0 they use the v13 predictors. The v13 predictors are more expensive than the v9 predictors and as such it is expected that PC-RTTOV runs more slowly in RTTOV v14.0 compared to v13.2.

As usual, the timing results exhibit a certain amount of noise. However, some clear patterns can be observed.

Table 2: 1 profile per call, v13.2 vs v14.0

There is a general indication that v14.0 is similar to or faster than v13.2 for clear-sky simulations. This is primarily due to the allocation optimisation described in note 1 above.

RTTOV v14.0 is significantly slower than v13.2 for the Chou-scaling solver, especially for aerosols (see note 3 above).

DOM simulations are also affected by the optical property interpolation, but the impact should not be seen because the solver run-time absolutely dominates. There is some indication of DOM aerosol direct and TL models running slower in v14.0, especially for gfortran. This is believed to be due to memory allocations: a simplification was made in the code which means that additional memory is allocated for direct model DOM simulations in v14.0. This will be investigated to see if the slowdown can be mitigated in a future release.

MFASIS-NN results in the single-profile case are mixed (see note 4 above). It appears that for single-profile calls, the AD/K are slower in v14.0 for gfortran builds, but this does not apply when multiple profiles are passed in (see Table 3).

For MW scattering, the general indication is for the direct and TL models to be slower in v14.0 as discussed in note 3 above (although it seems gfortran is not affected in the same way as ifort and Cray), and the AD/K run faster in v14.0.

PC-RTTOV results conform to expectations (see note 5 above).

Table 3: 50 profiles per call, v13.2 vs v14.0

The optimum number of profiles to pass per call to RTTOV for best performance is dependent on the system, compiler, and the type of simulation, and so users must run their own tests in cases where performance is critical. Here we compare RTTOV v14.0 and v13.2 for the case of multiple profiles per call.

For the MW, IR, and VIS clear-sky simulations, v14.0 and v13.2 are broadly similar in speed. The benefits of the allocation optimisation are not seen (as discussed in note 1 above). For the IASI test, the ifort and Cray results generally suggest that v14.0 is faster than v13.2. For gfortran v14.0 appears slower, but this is ***not*** replicated by subsequent ad-hoc tests which actually suggest v14.0 is slightly faster than v13.2.

For VIS/IR scattering simulations, the slower IR Chou-scaling aerosol simulations in v14.0 are again evident. The slowdown in v14.0 for Chou-scaling hydrometeor scattering is again ***not*** replicated by subsequent ad-hoc tests. DOM simulations follow a broadly similar pattern to the single profile case (Table 2).

As discussed in note 4 above MFASIS-NN has been optimised specifically for the multiple profile case and this is observed in these results showing that v14.0 is substantially faster than v13.2 in all models.

Results for MW scattering are consistent with the single profile case, as are the PC-RTTOV results. For PC-RTTOV there are indications that for gfortran and Cray compilers the difference in speed between v13 and v14 is larger for PC-RTTOV with multiple profiles than with a single profile per call.

Table 4: 1 profile per call, external trajectory structure allocation, v13.2 vs v14.0

See note 2 above. We generally expect a small improvement in v14.0 vs v13.2 for faster simulation types with the external allocation as v14.0 allows all three trajectory structures to be pre-allocated instead of just one.

For clear-sky simulations, comparing Tables 2 and 4 the benefit for v14.0 is most noticeable for the hyperspectral 7gas simulations for gfortran, though the ifort and Cray compilers also show some benefit too. The MW, IR and VIS cases are more similar for all compilers.

The external allocation has a clear benefit for IR Chou-scaling hydrometeor simulations in v14.0 for gfortran but causes a slight slowdown for ifort. There also appears to be a slowdown in v14.0 vs v13.2 for direct model DOM hydrometeor simulations (especially the VIS case) with external allocation. As discussed in note 2 above, these slowdowns could be due to the additional memory that must be allocated for hydrometeor simulations with maximum/random overlap which causes a net increase in run-time, despite the benefits of pre-allocating all trajectory structures.

MFASIS-NN results are quite similar to those without external allocation.

For MW scattering, the benefits in external allocation for gfortran in the direct and TL models lead to equal (TL) or better (direct) performance in v14.0 compared to v13.2, and the AD/K are even faster. However, ifort and Cray show similar differences to Table 2 without external allocation. (Recall that in v13.2, RTTOV-SCATT does not support the external allocation at all).

There are indications that for PC-RTTOV, the external allocation reduces the performance gap between v14.0 and v13.2.

Table 5: 1 profile per call, v14.0 without and with external trajectory structure allocation

This table demonstrates the benefits in v14.0 of external allocation of the trajectory structures. This gives an idea of when the external allocation can be beneficial and highlights a few cases where it would not be recommended.

Note that any results indicating a slow down with external allocation aside from VIS/IR hydrometeor simulations should be considered to be due to noise in the system when testing.

Generally, one sees greatest benefit for gfortran. The external allocation would be recommended for clear-sky simulations, Chou-scaling scattering simulations (aerosols and hydrometeors), DOM aerosol simulations, and PC-RTTOV simulations (especially for the PC-RTTOV K model). Small benefits may also be seen for MW scattering using delta-Eddington and the MFASIS-NN model. External allocation would not be recommended for DOM hydrometeor direct/TL model simulations.

Note however that users concerned about performance should run tests on their own system to determine the optimal configuration for running RTTOV in terms of external allocation and number of profiles per call, for example.

Additional speed comparisons

Additional tests have been run to see the impact of some additional optimisations in RTTOV v14.0 and to examine the speed of the interpolator since this must be used in all RTTOV v14.0 simulations.

- Calls to the SURFEM-Ocean MW sea surface emissivity model have been optimised for cases where non-SRF-based coefficients are used. Where the frequency of consecutive channels is identical and the polarisation differs (and some other conditions are fulfilled), the emissivity values from the previous call to SURFEM-Ocean are re-used in v14.0 instead of calling the entire emissivity model again.

- The RTTOV interpolation code has been refactored slightly, and some optimisations implemented that primarily affect the K model when pressure is an active TL/AD/K variable. This particular case has been very slow in RTTOV.

These tests have been run with external allocation of the trajectory structures to avoid the v14.0 allocation optimisations impacting the results. Table 4 below shows that for the ATMS no gas simulations - test 1 - v14.0 and v13.2 have very similar run-times (with v14.0 perhaps still slightly faster than v13.2 with gfortran). This test was also chosen because it is the cheapest simulation in RTTOV so any difference in run-time for the surface emissivity or interpolation calculations will be most visible for this case.

The results are shown in Table 6. The benefits of the SURFEM-Ocean optimisation in v14.0 are clearly seen. It is less clear that the modifications in the interpolation code have had a significant positive benefit, but the results at least suggest no detrimental effect of the changes in v14.0 in terms of run-time.

As a final note, in the context of the operational 4D-Var assimilation system at ECMWF, the changes in RTTOV performance between v13 and v14 are completely negligible, since the observation processing cost is such a small fraction of the whole. In summary, in the context of real-life performance monitoring, RTTOV v14 is broadly the same speed as RTTOV v13.

Test case	Model	Intel gfortran v13.2	Intel gfortran v14.0	Intel gfortran v14.0:v13.2	Intel ifort v13.2	Intel ifort v14.0	Intel ifort v14.0:v13.2	Cray v13.2	Cray v14.0	Cray v14.0:v13.2
1 MW clear no gas	Direct	0.302	0.23	0.76	0.193	0.2	1.04	0.245	0.246	1.00
	TL	0.581	0.531	0.91	0.367	0.369	1.01	0.495	0.478	0.97
	AD	0.637	0.586	0.92	0.449	0.435	0.97	0.54	0.517	0.96
	K	1.273	1.195	0.94	0.729	0.695	0.95	0.869	0.913	1.05
2 MW clear O3-only	Direct	0.17	0.171	1.01	0.148	0.152	1.03	0.195	0.194	1.00
	TL	0.424	0.315	0.74	0.284	0.282	0.99	0.38	0.383	1.01
	AD	0.457	0.353	0.77	0.341	0.328	0.96	0.411	0.398	0.97
	K	0.899	0.86	0.96	0.554	0.509	0.92	0.628	0.617	0.98
3 MW clear CLW abs	Direct	0.499	0.421	0.84	0.319	0.325	1.02	0.384	0.408	1.06
	TL	0.992	0.944	0.95	0.628	0.631	1.01	0.849	0.79	0.93
	AD	1.061	1.016	0.96	0.727	0.718	0.99	0.899	0.846	0.94
	K	1.974	1.867	0.95	1.104	1.074	0.97	1.466	1.425	0.97
4 IR clear O3+CO2	Direct	0.124	0.129	1.04	0.117	0.116	0.99	0.159	0.157	0.99
	TL	0.231	0.236	1.02	0.219	0.219	1.00	0.308	0.299	0.97
	AD	0.257	0.257	1.00	0.264	0.249	0.94	0.334	0.312	0.94
	K	0.597	0.385	0.64	0.418	0.385	0.92	0.506	0.478	0.95
5 VIS clear O3+CO2	Direct	0.256	0.256	1.00	0.18	0.174	0.97	0.236	0.212	0.90
	TL	0.557	0.532	0.95	0.363	0.343	0.94	0.443	0.404	0.91
	AD	0.624	0.569	0.91	0.42	0.381	0.91	0.476	0.429	0.90
	K	1.455	1.363	0.94	0.787	0.7	0.89	0.864	0.79	0.91
6 Hi-res clear v13pred 7gas	Direct	3.477	3.264	0.94	1.994	2.042	1.02	3.304	2.705	0.82
	TL	5.784	5.389	0.93	3.837	3.792	0.99	7.439	5.547	0.75
	AD	6.289	5.825	0.93	4.812	4.213	0.88	6.98	5.769	0.83
	K	35.706	33.191	0.93	19.933	17.605	0.88	27.053	21.293	0.79
7 Hi-res clear v9pred 7gas	Direct	2.682	2.595	0.97	1.687	1.704	1.01	2.483	2.188	0.88
	TL	4.576	4.447	0.97	3.161	3.138	0.99	5.981	4.201	0.70
	AD	5.44	4.814	0.89	4.044	3.559	0.88	5.93	4.564	0.77
	K	35.709	33.644	0.94	24.6	17.635	0.72	26.081	22.951	0.88
8 Hi-res clear v13pred no gas	Direct	3.389	3.244	0.96	1.961	2.009	1.02	3.437	2.842	0.83
	TL	5.749	5.369	0.93	3.779	3.754	0.99	6.926	5.51	0.80
	AD	6.138	5.846	0.95	4.808	4.191	0.87	6.905	5.665	0.82
	K	30.636	28.988	0.95	17.041	14.368	0.84	19.325	21.349	1.10
9 IR aerosol Chou-scaling	Direct	0.161	0.191	1.19	0.147	0.198	1.34	0.202	0.232	1.15
	TL	0.312	0.58	1.86	0.292	0.449	1.54	0.392	0.463	1.18
	AD	0.447	0.641	1.44	0.337	0.513	1.52	0.424	0.523	1.24
	K	0.82	1.012	1.23	0.521	0.693	1.33	0.666	0.742	1.11
10 IR hydro Chou-scaling	Direct	1.596	1.513	0.95	0.681	0.714	1.05	0.944	0.982	1.04
	TL	2.935	2.849	0.97	1.32	1.463	1.11	2.009	2.061	1.03
	AD	3.341	3.133	0.94	1.863	2.01	1.08	2.256	2.414	1.07
	K	3.443	3.499	1.02	1.885	1.989	1.05	2.594	2.627	1.01

Table 2 (continued below): Speed test results, 1 profile per call, v13.2 vs v14.0. Timings are ms per profile.

11 IR aerosol DOM	Direct	1.198	1.44	1.20	1.16	1.243	1.07	1.437	1.546	1.08
	TL	2.984	3.501	1.17	3.134	3.33	1.06	3.238	3.251	1.00
	AD	48.01	48.158	1.00	51.278	50.908	0.99	59.748	62.266	1.04
	K	48.778	48.962	1.00	50.948	50.88	1.00	60.992	61.35	1.01
12 IR hydro DOM	Direct	34.526	34.616	1.00	36.268	36.928	1.02	39.928	41.81	1.05
	TL	96.005	96.865	1.01	103.015	104.34	1.01	102.58	96.295	0.94
	AD	2017.3	1983.7	0.98	2149.8	2131.1	0.99	2505.9	2510.5	1.00
	K	2014.6	1988.2	0.99	2117.4	2119.1	1.00	2508.6	2569.6	1.02
13 VIS aerosol DOM	Direct	1.09	1.556	1.43	1.095	1.241	1.13	1.307	1.358	1.04
	TL	3.141	3.79	1.21	2.938	3.245	1.10	2.783	2.859	1.03
	AD	8.845	9.492	1.07	8.847	9.153	1.03	8.896	8.911	1.00
	K	9.827	10.465	1.06	9.151	9.474	1.04	9.571	9.172	0.96
14 VIS hydro DOM	Direct	21.066	21.304	1.01	18.202	18.358	1.01	18.972	19.324	1.02
	TL	61.98	62.195	1.00	50.58	50.875	1.01	48.38	49.955	1.03
	AD	302.96	297.38	0.98	310.4	310.58	1.00	324.14	323.58	1.00
	K	299.86	300.66	1.00	307.28	307.66	1.00	312.24	319.28	1.02
15 VIS aer+hyd+ray DOM	Direct	41.62	41.324	0.99	39.56	39.664	1.00	44.568	45.268	1.02
	TL	113.73	113.89	1.00	107.27	107.6	1.00	107.23	106.44	0.99
	AD	2012.6	1962.8	0.98	2172.6	2111	0.97	2617.4	2501.8	0.96
	K	1988.6	1996.6	1.00	2139.6	2126	0.99	2409.8	2534.4	1.05
16 VIS hydro MFASIS-NN	Direct	1.603	1.645	1.03	1.456	0.971	0.67	1.412	1.232	0.87
	TL	4.93	4.64	0.94	4.212	3.055	0.73	4.476	3.948	0.88
	AD	5.196	8.002	1.54	4.37	3.771	0.86	5.513	5.388	0.98
	K	5.484	8.635	1.57	4.482	3.981	0.89	5.345	5.424	1.01
17 MW hydro delta-Edd	Direct	0.756	0.662	0.88	0.503	0.548	1.09	0.636	0.733	1.15
	TL	1.401	1.411	1.01	0.916	1.278	1.40	1.134	1.611	1.42
	AD	2.915	1.879	0.64	2.06	1.672	0.81	2.582	2.178	0.84
	K	3.814	2.274	0.60	2.673	2.161	0.81	3.121	2.78	0.89
18 PC O3-only	Direct	2.991	3.878	1.30	2.701	3.507	1.30	4.403	5.237	1.19
	TL	5.483	6.986	1.27	5.429	6.695	1.23	9.858	10.475	1.06
	AD	6.862	7.74	1.13	6.702	7.261	1.08	8.627	10.903	1.26
	K	57.865	68.01	1.18	33.825	36.085	1.07	41.365	43.59	1.05
19 PC, rec rad O3-only	Direct	3.083	4.039	1.31	2.841	3.628	1.28	4.804	5.079	1.06
	TL	5.692	7.145	1.26	5.681	6.886	1.21	8.993	10.759	1.20
	AD	7.047	8.084	1.15	6.889	7.428	1.08	10.291	11.097	1.08
	K	82.085	92.61	1.13	46.2	50.545	1.09	66.88	124.7	1.86
20 PC 6gas	Direct	2.972	3.896	1.31	2.829	3.53	1.25	4.173	5.243	1.26
	TL	5.419	7.037	1.30	5.492	6.67	1.21	9.356	10.706	1.14
	AD	6.93	7.836	1.13	6.796	7.259	1.07	8.832	11.1	1.26
	K	89.405	92.485	1.03	54.725	52.32	0.96	54.855	52.445	0.96
21 PC, rec rad 6gas	Direct	3.069	3.995	1.30	2.874	3.674	1.28	4.583	5.489	1.20
	TL	5.688	7.186	1.26	5.704	6.889	1.21	9.892	10.551	1.07
	AD	7.167	7.908	1.10	6.935	7.516	1.08	9.985	11.127	1.11
	K	113.835	116.675	1.02	66.48	66.65	1.00	86.605	131.34	1.52

Table 2 (continued from above): Speed test results, 1 profile per call, v13.2 vs v14.0. Timings are ms per profile.

Test case	Model	Intel gfortran v13.2	Intel gfortran v14.0	Intel gfortran v14.0:v13.2	Intel ifort v13.2	Intel ifort v14.0	Intel ifort v14.0:v13.2	Cray v13.2	Cray v14.0	Cray v14.0:v13.2
1 MW clear no gas	Direct	0.288	0.282	0.98	0.155	0.167	1.08	0.194	0.209	1.08
	TL	0.516	0.494	0.96	0.304	0.312	1.03	0.454	0.434	0.96
	AD	0.563	0.536	0.95	0.38	0.372	0.98	0.474	0.467	0.99
	K	1.403	1.433	1.02	0.798	0.76	0.95	1.047	0.978	0.93
2 MW clear O3-only	Direct	0.2	0.2	1.00	0.108	0.119	1.10	0.134	0.142	1.06
	TL	0.348	0.349	1.00	0.211	0.222	1.05	0.319	0.29	0.91
	AD	0.378	0.383	1.01	0.258	0.259	1.00	0.314	0.318	1.01
	K	0.938	0.984	1.05	0.553	0.526	0.95	0.712	0.612	0.86
3 MW clear CLW abs	Direct	0.47	0.463	0.98	0.277	0.29	1.05	0.336	0.342	1.02
	TL	0.9	0.876	0.97	0.564	0.569	1.01	0.75	0.767	1.02
	AD	0.957	0.929	0.97	0.655	0.643	0.98	0.781	0.798	1.02
	K	2.09	2.124	1.02	1.282	1.143	0.89	1.489	1.491	1.00
4 IR clear O3+CO2	Direct	0.142	0.15	1.05	0.077	0.086	1.12	0.103	0.105	1.02
	TL	0.244	0.264	1.08	0.148	0.16	1.08	0.227	0.212	0.94
	AD	0.263	0.279	1.06	0.182	0.187	1.03	0.249	0.224	0.90
	K	0.633	0.648	1.02	0.378	0.359	0.95	0.5	0.51	1.02
5 VIS clear O3+CO2	Direct	0.245	0.257	1.05	0.132	0.132	1.00	0.152	0.171	1.13
	TL	0.448	0.452	1.01	0.275	0.259	0.94	0.309	0.307	0.99
	AD	0.483	0.501	1.04	0.315	0.285	0.90	0.353	0.336	0.95
	K	1.45	1.453	1.00	0.818	0.668	0.82	0.868	0.749	0.86
6 Hi-res clear v13pred 7gas	Direct	3.353	3.883	1.16	2.451	2.17	0.89	3.147	3.068	0.97
	TL	5.625	6.267	1.11	5.224	4.095	0.78	6.94	5.438	0.78
	AD	6.1	6.74	1.10	6.219	4.532	0.73	7.419	5.854	0.79
	K	33.144	37.266	1.12	40.27	26.473	0.66	29.313	24.686	0.84
7 Hi-res clear v9pred 7gas	Direct	2.596	2.5	0.96	2.052	1.756	0.86	2.196	2.094	0.95
	TL	5.104	5.029	0.99	3.949	3.278	0.83	4.884	4.171	0.85
	AD	5.408	5.438	1.01	4.61	3.748	0.81	4.945	4.869	0.98
	K	38.12	36.976	0.97	40.052	28.275	0.71	23.183	27.451	1.18
8 Hi-res clear v13pred no gas	Direct	3.224	3.868	1.20	2.448	2.153	0.88	2.789	2.814	1.01
	TL	5.543	6.264	1.13	5.175	4.064	0.79	6.315	5.425	0.86
	AD	6.025	6.74	1.12	5.773	4.508	0.78	6.953	5.794	0.83
	K	32.687	33.043	1.01	31.678	20.488	0.65	25.404	20.664	0.81
9 IR aerosol Chou-scaling	Direct	0.185	0.276	1.49	0.104	0.158	1.53	0.141	0.189	1.34
	TL	0.334	0.579	1.73	0.208	0.39	1.88	0.288	0.419	1.46
	AD	0.357	0.659	1.84	0.241	0.444	1.84	0.321	0.555	1.73
	K	0.845	1.2	1.42	0.531	0.726	1.37	0.64	0.826	1.29
10 IR hydro Chou-scaling	Direct	1.408	1.794	1.27	0.72	0.734	1.02	1.097	1.035	0.94
	TL	2.675	3.135	1.17	1.844	1.499	0.81	2.175	2.216	1.02
	AD	3.071	3.499	1.14	2.36	2.172	0.92	2.462	2.728	1.11
	K	3.548	4.074	1.15	2.462	2.154	0.87	2.737	2.811	1.03

Table 3 (continued below): Speed test results, 50 profiles per call, v13.2 vs v14.0. Timings are ms per profile.

11 IR aerosol DOM	Direct	1.065	1.112	1.04	1.096	1.255	1.15	1.367	1.531	1.12
	TL	2.885	3.611	1.25	3.068	3.369	1.10	3.239	3.415	1.05
	AD	47.748	47.636	1.00	51.474	50.736	0.99	59.79	60.46	1.01
	K	48.18	48.266	1.00	51.194	51.634	1.01	59.03	62.266	1.05
12 IR hydro DOM	Direct	34.158	34.658	1.01	36.69	36.974	1.01	38.952	43.618	1.12
	TL	96.885	97.965	1.01	106.295	105.97	1.00	100.64	99.42	0.99
	AD	2011.4	1976.9	0.98	2125.8	2141.3	1.01	2462.7	2714.9	1.10
	K	2009.8	1975.5	0.98	2140.1	2142.8	1.00	2444.4	2716.1	1.11
13 VIS aerosol DOM	Direct	1.039	1.497	1.44	0.931	1.127	1.21	1.146	1.353	1.18
	TL	3.076	3.938	1.28	2.769	3.008	1.09	2.853	2.973	1.04
	AD	8.512	9.387	1.10	9.121	9.2	1.01	8.92	9.305	1.04
	K	9.583	10.446	1.09	9.08	9.371	1.03	9.7	9.466	0.98
14 VIS hydro DOM	Direct	21.078	21.346	1.01	18.312	18.432	1.01	18.81	20.964	1.11
	TL	64.295	64.895	1.01	54.685	57.49	1.05	49.585	49.835	1.01
	AD	296.56	301.48	1.02	317.2	319.96	1.01	311.44	327.2	1.05
	K	300.16	307.2	1.02	314.52	317	1.01	317.76	334.46	1.05
15 VIS aer+hyd+ray DOM	Direct	41.948	41.74	1.00	39.424	39.78	1.01	41.36	46.744	1.13
	TL	116.66	115.96	0.99	113.69	111.59	0.98	105.84	103.66	0.98
	AD	1972.4	1992.2	1.01	2143.4	2129.2	0.99	2414.4	2575.8	1.07
	K	1977.6	1953	0.99	2164	2133.8	0.99	2492	2607.6	1.05
16 VIS hydro MFASIS-NN	Direct	1.619	1.072	0.66	1.279	0.784	0.61	1.49	1.047	0.70
	TL	4.636	3.348	0.72	3.999	2.717	0.68	4.596	3.385	0.74
	AD	5.064	3.821	0.75	4.321	2.94	0.68	4.949	4.045	0.82
	K	5.187	4.285	0.83	4.559	3.179	0.70	5.188	4.487	0.87
17 MW hydro delta-Edd	Direct	0.768	0.924	1.20	0.476	0.521	1.10	0.611	0.716	1.17
	TL	1.308	2.034	1.56	0.903	1.252	1.39	1.318	1.719	1.30
	AD	2.997	2.591	0.86	2.026	1.719	0.85	2.635	2.18	0.83
	K	4.305	3.762	0.87	2.912	2.389	0.82	3.479	3.063	0.88
18 PC O3-only	Direct	3.893	6.564	1.69	3.418	3.84	1.12	3.639	5.389	1.48
	TL	6.425	10.608	1.65	6.305	7.543	1.20	7.276	10.817	1.49
	AD	7.915	11.345	1.43	7.691	7.808	1.02	8.778	10.975	1.25
	K	61.78	73.755	1.19	60.135	57.835	0.96	44.855	44.35	0.99
19 PC, rec rad O3-only	Direct	4.872	6.701	1.38	3.447	3.886	1.13	3.983	5.438	1.37
	TL	7.78	10.873	1.40	6.529	7.195	1.10	8.099	10.104	1.25
	AD	9.242	9.655	1.04	7.826	7.964	1.02	7.932	11.327	1.43
	K	85.46	98.175	1.15	71.03	72.945	1.03	69.615	125.345	1.80
20 PC 6gas	Direct	4.786	6.63	1.39	3.352	3.945	1.18	3.742	5.118	1.37
	TL	7.627	10.594	1.39	5.807	7.151	1.23	7.49	10.357	1.38
	AD	9.134	11.38	1.25	7.167	7.856	1.10	7.878	11.184	1.42
	K	96.95	99.49	1.03	81.675	76.03	0.93	64.7	62.545	0.97
21 PC, rec rad 6gas	Direct	3.984	6.771	1.70	3.214	3.88	1.21	3.792	5.223	1.38
	TL	8.389	10.772	1.28	6.218	7.63	1.23	7.751	9.967	1.29
	AD	9.869	11.558	1.17	7.877	8.034	1.02	9.769	10.527	1.08
	K	113.83	123.79	1.09	95.115	90.12	0.95	85.395	137.105	1.61

Table 3 (continued from above): Speed test results, 50 profiles per call, v13.2 vs v14.0. Timings are ms per profile.

Test case	Model	Intel gfortran v13.2	Intel gfortran v14.0	Intel gfortran v14.0:v13.2	Intel ifort v13.2	Intel ifort v14.0	Intel ifort v14.0:v13.2	Cray v13.2	Cray v14.0	Cray v14.0:v13.2
1 MW clear no gas	Direct	0.221	0.222	1.00	0.177	0.182	1.03	0.233	0.239	1.02
	TL	0.443	0.397	0.90	0.341	0.343	1.01	0.466	0.45	0.97
	AD	0.503	0.45	0.90	0.422	0.403	0.95	0.513	0.5	0.97
	K	0.726	0.686	0.94	0.665	0.648	0.97	0.799	0.804	1.01
2 MW clear O3-only	Direct	0.156	0.165	1.06	0.132	0.134	1.01	0.18	0.175	0.97
	TL	0.292	0.295	1.01	0.257	0.257	1.00	0.352	0.339	0.96
	AD	0.352	0.33	0.94	0.311	0.3	0.96	0.381	0.373	0.98
	K	0.513	0.496	0.97	0.488	0.476	0.98	0.587	0.587	1.00
3 MW clear CLW abs	Direct	0.404	0.404	1.00	0.303	0.303	1.00	0.372	0.394	1.06
	TL	0.848	0.789	0.93	0.598	0.601	1.00	0.79	0.762	0.96
	AD	0.913	0.853	0.94	0.699	0.678	0.97	0.852	0.813	0.95
	K	1.33	1.278	0.96	1.032	1.005	0.97	1.355	1.369	1.01
4 IR clear O3+CO2	Direct	0.114	0.119	1.04	0.101	0.101	1.00	0.138	0.138	1.00
	TL	0.211	0.216	1.03	0.196	0.193	0.99	0.268	0.261	0.98
	AD	0.234	0.239	1.02	0.234	0.224	0.96	0.291	0.276	0.95
	K	0.35	0.357	1.02	0.36	0.345	0.96	0.438	0.428	0.98
5 VIS clear O3+CO2	Direct	0.211	0.209	0.99	0.16	0.153	0.96	0.2	0.196	0.98
	TL	0.399	0.39	0.98	0.323	0.307	0.95	0.391	0.391	1.00
	AD	0.435	0.427	0.98	0.382	0.345	0.90	0.417	0.39	0.93
	K	0.978	0.981	1.00	0.695	0.651	0.94	0.769	0.774	1.01
6 Hi-res clear v13pred 7gas	Direct	3.142	2.286	0.73	1.963	2.003	1.02	3.532	2.699	0.76
	TL	5.187	4.11	0.79	3.765	3.696	0.98	7.132	5.518	0.77
	AD	5.644	4.539	0.80	4.788	4.145	0.87	7.541	5.536	0.73
	K	18.39	14.963	0.81	19.094	17.777	0.93	25.861	23.194	0.90
7 Hi-res clear v9pred 7gas	Direct	2.27	1.861	0.82	1.615	1.692	1.05	2.846	2.028	0.71
	TL	3.883	3.355	0.86	3.111	3.082	0.99	5.688	4.032	0.71
	AD	4.797	3.756	0.78	3.967	3.513	0.89	6.106	4.636	0.76
	K	18.021	14.858	0.82	19.208	17.791	0.93	25.902	23.95	0.92
8 Hi-res clear v13pred no gas	Direct	3.059	2.283	0.75	1.934	1.996	1.03	3.188	2.538	0.80
	TL	5.038	4.092	0.81	3.729	3.722	1.00	6.385	5.766	0.90
	AD	5.579	4.498	0.81	4.683	4.114	0.88	7.12	5.571	0.78
	K	15.17	12.89	0.85	15.943	14.287	0.90	21.369	19.048	0.89
9 IR aerosol Chou-scaling	Direct	0.146	0.176	1.20	0.129	0.175	1.35	0.188	0.205	1.09
	TL	0.284	0.365	1.29	0.256	0.41	1.60	0.362	0.429	1.19
	AD	0.331	0.427	1.29	0.305	0.471	1.55	0.4	0.476	1.19
	K	0.471	0.582	1.24	0.469	0.649	1.38	0.594	0.687	1.16
10 IR hydro Chou-scaling	Direct	1.382	0.996	0.72	0.654	0.687	1.05	0.932	0.931	1.00
	TL	2.577	2.068	0.80	1.272	1.421	1.12	1.976	2.012	1.02
	AD	2.981	2.668	0.89	1.782	2.026	1.14	2.319	2.503	1.08
	K	3.119	2.814	0.90	1.793	1.981	1.10	2.466	2.554	1.04

Table 4 (continued below): Speed test results, 1 profile per call with external allocation of trajectory structures, v13.2 vs v14.0. Timings are ms per profile.

11 IR aerosol DOM	Direct	1.143	1.176	1.03	1.134	1.285	1.13	1.405	1.468	1.04
	TL	2.926	2.85	0.97	3.076	3.294	1.07	3.2	3.24	1.01
	AD	47.606	46.43	0.98	51.034	50.85	1.00	60.142	61.628	1.02
	K	47.442	47.14	0.99	51.156	50.83	0.99	60.612	61.31	1.01
12 IR hydro DOM	Direct	34.094	35.462	1.04	36.026	38.854	1.08	38.922	41.654	1.07
	TL	95.99	98.14	1.02	104.775	104.42	1.00	98.775	94.655	0.96
	AD	2004.3	1972.2	0.98	2191.6	2141.5	0.98	2522.2	2547.6	1.01
	K	2008.1	1978.9	0.99	2140.8	2110.3	0.99	2512.9	2577.8	1.03
13 VIS aerosol DOM	Direct	1.09	1.271	1.17	1.061	1.471	1.39	1.231	1.327	1.08
	TL	2.978	2.683	0.90	2.864	3.162	1.10	2.704	2.671	0.99
	AD	8.539	8.261	0.97	8.879	8.993	1.01	8.997	8.772	0.97
	K	9.146	8.804	0.96	9.102	9.345	1.03	9.686	9.646	1.00
14 VIS hydro DOM	Direct	20.78	23.59	1.14	18.462	25.652	1.39	19.466	25.768	1.32
	TL	62.125	59.34	0.96	50.945	55.495	1.09	49.465	52.55	1.06
	AD	293.8	297.7	1.01	311.86	313.04	1.00	314.6	305.26	0.97
	K	297.8	297.4	1.00	310.82	314.24	1.01	309.96	313.58	1.01
15 VIS aer+hyd+ray DOM	Direct	41.568	44.068	1.06	39.408	47.052	1.19	43.348	47.52	1.10
	TL	112.92	109.19	0.97	106.53	112.97	1.06	106.22	105.43	0.99
	AD	1982.6	1929.4	0.97	2155.2	2155.2	1.00	2483.2	2628.2	1.06
	K	2006.2	1941	0.97	2155.6	2127	0.99	2577.2	2461.4	0.96
16 VIS hydro MFASIS-NN	Direct	1.605	1.495	0.93	1.401	0.941	0.67	1.427	1.165	0.82
	TL	4.644	4.621	1.00	4.129	3.015	0.73	4.49	4.032	0.90
	AD	5.005	8.018	1.60	4.372	3.742	0.86	5.256	4.867	0.93
	K	5.216	8.233	1.58	4.505	3.942	0.88	5.215	5.115	0.98
17 MW hydro delta-Edd	Direct	0.791	0.632	0.80	0.502	0.521	1.04	0.627	0.718	1.14
	TL	1.346	1.383	1.03	0.914	1.231	1.35	1.158	1.607	1.39
	AD	2.93	1.83	0.62	2.062	1.619	0.79	2.563	2.092	0.82
	K	3.958	2.218	0.56	2.674	2.094	0.78	3.176	2.543	0.80
18 PC O3-only	Direct	2.892	3.829	1.32	2.661	3.485	1.31	4.241	4.644	1.10
	TL	5.324	6.975	1.31	5.313	6.536	1.23	8.255	9.678	1.17
	AD	6.884	7.593	1.10	6.629	7.261	1.10	9.033	11.011	1.22
	K	32.285	39.545	1.22	31.72	35.785	1.13	41.06	37.795	0.92
19 PC, rec rad O3-only	Direct	3.016	3.94	1.31	2.785	3.576	1.28	4.397	4.793	1.09
	TL	5.591	7.168	1.28	5.609	6.768	1.21	8.872	10.356	1.17
	AD	7.138	7.734	1.08	6.935	7.335	1.06	10.207	11.819	1.16
	K	55.74	63.195	1.13	44.735	49.95	1.12	67.16	120.95	1.80
20 PC 6gas	Direct	2.968	3.926	1.32	2.69	3.497	1.30	4.419	5.037	1.14
	TL	5.373	7.004	1.30	5.412	6.637	1.23	8.865	10.167	1.15
	AD	6.775	7.647	1.13	6.715	7.261	1.08	9.968	10.589	1.06
	K	62.645	62.52	1.00	52.315	51.61	0.99	51.5	55.77	1.08
21 PC, rec rad 6gas	Direct	3.02	3.929	1.30	2.832	3.575	1.26	4.609	4.84	1.05
	TL	5.557	7.088	1.28	5.603	6.772	1.21	9.626	10.503	1.09
	AD	6.996	7.867	1.12	6.861	7.385	1.08	10.154	10.604	1.04
	K	85.565	85.92	1.00	64.885	66.635	1.03	81.085	134.92	1.66

Table 4 (continued from above): Speed test results, 1 profile per call with external allocation of trajectory structures, v13.2 vs v14.0. Timings are ms per profile.

Test case	Model	Intel gfortran v14.0 no alloc	Intel gfortran v14.0 alloc	Intel gfortran alloc:no alloc	Intel ifort v14.0 no alloc	Intel ifort v14.0 alloc	Intel ifort alloc:no alloc	Cray v14.0 no alloc	Cray v14.0 alloc	Cray alloc:no alloc
1 MW clear no gas	Direct	0.23	0.222	0.96	0.2	0.182	0.91	0.246	0.239	0.97
	TL	0.531	0.397	0.75	0.369	0.343	0.93	0.478	0.45	0.94
	AD	0.586	0.45	0.77	0.435	0.403	0.93	0.517	0.5	0.97
	K	1.195	0.686	0.57	0.695	0.648	0.93	0.913	0.804	0.88
2 MW clear O3-only	Direct	0.171	0.165	0.96	0.152	0.134	0.88	0.194	0.175	0.90
	TL	0.315	0.295	0.94	0.282	0.257	0.91	0.383	0.339	0.89
	AD	0.353	0.33	0.93	0.328	0.3	0.91	0.398	0.373	0.94
	K	0.86	0.496	0.58	0.509	0.476	0.93	0.617	0.587	0.95
3 MW clear CLW abs	Direct	0.421	0.404	0.96	0.325	0.303	0.93	0.408	0.394	0.97
	TL	0.944	0.789	0.84	0.631	0.601	0.95	0.79	0.762	0.97
	AD	1.016	0.853	0.84	0.718	0.678	0.94	0.846	0.813	0.96
	K	1.867	1.278	0.68	1.074	1.005	0.94	1.425	1.369	0.96
4 IR clear O3+CO2	Direct	0.129	0.119	0.92	0.116	0.101	0.87	0.157	0.138	0.88
	TL	0.236	0.216	0.92	0.219	0.193	0.88	0.299	0.261	0.88
	AD	0.257	0.239	0.93	0.249	0.224	0.90	0.312	0.276	0.88
	K	0.385	0.357	0.93	0.385	0.345	0.90	0.478	0.428	0.89
5 VIS clear O3+CO2	Direct	0.256	0.209	0.82	0.174	0.153	0.88	0.212	0.196	0.92
	TL	0.532	0.39	0.73	0.343	0.307	0.89	0.404	0.391	0.97
	AD	0.569	0.427	0.75	0.381	0.345	0.90	0.429	0.39	0.91
	K	1.363	0.981	0.72	0.7	0.651	0.93	0.79	0.774	0.98
6 Hi-res clear v13pred 7gas	Direct	3.264	2.286	0.70	2.042	2.003	0.98	2.705	2.699	1.00
	TL	5.389	4.11	0.76	3.792	3.696	0.97	5.547	5.518	0.99
	AD	5.825	4.539	0.78	4.213	4.145	0.98	5.769	5.536	0.96
	K	33.191	14.963	0.45	17.605	17.777	1.01	21.293	23.194	1.09
7 Hi-res clear v9pred 7gas	Direct	2.595	1.861	0.72	1.704	1.692	0.99	2.188	2.028	0.93
	TL	4.447	3.355	0.75	3.138	3.082	0.98	4.201	4.032	0.96
	AD	4.814	3.756	0.78	3.559	3.513	0.99	4.564	4.636	1.02
	K	33.644	14.858	0.44	17.635	17.791	1.01	22.951	23.95	1.04
8 Hi-res clear v13pred no gas	Direct	3.244	2.283	0.70	2.009	1.996	0.99	2.842	2.538	0.89
	TL	5.369	4.092	0.76	3.754	3.722	0.99	5.51	5.766	1.05
	AD	5.846	4.498	0.77	4.191	4.114	0.98	5.665	5.571	0.98
	K	28.988	12.89	0.44	14.368	14.287	0.99	21.349	19.048	0.89
9 IR aerosol Chou-scaling	Direct	0.191	0.176	0.92	0.198	0.175	0.89	0.232	0.205	0.88
	TL	0.58	0.365	0.63	0.449	0.41	0.91	0.463	0.429	0.93
	AD	0.641	0.427	0.67	0.513	0.471	0.92	0.523	0.476	0.91
	K	1.012	0.582	0.58	0.693	0.649	0.94	0.742	0.687	0.93
10 IR hydro Chou-scaling	Direct	1.513	0.996	0.66	0.714	0.687	0.96	0.982	0.931	0.95
	TL	2.849	2.068	0.73	1.463	1.421	0.97	2.061	2.012	0.98
	AD	3.133	2.668	0.85	2.01	2.026	1.01	2.414	2.503	1.04
	K	3.499	2.814	0.80	1.989	1.981	1.00	2.627	2.554	0.97

Table 5 (continued below): Speed test results, 1 profile per call, v14.0 without vs with external allocation of trajectory structures. Timings are ms per profile.

11 IR aerosol DOM	Direct	1.44	1.176	0.82	1.243	1.285	1.03	1.546	1.468	0.95
	TL	3.501	2.85	0.81	3.33	3.294	0.99	3.251	3.24	1.00
	AD	48.158	46.43	0.96	50.908	50.85	1.00	62.266	61.628	0.99
	K	48.962	47.14	0.96	50.88	50.83	1.00	61.35	61.31	1.00
12 IR hydro DOM	Direct	34.616	35.462	1.02	36.928	38.854	1.05	41.81	41.654	1.00
	TL	96.865	98.14	1.01	104.34	104.42	1.00	96.295	94.655	0.98
	AD	1983.7	1972.2	0.99	2131.1	2141.5	1.00	2510.5	2547.6	1.01
	K	1988.2	1978.9	1.00	2119.1	2110.3	1.00	2569.6	2577.8	1.00
13 VIS aerosol DOM	Direct	1.556	1.271	0.82	1.241	1.471	1.18	1.358	1.327	0.98
	TL	3.79	2.683	0.71	3.245	3.162	0.97	2.859	2.671	0.93
	AD	9.492	8.261	0.87	9.153	8.993	0.98	8.911	8.772	0.98
	K	10.465	8.804	0.84	9.474	9.345	0.99	9.172	9.646	1.05
14 VIS hydro DOM	Direct	21.304	23.59	1.11	18.358	25.652	1.40	19.324	25.768	1.33
	TL	62.195	59.34	0.95	50.875	55.495	1.09	49.955	52.55	1.05
	AD	297.38	297.7	1.00	310.58	313.04	1.01	323.58	305.26	0.94
	K	300.66	297.4	0.99	307.66	314.24	1.02	319.28	313.58	0.98
15 VIS aer+hyd+ray DOM	Direct	41.324	44.068	1.07	39.664	47.052	1.19	45.268	47.52	1.05
	TL	113.89	109.19	0.96	107.6	112.97	1.05	106.44	105.43	0.99
	AD	1962.8	1929.4	0.98	2111	2155.2	1.02	2501.8	2628.2	1.05
	K	1996.6	1941	0.97	2126	2127	1.00	2534.4	2461.4	0.97
16 VIS hydro MFASIS-NN	Direct	1.645	1.495	0.91	0.971	0.941	0.97	1.232	1.165	0.95
	TL	4.64	4.621	1.00	3.055	3.015	0.99	3.948	4.032	1.02
	AD	8.002	8.018	1.00	3.771	3.742	0.99	5.388	4.867	0.90
	K	8.635	8.233	0.95	3.981	3.942	0.99	5.424	5.115	0.94
17 MW hydro delta-Edd	Direct	0.662	0.632	0.95	0.548	0.521	0.95	0.733	0.718	0.98
	TL	1.411	1.383	0.98	1.278	1.231	0.96	1.611	1.607	1.00
	AD	1.879	1.83	0.97	1.672	1.619	0.97	2.178	2.092	0.96
	K	2.274	2.218	0.98	2.161	2.094	0.97	2.78	2.543	0.91
18 PC O3-only	Direct	3.878	3.829	0.99	3.507	3.485	0.99	5.237	4.644	0.89
	TL	6.986	6.975	1.00	6.695	6.536	0.98	10.475	9.678	0.92
	AD	7.74	7.593	0.98	7.261	7.261	1.00	10.903	11.011	1.01
	K	68.01	39.545	0.58	36.085	35.785	0.99	43.59	37.795	0.87
19 PC, rec rad O3-only	Direct	4.039	3.94	0.98	3.628	3.576	0.99	5.079	4.793	0.94
	TL	7.145	7.168	1.00	6.886	6.768	0.98	10.759	10.356	0.96
	AD	8.084	7.734	0.96	7.428	7.335	0.99	11.097	11.819	1.07
	K	92.61	63.195	0.68	50.545	49.95	0.99	124.7	120.95	0.97
20 PC 6gas	Direct	3.896	3.926	1.01	3.53	3.497	0.99	5.243	5.037	0.96
	TL	7.037	7.004	1.00	6.67	6.637	1.00	10.706	10.167	0.95
	AD	7.836	7.647	0.98	7.259	7.261	1.00	11.1	10.589	0.95
	K	92.485	62.52	0.68	52.32	51.61	0.99	52.445	55.77	1.06
21 PC, rec rad 6gas	Direct	3.995	3.929	0.98	3.674	3.575	0.97	5.489	4.84	0.88
	TL	7.186	7.088	0.99	6.889	6.772	0.98	10.551	10.503	1.00
	AD	7.908	7.867	0.99	7.516	7.385	0.98	11.127	10.604	0.95
	K	116.675	85.92	0.74	66.65	66.635	1.00	131.34	134.92	1.03

Table 5 (continued from above): Speed test results, 1 profile per call, v14.0 without vs with external allocation of trajectory structures. Timings are ms per profile.

Test case	Model	Intel gfortran v13.2	Intel gfortran v14.0	Intel gfortran v14.0:v13.2	Intel ifort v13.2	Intel ifort v14.0	Intel ifort v14.0:v13.2	Cray v13.2	Cray v14.0	Cray v14.0:v13.2
1 SURFEM-Ocean	Direct	0.419	0.331	0.79	0.264	0.229	0.87	0.317	0.26	0.82
	TL	0.864	0.63	0.73	0.583	0.471	0.81	0.647	0.578	0.89
	AD	1.214	0.99	0.82	0.79	0.697	0.88	0.804	0.724	0.90
	K	1.445	1.221	0.85	1.029	0.941	0.91	1.098	1.082	0.98
2 Interp mode 1	Direct	0.212	0.218	1.03	0.17	0.178	1.05	0.227	0.217	0.96
	TL	0.433	0.388	0.90	0.317	0.327	1.03	0.44	0.429	0.98
	AD	0.489	0.432	0.88	0.408	0.398	0.97	0.475	0.464	0.98
	K	0.711	0.674	0.95	0.64	0.649	1.01	0.772	0.787	1.02
3 Interp mode 2	Direct	0.208	0.213	1.02	0.163	0.173	1.06	0.218	0.211	0.97
	TL	0.425	0.377	0.89	0.308	0.321	1.04	0.441	0.415	0.94
	AD	0.479	0.422	0.88	0.396	0.39	0.99	0.483	0.453	0.94
	K	0.703	0.655	0.93	0.626	0.637	1.02	0.763	0.755	0.99
4 Interp mode 3	Direct	0.211	0.212	1.00	0.165	0.175	1.06	0.217	0.226	1.04
	TL	0.43	0.381	0.89	0.313	0.326	1.04	0.433	0.424	0.98
	AD	0.484	0.425	0.88	0.398	0.394	0.99	0.48	0.469	0.98
	K	0.708	0.666	0.94	0.639	0.641	1.00	0.782	0.78	1.00
5 Interp mode 4	Direct	0.215	0.22	1.02	0.177	0.183	1.03	0.225	0.226	1.00
	TL	0.444	0.402	0.90	0.339	0.341	1.01	0.476	0.452	0.95
	AD	0.506	0.447	0.88	0.42	0.409	0.97	0.515	0.484	0.94
	K	0.741	0.684	0.92	0.662	0.65	0.98	0.821	0.793	0.97
6 Interp mode 5	Direct	0.215	0.22	1.02	0.175	0.18	1.03	0.223	0.217	0.97
	TL	0.439	0.394	0.90	0.33	0.338	1.02	0.452	0.445	0.98
	AD	0.5	0.446	0.89	0.416	0.401	0.96	0.491	0.479	0.97
	K	0.724	0.677	0.94	0.655	0.647	0.99	0.771	0.818	1.06
7 Interp mode 1 Pressure grad	Direct	0.215	0.215	1.00	0.168	0.179	1.07	0.218	0.212	0.97
	TL	0.461	0.407	0.88	0.333	0.347	1.04	0.46	0.45	0.98
	AD	0.557	0.485	0.87	0.446	0.436	0.98	0.555	0.522	0.94
	K	1.261	1.171	0.93	1.169	1.136	0.97	1.419	1.408	0.99
8 Interp mode 2 Pressure grad	Direct	0.211	0.213	1.01	0.163	0.172	1.05	0.212	0.207	0.98
	TL	0.44	0.387	0.88	0.317	0.333	1.05	0.451	0.429	0.95
	AD	0.513	0.443	0.86	0.416	0.405	0.97	0.489	0.464	0.95
	K	0.882	0.808	0.92	0.781	0.753	0.96	0.907	0.888	0.98
9 Interp mode 3 Pressure grad	Direct	0.21	0.212	1.01	0.172	0.174	1.02	0.218	0.209	0.96
	TL	0.451	0.397	0.88	0.324	0.339	1.04	0.481	0.441	0.92
	AD	0.537	0.461	0.86	0.428	0.414	0.97	0.537	0.538	1.00
	K	1.058	0.981	0.93	0.98	0.944	0.96	1.183	1.222	1.03
10 Interp mode 4 Pressure grad	Direct	0.218	0.221	1.01	0.177	0.182	1.03	0.228	0.22	0.96
	TL	0.468	0.42	0.90	0.365	0.368	1.01	0.509	0.468	0.92
	AD	0.576	0.496	0.86	0.473	0.454	0.96	0.568	0.564	0.99
	K	1.262	1.171	0.93	1.194	1.145	0.96	1.475	1.495	1.01
11 Interp mode 5 Pressure grad	Direct	0.216	0.219	1.01	0.175	0.18	1.03	0.225	0.217	0.96
	TL	0.466	0.409	0.88	0.353	0.356	1.01	0.509	0.451	0.89
	AD	0.559	0.478	0.86	0.449	0.439	0.98	0.565	0.538	0.95
	K	1.085	0.989	0.91	1.001	0.954	0.95	1.217	1.225	1.01

Table 6: Additional speed test results, 1 profile per call with external allocation of trajectory structures, v13.2 vs v14.0. Timings are ms per profile.

2. Memory comparisons

Peak memory usage was measured using valgrind's massif tool. This is intended to give a rough idea of memory requirements for different types of simulation and, more importantly, to enable comparisons between different versions of RTTOV and between RTTOV configurations. Tests were performed on an Intel desktop using the gfortran v11.2.0 compiler and the results are shown in Table 7. The colour-coding is as follows:

- green => peak memory for v14.0 90% or less than that for v13.2
- blue => peak memory for v14.0 90-95% than that for v13.2
- white => peak memory for v14.0 within +/-5% that of v13.2
- orange => peak memory for v14.0 105-110% than that for v13.2
- red => peak memory for v14.0 110% or more than that for v13.2

The IASI tests are run after extracting coefficients for the required channels for each test to separate "binary" (Fortran unformatted) files. This gives a more representative idea of the memory usage of the simulation itself, otherwise the peak memory is dominated by that required to read in the full netCDF coefficient files.

RTTOV v14.0 requires less memory than v13.2 for all simulation types (in many cases significantly so) except for MFASIS-NN.

Optical depth coefficients, PC-RTTOV coefficients, and aerosol and hydrometeor optical property values are all stored in single precision arrays in RTTOV v14.0 while they are double precision in RTTOV v13 and earlier. These data therefore require half the memory in v14.0 compared to v13.2. For simulations where memory consumption is dominated by the coefficients and/or optical properties (such as MW scattering, and simulations involving hyperspectral sounders) the results are substantial.

There are some other changes in RTTOV v14.0 which require additional memory (such as changes made to simplify the code), and some changes that reduce the memory requirements (such as being more careful about allocating only the memory required for the TL/AD/K, and no longer requiring additional data specifically related to the near-surface layer). However, the impacts of these changes are relatively small compared to the change in precision described above for most simulation types.

For MFASIS-NN, the run-time optimisation has resulted in a significant increase in the memory footprint.

Test case	Model	v13.2 peak memory (MB)	v14.0 peak memory (MB)	v14.0:v13.2
1 MW clear no gas	Direct	1.953	1.875	0.96
	TL	2.062	1.875	0.90
	AD	2.086	1.875	0.89
	K	3.076	2.881	0.93
2 MW clear O3-only	Direct	1.624	1.566	0.96
	TL	1.799	1.67	0.92
	AD	1.813	1.68	0.92
	K	2.467	2.404	0.97
3 MW clear CLW abs	Direct	1.953	1.875	0.96
	TL	2.079	1.875	0.90
	AD	2.103	1.875	0.89
	K	3.268	3.16	0.96
4 IR clear O3+CO2	Direct	1.834	1.685	0.91
	TL	1.914	1.71	0.89
	AD	1.923	1.716	0.89
	K	2.344	2.2	0.93
5 VIS clear O3+CO2	Direct	1.839	1.649	0.89
	TL	2.071	1.868	0.90
	AD	2.08	1.874	0.90
	K	2.85	2.686	0.94
6 Hi-res clear v13pred 7gas	Direct	16.59	10.68	0.64
	TL	18.64	11.76	0.63
	AD	18.83	11.96	0.63
	K	52.94	47.06	0.88
7 Hi-res clear v9pred 7gas	Direct	14.05	8.641	0.61
	TL	16.11	9.822	0.60
	AD	16.29	9.927	0.60
	K	51.63	46.27	0.89
8 Hi-res clear v13pred no gas	Direct	16.57	10.67	0.64
	TL	18.61	11.73	0.63
	AD	18.8	11.93	0.63
	K	50.84	45.16	0.88
9 IR aerosol Chou-scaling	Direct	2.573	2.006	0.77
	TL	2.606	2.349	0.90
	AD	2.603	2.353	0.90
	K	3.131	2.943	0.93
10 IR hydro Chou-scaling	Direct	4.501	3.677	0.81
	TL	5.632	4.699	0.83
	AD	5.64	4.703	0.83
	K	7.926	7.185	0.90

Table 7 (continued below): Memory test results.

11 IR aerosol DOM	Direct	2.667	2.006	0.75
	TL	3.586	2.349	0.65
	AD	5.357	2.353	0.43
	K	5.897	2.943	0.49
12 IR hydro DOM	Direct	4.428	3.677	0.83
	TL	13.64	4.699	0.34
	AD	15.47	4.703	0.30
	K	17.76	7.185	0.40
13 VIS aerosol DOM	Direct	4.174	3.786	0.90
	TL	8.766	7.072	0.80
	AD	8.953	7.256	0.81
	K	9.819	8.235	0.83
14 VIS hydro DOM	Direct	7.681	5.144	0.66
	TL	33.74	19.23	0.56
	AD	34.32	19.8	0.57
	K	36.93	22.61	0.61
15 VIS aer+hyd+ray DOM	Direct	9.77	6.304	0.64
	TL	36.2	20.87	0.57
	AD	38.35	23.13	0.60
	K	41.06	25.95	0.63
16 VIS hydro MFASIS-NN	Direct	4.199	4.706	1.12
	TL	4.439	13.7	3.08
	AD	4.444	13.72	3.08
	K	5.912	15.32	2.59
17 MW hydro delta-Edd	Direct	72.03	35.12	0.48
	TL	72.73	35.12	0.48
	AD	72.74	35.12	0.48
	K	73.47	35.12	0.47
18 PC O3-only	Direct	104.9	56.83	0.54
	TL	104.9	56.83	0.54
	AD	104.9	56.83	0.54
	K	137.1	109.5	0.79
19 PC, rec rad O3-only	Direct	42.79	25.56	0.59
	TL	42.79	25.82	0.60
	AD	42.79	25.83	0.60
	K	87.59	84.93	0.96
20 PC 6gas	Direct	104.9	56.83	0.54
	TL	104.9	56.83	0.54
	AD	104.9	56.83	0.54
	K	140.7	112.4	0.79
21 PC, rec rad 6gas	Direct	42.79	25.56	0.59
	TL	42.79	25.84	0.60
	AD	42.79	25.85	0.60
	K	91.22	87.79	0.96

Table 7 (continued from above): Memory test results.