RTTOV v14.1 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 v14.1 with that of RTTOV v14.0. This includes comparisons of execution speed and peak memory usage.

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. The ATMS, ICI, and FCI coefficients are on 54L, and the IASI coefficients are on 101L. FCI MFASIS-NN simulations used the v14.0 MFASIS-NN coefficients. 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.
- SURFEM-Ocean 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 was run with 300 predictor channels and 300 PC scores.
- PC-RTTOV reconstructed radiances were calculated for 300 channels.

Unless stated otherwise, all options use the RTTOV v14 default values.

1. Speed comparisons

Tests were performed on an AMD compute cluster (Milan) using gfortran v11.5.0 and ifort v19.0.0, and a Cray EX HPC (AMD Milan) using the Cray Fortran compiler v15.0.0.

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 v14.1 and v14.0, and Table 5 compares RTTOV v14.1 without and with the external allocation.

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 => v14.1 more than 10% faster than v14.0
- blue => v14.1 5-10% faster than v14.0
- white => v14.1 run-time within +/-5% that of v14.0
- orange => v14.1 5-10% slower than v14.0
- red => v14.1 more than 10% slower than v14.0

Note the following known/expected impact of specific code changes in RTTOV v14.1 on the timing results:

1. The SURFEM-Ocean MW sea surface emissivity model was modified to exploit vector array operations in place of loops within the neural network inference. In testing during development, this improved the performance with gfortran which is by far the most commonly-used compiler among users according to the user surveys, but there was evidence of a slight degradation in performance with ifort.

2. Updates to the cloud overlap schemes revealed that the existing maximum-random overlap code was in some cases generating redundant cloud columns with zero width. These require additional memory, and a full radiance calculation for each additional column with no impact on simulated radiance. Therefore VIS/IR hydrometeor simulations (all solvers) are expected to run more quickly in v14.1.

3. The DOM solar solver was optimised when Rayleigh multiple scattering is enabled. Therefore, the test that includes Rayleigh multiple scattering (which also includes aerosol and hydrometeors) is expected to be faster due to the cloud columns update described above and the DOM optimisation. Testing during development indicated that the refactoring involved in this update resulted in a modest slow-down for DOM solar simulations with Rayleigh single scattering.

Some additional code changes may contribute to unintentional changes in run-time performance:

4. As part of the cloud overlap updates, the code was refactored to allow for in-cloud inhomogeneity. This was done in anticipation of future developments. These changes to do increase memory requirements or introduce significant additional computations for the existing cloud overlap schemes, but it is possible that the changes may interfere with certain compiler optimisations that were previously possible.

5. MFASIS-NN has undergone various updates and the memory requirements increased which may affect run-time performance.

6. The changes to allow over-allocation of the trajectory structures in *nprofiles* required explicitly specifying array bounds in numerous places which may have some impact on performance, although if so, it is not a consistent impact throughout the tests carried out here as might be expected.

As usual, the timing results exhibit some noise which hinders interpretation of the results. **It is important to read the text descriptions below as subsequent ad-hoc testing indicates that not all results from the testing scripts shown in the tables are replicable.**

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

For the clear-sky MW simulations, the SURFEM-Ocean optimisation has improved performance with gfortran as expected. Testing during development indicated a small degradation in performance with ifort. The performance testing run here shows that the Cray compiler is impacted to a greater extent.

For multi-spectral VIS/IR clear-sky simulations, there is little difference in run-time as expected.

Results for hi-res clear-sky simulations mostly show no change. However, the unexpected increase in K model run-times for the 7gas cases with gfortran are replicable. As in many other cases, the differences appear to be in the time spent in system calls rather in RTTOV itself, so perhaps is related to the way the compilers are managing memory, and it could be related to some interaction of specific simulations with the specific hardware (CPU cache etc) in the test system. The slowdown in the TL model with the v9 predictor file is also replicable although the ad-hoc testing suggests the amount of slowdown is less than shown in this table. The speed-up for the K model in the "no gas" test with gfortran is also replicable and similarly unexpected.

The apparently systematic slight slowdown for IR Chou-scaling aerosol simulations across all models and compilers is not supported by ad-hoc testing which indicates similar run-times for v14.0 and v14.1.

The VIS and IR DOM aerosol results show similar run-times for v14.0 and v14.1. The TL slow-down for ifort for the IR simulations was not replicated in ad-hoc testing. The TL slow-down with gfortran is replicated but may not be as large as that shown in the table. Note that testing during development indicated that the DOM Rayleigh multiple scattering optimisation resulted in a slight slow-down for Rayleigh single-scattering DOM simulations, which may be the reason for the marginally slower performance in the VIS aerosol runs in some cases.

The reduction in run-time observed for the IR Chou-scaling and VIS and IR DOM hydrometeor simulations is expected due to the elimination of redundant cloud columns described above. The further reduction in run-time when Rayleigh multiple scattering is included is also expected.

The MFASIS-NN results show a speed-up for ifort and Cray which can be explained by the elimination of redundant cloud columns. It is not clear why for gfortran there is a significant slow-down. It should be noted though that MFASIS-NN has been optimised for multiple profiles per call, so it is recommended to pass in multiple profiles rather than one profile as in this test for best performance.

The MW hydrometeor simulations with delta-Eddington show a speed-up for gfortran and a degradation for ifort and Cray. Since SURFEM-Ocean is used here this will have an impact. For the Cray compiler, ad-hoc testing suggests there may be some additional contribution to the slow-down beyond the SURFEM-Ocean changes. It is conceivable that this is due to the refactoring to support in-cloud inhomogeneity described above.

The PC-RTTOV results show no change for ifort and Cray compilers. The degradation for gfortran is not replicable.

Table 3: 50 profiles per call, v14.0 vs v14.1

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 v14.1 and v14.0 for the case of multiple profiles per call.

The results for clear-sky MW simulations are somewhat mixed. The impact of the SURFEM-Ocean optimisation discussed above is evident again. The slowdown for the TL model with gfortran is a replicable result and is not related to SURFEM-Ocean, i.e., it can be seen in the same simulation with a fixed surface emissivity meaning the emissivity model is not called. The reasons for this are unclear even after profiling, as there have been no obvious substantive code changes in relevant routines for this type of simulation and it is not observed in the single-profile calls. The test suite timing output indicates that the increase in run-time is seen in system calls rather than the time spent in the RTTOV code itself which suggests it could be related to memory management by the compiler.

For multi-spectral VIS/IR clear-sky simulations, the results are mixed. For gfortran clear-sky IR, the TL slowdown is replicable, as is the K model speed-up, though in ad-hoc runs the performance gain is not as large as reported in the table. Neither change is expected. The slowdown for ifort K model IR clear-sky is not replicated by ad-hoc testing. The slow-downs for clear-sky VIS with gfortran appear to be replicable in ad-hoc testing, but the slow-down may not be as large as indicated in the table. The VIS clear-sky direct and TL slowdown with the Cray compiler is not replicated by ad-hoc testing.

The hi-res clear-sky tests show broadly neutral results for ifort and Cray compilers, but a substantial and, again unexpected, improvement in run-time for gfortran. These gfortran results are not supported by ad-hoc testing which suggest broadly similar run-times for v14.0 and v14.1.

The IR Chou-scaling aerosol results are mixed. The slight slow-down for Cray is supported by ad-hoc testing, but the slow-down for ifort is not. The speed-up for gfortran is not supported by ad-hoc testing, but the slow-down in the AD with gfortran is replicable.

The VIS and IR DOM aerosol results show similar run-times for v14.0 and v14.1. The slow-down for the TL model for IR simulations with ifort is supported by ad-hoc testing, although the slow-down may be less than indicated in the table. Note that testing during development indicated that the DOM Rayleigh multiple scattering optimisation resulted in a slight slow-down for Rayleigh single-scattering DOM simulations, which may be the reason for the marginally slower performance in the VIS aerosol runs in some cases.

The reduction in run-time observed for the IR Chou-scaling and VIS and IR DOM hydrometeor simulations is expected due to the elimination of redundant cloud columns described above. The further reduction in run-time when Rayleigh multiple scattering is included is also expected.

The MFASIS-NN results show a speed-up for all models and compilers which can be explained by the elimination of the redundant cloud columns. The dramatic speed-up for ifort is borne out by ad-hoc testing. This seems unlikely to be solely due to the cloud columns optimisation, so the cause is not fully understood.

The MW hydrometeor simulation results are consistent with those for the single-profile case above.

The PC-RTTOV results show no change for ifort and Cray compilers. The speed-up for gfortran is not replicable.

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

Clear-sky MW simulations show similar results to the single-profile case without external trajectory structure allocation.

For multi-spectral VIS/IR clear-sky simulations, gfortran and Cray show similar run-times while a small slow-down is observed for ifort.

The results for hi-res clear-sky simulations indicate broadly similar performance in v14.0 and v14.1 especially when considering variable results for the single- and multiple-profile tests described above.

The IR Chou-scaling aerosol results for Cray are not strongly supported by ad-hoc testing which suggests similar run-times. The degradation in performance for ifort is also not supported by ad-hoc testing.

The VIS and IR DOM aerosol results show similar run-times for v14.0 and v14.1. Note that testing during development indicated that the DOM Rayleigh multiple scattering optimisation resulted in a slight slow-down for Rayleigh single-scattering DOM simulations, which may be the reason for the marginally slower performance in the VIS aerosol runs in some cases.

The reduction in run-time observed for the IR Chou-scaling and VIS and IR DOM hydrometeor simulations is expected due to the elimination of redundant cloud columns described above. The further reduction in run-time when Rayleigh multiple scattering is included is also expected.

For MFASIS-NN, again we see an improvement for ifort and Cray. The results for gfortran are quite neutral suggesting that the benefits of the trajectory allocation are roughly balancing the degradation observed in the single-profile calls without trajectory allocation above.

The MW hydrometeor simulation results are consistent with those for the single-profile case above.

The PC-RTTOV results show essentially no change in performance.

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

This table demonstrates the benefits in v14.1 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. This is because the calls without trajectory allocation (aside from the caveated cases) allocate the same amount of memory, but they do this in every call to RTTOV instead of once before all calls, so they cannot be any faster than the calls with external allocation.

Generally, greatest benefit is obtained for gfortran and indeed the results indicate that benefits may be obtained across all simulation types with gfortran. It is particularly with ifort that one may see a degradation with VIS/IR scattering simulations.

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.

Test case	Model	Intel gfortran v14.0	Intel gfortran v14.1	Intel gfortran v14.1:v14.0	Intel ifort v14.0	Intel ifort v14.1	Intel ifort v14.1:v14.0	Cray v14.0	Cray v14.1	Cray v14.1:v14.0
1 MW clear no gas	Direct	0.187	0.168	0.90	0.206	0.221	1.07	0.112	0.125	1.12
	TL	0.382	0.339	0.89	0.442	0.442	1.00	0.228	0.268	1.18
	AD	0.557	0.443	0.79	0.653	0.68	1.04	0.351	0.361	1.03
	K	0.769	0.645	0.84	0.853	0.884	1.04	0.486	0.511	1.05
2 MW clear O3-only	Direct	0.116	0.11	0.95	0.134	0.142	1.05	0.079	0.087	1.10
	TL	0.236	0.22	0.94	0.283	0.277	0.98	0.155	0.172	1.11
	AD	0.351	0.297	0.85	0.416	0.423	1.02	0.223	0.235	1.05
	K	0.497	0.444	0.89	0.56	0.574	1.02	0.34	0.341	1.00
3 MW clear CLW abs	Direct	0.263	0.244	0.93	0.318	0.328	1.03	0.17	0.184	1.08
	TL	0.558	0.539	0.97	0.684	0.678	0.99	0.356	0.397	1.11
	AD	0.742	0.665	0.90	0.902	0.922	1.02	0.471	0.514	1.09
	K	1.284	1.168	0.91	1.458	1.521	1.04	0.739	0.802	1.08
4 IR clear O3+CO2	Direct	0.074	0.076	1.03	0.091	0.092	1.01	0.06	0.06	1.00
	TL	0.146	0.15	1.02	0.175	0.176	1.00	0.114	0.114	1.00
	AD	0.164	0.169	1.03	0.207	0.21	1.02	0.125	0.13	1.04
	K	0.269	0.276	1.03	0.314	0.316	1.01	0.198	0.204	1.03
5 VIS clear O3+CO2	Direct	0.118	0.12	1.02	0.143	0.143	1.00	0.085	0.088	1.04
	TL	0.24	0.243	1.01	0.28	0.283	1.01	0.163	0.166	1.02
	AD	0.262	0.266	1.01	0.331	0.334	1.01	0.182	0.183	1.01
	K	0.62	0.58	0.94	0.722	0.731	1.01	0.346	0.347	1.00
6 Hi-res clear v13pred 7gas	Direct	1.55	1.567	1.01	1.6	1.603	1.00	1.077	1.091	1.01
	TL	2.893	2.959	1.02	2.978	2.977	1.00	2.15	2.154	1.00
	AD	3.311	3.46	1.04	3.538	3.607	1.02	2.328	2.347	1.01
	K	18.966	24.551	1.29	26.717	27.13	1.02	12.06	11.429	0.95
7 Hi-res clear v9pred 7gas	Direct	1.678	1.542	0.92	1.829	1.86	1.02	0.885	0.873	0.99
	TL	2.339	2.887	1.23	2.742	2.743	1.00	1.728	1.77	1.02
	AD	3.107	3.202	1.03	3.282	3.275	1.00	1.918	1.941	1.01
	K	13.338	17.885	1.34	26.29	26.797	1.02	11.783	11.159	0.95
8 Hi-res clear v13pred no gas	Direct	1.514	1.568	1.04	1.591	1.597	1.00	1.08	1.091	1.01
	TL	2.875	2.95	1.03	2.939	2.937	1.00	2.12	2.223	1.05
	AD	3.565	3.897	1.09	3.481	3.556	1.02	2.322	2.297	0.99
	K	15.958	13.721	0.86	22.887	21.078	0.92	9.929	9.267	0.93
9 IR aerosol Chou-scaling	Direct	0.124	0.134	1.08	0.155	0.168	1.08	0.101	0.108	1.06
	TL	0.263	0.284	1.08	0.329	0.35	1.06	0.244	0.258	1.06
	AD	0.31	0.334	1.08	0.384	0.415	1.08	0.288	0.315	1.09
	K	0.435	0.466	1.07	0.555	0.582	1.05	0.383	0.421	1.10
10 IR hydro Chou-scaling	Direct	0.75	0.522	0.70	1.036	0.669	0.65	0.397	0.295	0.74
	TL	1.571	1.106	0.70	1.752	0.907	0.52	0.874	0.68	0.78
	AD	1.848	1.209	0.65	2.541	1.371	0.54	1.167	0.848	0.73
	K	1.641	1.505	0.92	2.485	1.635	0.66	1.296	0.983	0.76

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

11 IR aerosol DOM	Direct	0.82	0.865	1.05	1.046	1.066	1.02	0.781	0.816	1.04
	TL	1.92	2.512	1.31	2.456	2.822	1.15	1.86	1.832	0.98
	AD	38.718	39.942	1.03	39.578	40.172	1.02	25.02	26.196	1.05
	K	38.824	40.616	1.05	39.716	40.072	1.01	24.96	25.402	1.02
12 IR hydro DOM	Direct	22.76	14.51	0.64	28.476	17.392	0.61	21.298	12.646	0.59
	TL	58.675	37.68	0.64	73.34	44.095	0.60	48.2	28.99	0.60
	AD	1642.4	979.7	0.60	1668.3	969.9	0.58	1056.1	610.9	0.58
	K	1633.5	1001.1	0.61	1664.2	974.5	0.59	1068.5	618.8	0.58
13 VIS aerosol DOM	Direct	3.62	3.913	1.08	4.46	4.64	1.04	3.428	3.505	1.02
	TL	8.652	8.647	1.00	10.698	10.374	0.97	7.529	7.731	1.03
	AD	39.29	41.294	1.05	46.991	46.9	1.00	25.9	26.294	1.02
	K	40.415	41.448	1.03	46.967	47.783	1.02	26.057	26.285	1.01
14 VIS hydro DOM	Direct	50.382	31.926	0.63	60.912	38.148	0.63	45.26	26.334	0.58
	TL	124.215	82.67	0.67	160.265	98.81	0.62	101.125	62.625	0.62
	AD	1479.64	722.62	0.49	1682.54	806.5	0.48	945.68	449.18	0.47
	K	1477.72	720.58	0.49	1675.56	813.1	0.49	926.84	454.48	0.49
15 VIS aer+hyd+ray DOM	Direct	136.208	68.272	0.50	166.02	83.288	0.50	126.576	59.2	0.47
	TL	334.64	163.97	0.49	415.4	202.6	0.49	285.68	136.48	0.48
	AD	12203.8	3932.6	0.32	12809.2	4070.6	0.32	7895.4	2414.4	0.31
	K	12205	3912.6	0.32	12769.8	4051.4	0.32	7843.6	2431.4	0.31
16 VIS hydro MFASIS-NN	Direct	0.77	1.022	1.33	0.742	0.53	0.71	0.504	0.384	0.76
	TL	3.332	3.118	0.94	2.3	1.556	0.68	1.572	1.139	0.72
	AD	6.264	9.373	1.50	2.725	2.014	0.74	1.913	1.558	0.81
	K	6.897	9.734	1.41	3.16	2.402	0.76	2.039	1.606	0.79
17 MW hydro delta-Edd	Direct	0.57	0.521	0.91	0.59	0.667	1.13	0.461	0.555	1.21
	TL	1.294	1.201	0.93	1.411	1.48	1.05	1.109	1.374	1.24
	AD	2.003	1.742	0.87	2.079	2.219	1.07	1.595	1.776	1.11
	K	2.332	2.086	0.89	2.58	2.732	1.06	1.875	2.126	1.13
18 PC O3-only	Direct	2.642	2.85	1.08	2.81	2.833	1.01	1.877	1.903	1.01
	TL	5.06	5.646	1.12	5.223	5.276	1.01	3.825	3.824	1.00
	AD	5.747	6.534	1.14	6.132	6.278	1.02	4.108	4.149	1.01
	K	35.015	36.265	1.04	50.035	48.8	0.98	25.18	24.82	0.99
19 PC, rec rad O3-only	Direct	2.735	3.046	1.11	2.929	2.929	1.00	1.929	1.923	1.00
	TL	5.195	5.95	1.15	5.413	5.476	1.01	3.882	3.835	0.99
	AD	5.888	6.756	1.15	6.29	6.421	1.02	4.23	4.259	1.01
	K	59.9	62.15	1.04	48.55	48.5	1.00	54.39	54.92	1.01
20 PC 6gas	Direct	2.632	2.995	1.14	2.825	2.836	1.00	1.891	1.892	1.00
	TL	5.004	5.67	1.13	5.271	5.234	0.99	3.783	3.84	1.02
	AD	5.697	6.523	1.15	6.168	6.356	1.03	4.111	4.062	0.99
	K	57.895	59.175	1.02	75.87	76.305	1.01	34.845	34.925	1.00
21 PC, rec rad 6gas	Direct	2.729	2.985	1.09	2.968	2.96	1.00	1.913	1.92	1.00
	TL	5.167	5.908	1.14	5.497	5.505	1.00	3.899	3.848	0.99
	AD	5.855	6.71	1.15	6.314	6.47	1.02	4.24	4.225	1.00
	K	82.515	85.315	1.03	73.665	73.855	1.00	65.02	64.33	0.99

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

Test case	Model	Intel gfortran v14.0	Intel gfortran v14.1	Intel gfortran v14.1:v14.0	Intel ifort v14.0	Intel ifort v14.1	Intel ifort v14.1:v14.0	Cray v14.0	Cray v14.1	Cray v14.1:v14.0
1 MW clear no gas	Direct	0.272	0.227	0.83	0.27	0.294	1.09	0.1	0.108	1.08
	TL	0.385	0.437	1.14	0.534	0.549	1.03	0.204	0.243	1.19
	AD	0.621	0.543	0.87	0.729	0.777	1.06	0.315	0.343	1.09
	K	1.481	1.095	0.74	1.294	1.618	1.25	0.66	0.704	1.07
2 MW clear O3-only	Direct	0.18	0.159	0.88	0.173	0.185	1.07	0.067	0.071	1.05
	TL	0.229	0.229	1.00	0.334	0.347	1.04	0.132	0.147	1.11
	AD	0.423	0.295	0.70	0.467	0.495	1.06	0.197	0.211	1.07
	K	0.509	0.431	0.85	0.918	1.076	1.17	0.415	0.427	1.03
3 MW clear CLW abs	Direct	0.352	0.313	0.89	0.382	0.406	1.06	0.156	0.167	1.07
	TL	0.569	0.637	1.12	0.778	0.796	1.02	0.333	0.377	1.13
	AD	0.881	0.736	0.84	0.996	1.04	1.04	0.45	0.475	1.06
	K	1.396	1.393	1.00	1.708	2.138	1.25	0.964	0.999	1.04
4 IR clear O3+CO2	Direct	0.115	0.114	0.99	0.126	0.133	1.05	0.045	0.045	1.00
	TL	0.109	0.125	1.15	0.224	0.235	1.05	0.088	0.088	0.99
	AD	0.125	0.129	1.03	0.252	0.267	1.06	0.097	0.105	1.08
	K	0.466	0.262	0.56	0.594	0.665	1.12	0.229	0.218	0.95
5 VIS clear O3+CO2	Direct	0.126	0.183	1.45	0.192	0.199	1.04	0.07	0.077	1.10
	TL	0.193	0.209	1.08	0.35	0.363	1.04	0.133	0.147	1.11
	AD	0.216	0.249	1.16	0.408	0.429	1.05	0.151	0.156	1.04
	K	0.544	0.584	1.07	1.07	1.108	1.04	0.405	0.392	0.97
6 Hi-res clear v13pred 7gas	Direct	2.613	2.082	0.80	3.05	3.087	1.01	1.323	1.295	0.98
	TL	4.664	3.256	0.70	4.892	5.017	1.03	2.645	2.674	1.01
	AD	5.166	3.73	0.72	5.453	5.715	1.05	2.948	2.962	1.00
	K	32.845	15.952	0.49	33.456	34.884	1.04	12.984	13.179	1.02
7 Hi-res clear v9pred 7gas	Direct	1.676	1.685	1.00	2.336	2.405	1.03	1.149	0.989	0.86
	TL	3.569	2.645	0.74	3.839	3.957	1.03	1.968	2.005	1.02
	AD	4.029	3.015	0.75	4.451	4.584	1.03	2.309	2.308	1.00
	K	31.956	15.907	0.50	33.745	34.948	1.04	13.061	13.894	1.06
8 Hi-res clear v13pred no gas	Direct	2.852	1.941	0.68	3.038	3.11	1.02	1.284	1.354	1.05
	TL	4.727	3.106	0.66	4.861	4.988	1.03	2.547	2.63	1.03
	AD	5.238	3.657	0.70	5.397	5.63	1.04	2.852	2.891	1.01
	K	28.573	13.756	0.48	28.098	29.017	1.03	10.378	10.997	1.06
9 IR aerosol Chou-scaling	Direct	0.149	0.133	0.89	0.263	0.284	1.08	0.084	0.089	1.06
	TL	0.262	0.26	0.99	0.551	0.586	1.06	0.233	0.242	1.04
	AD	0.29	0.327	1.13	0.608	0.663	1.09	0.305	0.312	1.02
	K	0.459	0.46	1.00	1.108	1.174	1.06	0.505	0.533	1.06
10 IR hydro Chou-scaling	Direct	0.637	0.5	0.79	1.302	0.884	0.68	0.465	0.324	0.70
	TL	1.734	0.906	0.52	2.167	1.504	0.69	1.065	0.736	0.69
	AD	1.794	1.067	0.60	3.008	2.034	0.68	1.398	0.965	0.69
	K	1.932	1.452	0.75	3.137	2.431	0.78	1.655	1.194	0.72

Table 3 (continued below): Speed test results, 50 profiles per call, v14.0 vs v14.1. Timings are ms per profile.

11 IR aerosol DOM	Direct	0.82	0.816	1.00	1.016	1.074	1.06	0.789	0.782	0.99
	TL	1.925	1.881	0.98	2.423	3.196	1.32	1.95	1.957	1.00
	AD	39.268	38.99	0.99	39.464	41.452	1.05	25.364	25.342	1.00
	K	38.938	39.214	1.01	39.71	41.95	1.06	25.406	25.274	0.99
12 IR hydro DOM	Direct	22.856	14.248	0.62	28.294	18.354	0.65	21.406	12.466	0.58
	TL	59.05	36.625	0.62	72.575	45.83	0.63	49.62	29.75	0.60
	AD	1647.4	965.8	0.59	1664.3	994.7	0.60	1052.3	618.6	0.59
	K	1648.7	965	0.59	1661.9	996.4	0.60	1057.2	613.7	0.58
13 VIS aerosol DOM	Direct	3.603	3.776	1.05	4.832	5.186	1.07	3.626	3.463	0.96
	TL	8.316	8.437	1.01	10.937	11.528	1.05	8.502	7.914	0.93
	AD	38.943	39.657	1.02	46.5	48.839	1.05	27.657	26.583	0.96
	K	39.387	40.092	1.02	46.379	49.85	1.07	27.174	27.046	1.00
14 VIS hydro DOM	Direct	50.342	31.034	0.62	61.618	39.466	0.64	45.094	28.888	0.64
	TL	125	78.9	0.63	154.92	102.99	0.66	105.41	64.02	0.61
	AD	1492.18	703.1	0.47	1669.16	833.74	0.50	934.22	453.72	0.49
	K	1492.42	705.68	0.47	1672.9	831.74	0.50	948.46	451.78	0.48
15 VIS aer+hyd+ray DOM	Direct	138.012	66.524	0.48	165.224	86.54	0.52	124.044	59.392	0.48
	TL	338.68	159.61	0.47	415.72	208.82	0.50	286.2	137.72	0.48
	AD	12282.2	3829.8	0.31	12728.2	4178	0.33	7839.4	2419.6	0.31
	K	12294.6	3840.8	0.31	12706.4	4185.6	0.33	7809.4	2430.8	0.31
16 VIS hydro MFASIS-NN	Direct	0.842	0.537	0.64	0.782	0.251	0.32	0.422	0.269	0.64
	TL	2.378	1.455	0.61	2.299	0.465	0.20	1.421	0.839	0.59
	AD	2.89	1.725	0.60	2.555	1.309	0.51	1.682	1.028	0.61
	K	2.884	2.002	0.69	2.832	1.566	0.55	1.726	1.16	0.67
17 MW hydro delta-Edd	Direct	0.706	0.618	0.88	0.655	0.747	1.14	0.471	0.531	1.13
	TL	1.586	1.41	0.89	1.546	1.664	1.08	1.18	1.311	1.11
	AD	2.355	1.977	0.84	2.232	2.422	1.09	1.73	1.878	1.09
	K	3.221	2.584	0.80	3.214	3.503	1.09	2.257	2.398	1.06
18 PC O3-only	Direct	4.959	3.147	0.63	5.199	5.374	1.03	2.303	2.323	1.01
	TL	7.746	5.675	0.73	8.254	8.42	1.02	4.589	4.627	1.01
	AD	8.6	6.459	0.75	9.095	9.366	1.03	5.131	5.184	1.01
	K	68.195	45.54	0.67	65.32	67.595	1.03	25.99	26.6	1.02
19 PC, rec rad O3-only	Direct	4.941	3.241	0.66	4.839	4.939	1.02	2.331	2.354	1.01
	TL	7.784	5.856	0.75	6.626	6.812	1.03	4.686	4.684	1.00
	AD	8.525	6.609	0.78	7.542	8.012	1.06	5.284	5.312	1.01
	K	91.765	69.955	0.76	77.375	80.365	1.04	56.36	55.95	0.99
20 PC 6gas	Direct	4.813	3.216	0.67	5.185	5.336	1.03	2.301	2.304	1.00
	TL	7.532	5.784	0.77	8.293	8.546	1.03	4.612	4.622	1.00
	AD	8.384	6.459	0.77	9.222	9.53	1.03	5.148	5.164	1.00
	K	93.92	68.445	0.73	94.53	97.355	1.03	36.655	37.655	1.03
21 PC, rec rad 6gas	Direct	4.825	3.232	0.67	5.432	5.043	0.93	2.389	2.336	0.98
	TL	7.774	5.805	0.75	7.402	6.979	0.94	4.653	4.658	1.00
	AD	8.664	6.592	0.76	8.695	7.978	0.92	5.315	5.257	0.99
	K	119.475	92.36	0.77	106.005	109.39	1.03	65.775	65.43	0.99

Table 3 (continued from above): Speed test results, 50 profiles per call, v14.0 vs v14.1. Timings are ms per profile.

Test case	Model	Intel gfortran v14.0	Intel gfortran v14.1	Intel gfortran v14.1:v14.0	Intel ifort v14.0	Intel ifort v14.1	Intel ifort v14.1:v14.0	Cray v14.0	Cray v14.1	Cray v14.1:v14.0
1 MW clear no gas	Direct	0.175	0.151	0.87	0.198	0.226	1.14	0.106	0.117	1.10
	TL	0.362	0.299	0.83	0.425	0.454	1.07	0.216	0.252	1.17
	AD	0.533	0.399	0.75	0.625	0.693	1.11	0.323	0.348	1.08
	K	0.739	0.59	0.80	0.828	0.923	1.12	0.468	0.492	1.05
2 MW clear O3-only	Direct	0.109	0.097	0.89	0.125	0.142	1.14	0.072	0.077	1.08
	TL	0.22	0.194	0.88	0.259	0.28	1.08	0.148	0.161	1.09
	AD	0.331	0.265	0.80	0.396	0.436	1.10	0.213	0.222	1.04
	K	0.474	0.399	0.84	0.538	0.595	1.11	0.315	0.326	1.04
3 MW clear CLW abs	Direct	0.255	0.221	0.87	0.308	0.337	1.10	0.162	0.174	1.07
	TL	0.537	0.467	0.87	0.663	0.709	1.07	0.343	0.385	1.12
	AD	0.719	0.575	0.80	0.882	0.956	1.08	0.454	0.48	1.06
	K	0.992	0.842	0.85	1.186	1.303	1.10	0.718	0.75	1.04
4 IR clear O3+CO2	Direct	0.068	0.065	0.96	0.082	0.087	1.07	0.052	0.051	0.98
	TL	0.13	0.126	0.97	0.158	0.171	1.08	0.101	0.102	1.01
	AD	0.148	0.143	0.97	0.188	0.204	1.08	0.113	0.112	0.99
	K	0.25	0.24	0.96	0.297	0.325	1.09	0.184	0.197	1.07
5 VIS clear O3+CO2	Direct	0.109	0.106	0.97	0.132	0.144	1.09	0.076	0.075	0.99
	TL	0.219	0.209	0.96	0.259	0.279	1.08	0.147	0.147	0.99
	AD	0.239	0.232	0.97	0.31	0.333	1.08	0.165	0.165	1.00
	K	0.537	0.525	0.98	0.587	0.634	1.08	0.329	0.331	1.01
6 Hi-res clear v13pred 7gas	Direct	1.502	1.441	0.96	1.59	1.666	1.05	1.067	1.084	1.02
	TL	3.122	2.786	0.89	2.95	3.127	1.06	2.164	2.105	0.97
	AD	3.356	3.172	0.95	3.506	3.812	1.09	2.294	2.302	1.00
	K	12.15	11.671	0.96	13.689	14.368	1.05	11.804	11.823	1.00
7 Hi-res clear v9pred 7gas	Direct	1.093	1.068	0.98	1.301	1.364	1.05	0.865	0.861	1.00
	TL	2.31	2.251	0.97	2.368	2.475	1.05	1.701	1.702	1.00
	AD	2.568	2.47	0.96	2.954	3.081	1.04	1.902	1.909	1.00
	K	12.085	11.096	0.92	13.571	14.372	1.06	11.744	11.662	0.99
8 Hi-res clear v13pred no gas	Direct	1.522	1.438	0.94	1.594	1.653	1.04	1.068	1.07	1.00
	TL	2.863	2.932	1.02	2.926	3.047	1.04	2.1	2.099	1.00
	AD	3.268	3.116	0.95	3.455	3.677	1.06	2.298	2.278	0.99
	K	10.46	9.824	0.94	10.431	10.976	1.05	9.615	9.836	1.02
9 IR aerosol Chou-scaling	Direct	0.12	0.116	0.97	0.143	0.159	1.11	0.089	0.097	1.08
	TL	0.249	0.245	0.98	0.305	0.34	1.11	0.231	0.24	1.04
	AD	0.296	0.29	0.98	0.356	0.409	1.15	0.272	0.3	1.10
	K	0.425	0.411	0.97	0.523	0.581	1.11	0.363	0.396	1.09
10 IR hydro Chou-scaling	Direct	0.763	0.488	0.64	0.54	0.404	0.75	0.39	0.283	0.73
	TL	1.64	1.072	0.65	1.101	0.836	0.76	0.856	0.62	0.72
	AD	2.156	1.584	0.73	1.918	1.367	0.71	1.235	0.846	0.68
	K	2.27	1.768	0.78	1.683	1.332	0.79	1.32	0.98	0.74

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

11 IR aerosol DOM	Direct	0.895	0.831	0.93	1.114	1.185	1.06	0.773	0.775	1.00
	TL	1.934	1.93	1.00	2.4	2.476	1.03	1.808	1.826	1.01
	AD	39.444	38.368	0.97	40.252	41.684	1.04	24.788	24.684	1.00
	K	39.47	38.552	0.98	39.802	41.658	1.05	24.952	24.812	0.99
12 IR hydro DOM	Direct	23.996	14.45	0.60	31.452	20.744	0.66	21.86	12.766	0.58
	TL	60.245	35.86	0.60	73.325	47.49	0.65	48.84	29.295	0.60
	AD	1664	947.8	0.57	1672	1046.2	0.63	1047.5	648.4	0.62
	K	1664.9	947.1	0.57	1673	1018.4	0.61	1053.2	615.1	0.58
13 VIS aerosol DOM	Direct	3.827	3.747	0.98	4.944	5.211	1.05	3.467	3.558	1.03
	TL	8.425	8.175	0.97	10.291	10.81	1.05	7.424	7.551	1.02
	AD	38.661	38.815	1.00	46.296	48.948	1.06	25.554	25.833	1.01
	K	39.019	39.079	1.00	46.552	49.926	1.07	25.909	26.146	1.01
14 VIS hydro DOM	Direct	52.958	32.548	0.61	73.902	53.15	0.72	47.3	27.976	0.59
	TL	124.585	78.54	0.63	162.16	109.615	0.68	102.045	63.68	0.62
	AD	1467.98	691.88	0.47	1693.98	856.64	0.51	930.82	447.38	0.48
	K	1467.28	692.08	0.47	1686.54	849.62	0.50	933.16	446.84	0.48
15 VIS aer+hyd+ray DOM	Direct	140.244	67.14	0.48	180.884	101.024	0.56	126.688	61.496	0.49
	TL	336.21	159.69	0.47	423.36	216.02	0.51	287.17	136.06	0.47
	AD	12164.4	3777.8	0.31	12790.6	4316.4	0.34	7828.8	2484	0.32
	K	12126.6	3763.8	0.31	12794.8	4246.8	0.33	7854	2524.8	0.32
16 VIS hydro MFASIS-NN	Direct	0.748	0.751	1.00	0.727	0.537	0.74	0.512	0.387	0.76
	TL	3.448	2.751	0.80	2.274	1.604	0.71	1.56	1.179	0.76
	AD	6.208	6.362	1.02	2.747	2.119	0.77	1.916	1.569	0.82
	K	6.361	6.502	1.02	2.876	2.345	0.82	2.063	1.618	0.78
17 MW hydro delta-Edd	Direct	0.552	0.478	0.87	0.575	0.676	1.18	0.449	0.528	1.18
	TL	1.257	1.106	0.88	1.38	1.519	1.10	1.08	1.317	1.22
	AD	1.963	1.62	0.83	2.046	2.269	1.11	1.587	1.747	1.10
	K	2.275	1.945	0.86	2.535	2.793	1.10	1.826	2.004	1.10
18 PC O3-only	Direct	2.552	2.589	1.01	2.803	2.939	1.05	1.868	1.87	1.00
	TL	4.849	4.894	1.01	5.259	5.549	1.06	3.83	3.764	0.98
	AD	5.435	5.52	1.02	6.152	6.555	1.07	3.972	4.059	1.02
	K	33.735	33.69	1.00	35.555	37.315	1.05	25.075	23.22	0.93
19 PC, rec rad O3-only	Direct	2.64	2.663	1.01	2.89	3.037	1.05	1.895	1.968	1.04
	TL	4.993	5.059	1.01	5.42	5.73	1.06	3.815	3.872	1.01
	AD	5.668	5.744	1.01	6.28	6.69	1.07	4.193	4.216	1.01
	K	58.53	58.79	1.00	48.835	50.735	1.04	54.605	53.375	0.98
20 PC 6gas	Direct	2.584	2.578	1.00	2.809	2.995	1.07	1.889	1.899	1.01
	TL	4.826	4.872	1.01	5.238	5.555	1.06	3.794	3.784	1.00
	AD	5.521	5.555	1.01	6.147	6.624	1.08	3.965	4.218	1.06
	K	56.96	56.86	1.00	60.565	62.07	1.02	35.26	32.225	0.91
21 PC, rec rad 6gas	Direct	2.657	2.679	1.01	2.891	3.06	1.06	1.918	1.917	1.00
	TL	5.097	5.094	1.00	5.413	5.763	1.06	3.816	4.021	1.05
	AD	5.702	5.742	1.01	6.302	6.884	1.09	4.133	4.482	1.08
	K	81.715	82.475	1.01	73.74	75.51	1.02	64.04	61.945	0.97

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

Test case	Model	Intel gfortran v14.1 no alloc	Intel gfortran v14.1 alloc	Intel gfortran alloc:no alloc	Intel ifort v14.1 no alloc	Intel ifort v14.1 alloc	Intel ifort alloc:no alloc	Cray v14.1 no alloc	Cray v14.1 alloc	Cray alloc:no alloc
1 MW clear no gas	Direct	0.168	0.151	0.90	0.221	0.226	1.03	0.125	0.117	0.93
	TL	0.339	0.299	0.88	0.442	0.454	1.03	0.268	0.252	0.94
	AD	0.443	0.399	0.90	0.68	0.693	1.02	0.361	0.348	0.97
	K	0.645	0.59	0.91	0.884	0.923	1.04	0.511	0.492	0.96
2 MW clear O3-only	Direct	0.11	0.097	0.88	0.142	0.142	1.01	0.087	0.077	0.89
	TL	0.22	0.194	0.88	0.277	0.28	1.01	0.172	0.161	0.94
	AD	0.297	0.265	0.89	0.423	0.436	1.03	0.235	0.222	0.95
	K	0.444	0.399	0.90	0.574	0.595	1.04	0.341	0.326	0.96
3 MW clear CLW abs	Direct	0.244	0.221	0.91	0.328	0.337	1.03	0.184	0.174	0.95
	TL	0.539	0.467	0.87	0.678	0.709	1.05	0.397	0.385	0.97
	AD	0.665	0.575	0.86	0.922	0.956	1.04	0.514	0.48	0.93
	K	1.168	0.842	0.72	1.521	1.303	0.86	0.802	0.75	0.94
4 IR clear O3+CO2	Direct	0.076	0.065	0.86	0.092	0.087	0.95	0.06	0.051	0.85
	TL	0.15	0.126	0.84	0.176	0.171	0.97	0.114	0.102	0.90
	AD	0.169	0.143	0.85	0.21	0.204	0.97	0.13	0.112	0.87
	K	0.276	0.24	0.87	0.316	0.325	1.03	0.204	0.197	0.97
5 VIS clear O3+CO2	Direct	0.12	0.106	0.88	0.143	0.144	1.01	0.088	0.075	0.85
	TL	0.243	0.209	0.86	0.283	0.279	0.99	0.166	0.147	0.88
	AD	0.266	0.232	0.87	0.334	0.333	1.00	0.183	0.165	0.90
	K	0.58	0.525	0.91	0.731	0.634	0.87	0.347	0.331	0.95
6 Hi-res clear v13pred 7gas	Direct	1.567	1.441	0.92	1.603	1.666	1.04	1.091	1.084	0.99
	TL	2.959	2.786	0.94	2.977	3.127	1.05	2.154	2.105	0.98
	AD	3.46	3.172	0.92	3.607	3.812	1.06	2.347	2.302	0.98
	K	24.551	11.671	0.48	27.13	14.368	0.53	11.429	11.823	1.03
7 Hi-res clear v9pred 7gas	Direct	1.542	1.068	0.69	1.86	1.364	0.73	0.873	0.861	0.99
	TL	2.887	2.251	0.78	2.743	2.475	0.90	1.77	1.702	0.96
	AD	3.202	2.47	0.77	3.275	3.081	0.94	1.941	1.909	0.98
	K	17.885	11.096	0.62	26.797	14.372	0.54	11.159	11.662	1.05
8 Hi-res clear v13pred no gas	Direct	1.568	1.438	0.92	1.597	1.653	1.04	1.091	1.07	0.98
	TL	2.95	2.932	0.99	2.937	3.047	1.04	2.223	2.099	0.94
	AD	3.897	3.116	0.80	3.556	3.677	1.03	2.297	2.278	0.99
	K	13.721	9.824	0.72	21.078	10.976	0.52	9.267	9.836	1.06
9 IR aerosol Chou-scaling	Direct	0.134	0.116	0.87	0.168	0.159	0.95	0.108	0.097	0.90
	TL	0.284	0.245	0.86	0.35	0.34	0.97	0.258	0.24	0.93
	AD	0.334	0.29	0.87	0.415	0.409	0.99	0.315	0.3	0.95
	K	0.466	0.411	0.88	0.582	0.581	1.00	0.421	0.396	0.94
10 IR hydro Chou-scaling	Direct	0.522	0.488	0.94	0.669	0.404	0.60	0.295	0.283	0.96
	TL	1.106	1.072	0.97	0.907	0.836	0.92	0.68	0.62	0.91
	AD	1.209	1.584	1.31	1.371	1.367	1.00	0.848	0.846	1.00
	K	1.505	1.768	1.17	1.635	1.332	0.81	0.983	0.98	1.00

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

11 IR aerosol DOM	Direct	0.865	0.831	0.96	1.066	1.185	1.11	0.816	0.775	0.95
	TL	2.512	1.93	0.77	2.822	2.476	0.88	1.832	1.826	1.00
	AD	39.942	38.368	0.96	40.172	41.684	1.04	26.196	24.684	0.94
	K	40.616	38.552	0.95	40.072	41.658	1.04	25.402	24.812	0.98
12 IR hydro DOM	Direct	14.51	14.45	1.00	17.392	20.744	1.19	12.646	12.766	1.01
	TL	37.68	35.86	0.95	44.095	47.49	1.08	28.99	29.295	1.01
	AD	979.7	947.8	0.97	969.9	1046.2	1.08	610.9	648.4	1.06
	K	1001.1	947.1	0.95	974.5	1018.4	1.05	618.8	615.1	0.99
13 VIS aerosol DOM	Direct	3.913	3.747	0.96	4.64	5.211	1.12	3.505	3.558	1.02
	TL	8.647	8.175	0.95	10.374	10.81	1.04	7.731	7.551	0.98
	AD	41.294	38.815	0.94	46.9	48.948	1.04	26.294	25.833	0.98
	K	41.448	39.079	0.94	47.783	49.926	1.04	26.285	26.146	0.99
14 VIS hydro DOM	Direct	31.926	32.548	1.02	38.148	53.15	1.39	26.334	27.976	1.06
	TL	82.67	78.54	0.95	98.81	109.615	1.11	62.625	63.68	1.02
	AD	722.62	691.88	0.96	806.5	856.64	1.06	449.18	447.38	1.00
	K	720.58	692.08	0.96	813.1	849.62	1.04	454.48	446.84	0.98
15 VIS aer+hyd+ray DOM	Direct	68.272	67.14	0.98	83.288	101.024	1.21	59.2	61.496	1.04
	TL	163.97	159.69	0.97	202.6	216.02	1.07	136.48	136.06	1.00
	AD	3932.6	3777.8	0.96	4070.6	4316.4	1.06	2414.4	2484	1.03
	K	3912.6	3763.8	0.96	4051.4	4246.8	1.05	2431.4	2524.8	1.04
16 VIS hydro MFASIS-NN	Direct	1.022	0.751	0.73	0.53	0.537	1.01	0.384	0.387	1.01
	TL	3.118	2.751	0.88	1.556	1.604	1.03	1.139	1.179	1.04
	AD	9.373	6.362	0.68	2.014	2.119	1.05	1.558	1.569	1.01
	K	9.734	6.502	0.67	2.402	2.345	0.98	1.606	1.618	1.01
17 MW hydro delta-Edd	Direct	0.521	0.478	0.92	0.667	0.676	1.01	0.555	0.528	0.95
	TL	1.201	1.106	0.92	1.48	1.519	1.03	1.374	1.317	0.96
	AD	1.742	1.62	0.93	2.219	2.269	1.02	1.776	1.747	0.98
	K	2.086	1.945	0.93	2.732	2.793	1.02	2.126	2.004	0.94
18 PC O3-only	Direct	2.85	2.589	0.91	2.833	2.939	1.04	1.903	1.87	0.98
	TL	5.646	4.894	0.87	5.276	5.549	1.05	3.824	3.764	0.98
	AD	6.534	5.52	0.84	6.278	6.555	1.04	4.149	4.059	0.98
	K	36.265	33.69	0.93	48.8	37.315	0.76	24.82	23.22	0.94
19 PC, rec rad O3-only	Direct	3.046	2.663	0.87	2.929	3.037	1.04	1.923	1.968	1.02
	TL	5.95	5.059	0.85	5.476	5.73	1.05	3.835	3.872	1.01
	AD	6.756	5.744	0.85	6.421	6.69	1.04	4.259	4.216	0.99
	K	62.15	58.79	0.95	48.5	50.735	1.05	54.92	53.375	0.97
20 PC 6gas	Direct	2.995	2.578	0.86	2.836	2.995	1.06	1.892	1.899	1.00
	TL	5.67	4.872	0.86	5.234	5.555	1.06	3.84	3.784	0.99
	AD	6.523	5.555	0.85	6.356	6.624	1.04	4.062	4.218	1.04
	K	59.175	56.86	0.96	76.305	62.07	0.81	34.925	32.225	0.92
21 PC, rec rad 6gas	Direct	2.985	2.679	0.90	2.96	3.06	1.03	1.92	1.917	1.00
	TL	5.908	5.094	0.86	5.505	5.763	1.05	3.848	4.021	1.05
	AD	6.71	5.742	0.86	6.47	6.884	1.06	4.225	4.482	1.06
	K	85.315	82.475	0.97	73.855	75.51	1.02	64.33	61.945	0.96

Table 5 (continued from above): Speed test results, 1 profile per call, v14.1 without vs with external allocation of trajectory structures. 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 AMD compute cluster using the gfortran v11.5.0 compiler and the results are shown in Table 6. The colour-coding is as follows:

- green => peak memory for v14.1 90% or less than that for v14.0
- blue => peak memory for v14.1 90-95% than that for v14.0
- white => peak memory for v14.1 within +/-5% that of v14.0
- orange => peak memory for v14.1 105-110% than that for v14.0
- red => peak memory for v14.1 110% or more than that for v14.0

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.

The main code changes that result in changes in memory usage are:

1. The elimination of redundant zero-width cloud columns in maximum-random overlap reduces the memory requirements for VIS/IR hydrometeor (cloudy) simulations.

2. The refactoring of data for the DOM solver in order to implement the Rayleigh multiple scattering optimisation has a mixed impact on the VIS DOM aerosol simulations. The direct and TL models require slightly less memory while the AD and K models require slightly more.

3. Updates to the MFASIS-NN solver to extend support to additional VIS/NIR channels has resulted in an increase in memory requirements for all MFASIS-NN simulations.

Test case	Model	v14.0 peak memory (MB)	v14.1 peak memory (MB)	v14.1:v14.0
1 MW clear no gas	Direct	1.636	1.644	1.00
	TL	1.636	1.644	1.00
	AD	1.636	1.644	1.00
	K	2.655	2.682	1.01
2 MW clear O3-only	Direct	1.343	1.351	1.00
	TL	1.44	1.451	1.00
	AD	1.449	1.461	1.00
	K	2.174	2.197	1.01
3 MW clear CLW abs	Direct	1.636	1.644	1.00
	TL	1.636	1.644	1.00
	AD	1.636	1.644	1.00
	K	2.929	2.961	1.01
4 IR clear O3+CO2	Direct	1.457	1.465	1.00
	TL	1.479	1.491	1.00
	AD	1.486	1.497	1.00
	K	1.97	1.988	1.00
5 VIS clear O3+CO2	Direct	1.418	1.427	1.00
	TL	1.637	1.648	1.00
	AD	1.644	1.655	1.00
	K	2.455	2.474	1.00
6 Hi-res clear v13pred 7gas	Direct	10.45	10.46	1.00
	TL	11.53	11.54	1.00
	AD	11.73	11.75	1.00
	K	46.83	47.08	1.00
7 Hi-res clear v9pred 7gas	Direct	8.41	8.42	1.00
	TL	9.589	9.601	1.00
	AD	9.697	9.709	1.00
	K	46.17	46.3	1.00
8 Hi-res clear v13pred no gas	Direct	10.44	10.45	1.00
	TL	11.5	11.52	1.00
	AD	11.7	11.71	1.00
	K	44.93	45.18	1.00
9 IR aerosol Chou-scaling	Direct	1.776	1.786	1.00
	TL	2.119	2.132	1.00
	AD	2.123	2.136	1.00
	K	2.712	2.732	1.00
10 IR hydro Chou-scaling	Direct	3.447	2.911	0.84
	TL	4.469	3.73	0.83
	AD	4.472	3.734	0.83
	K	6.955	6.223	0.89

Table 6 (continued below): Memory test results.

11 IR aerosol DOM	Direct	1.776	1.786	1.00
	TL	2.119	2.132	1.00
	AD	2.123	2.136	1.00
	K	2.712	2.732	1.00
12 IR hydro DOM	Direct	3.447	2.911	0.84
	TL	4.469	3.73	0.83
	AD	4.472	3.734	0.83
	K	6.955	6.223	0.89
13 VIS aerosol DOM	Direct	3.556	3.372	0.94
	TL	6.842	5.733	0.83
	AD	7.025	7.673	1.09
	K	7.942	8.595	1.08
14 VIS hydro DOM	Direct	4.914	4.403	0.89
	TL	19	13.89	0.73
	AD	19.57	15.96	0.81
	K	22.38	18.77	0.83
15 VIS aer+hyd+ray DOM	Direct	6.074	5.639	0.92
	TL	20.64	15.55	0.75
	AD	22.9	17.82	0.77
	K	25.83	20.75	0.80
16 VIS hydro MFASIS-NN	Direct	4.478	7.209	1.60
	TL	13.47	18.74	1.39
	AD	13.49	19.52	1.44
	K	15.09	21.19	1.40
17 MW hydro delta-Edd	Direct	38.75	38.76	1.00
	TL	38.75	38.76	1.00
	AD	38.75	38.76	1.00
	K	38.75	38.75	1.00
18 PC O3-only	Direct	56.6	56.61	1.00
	TL	56.6	56.61	1.00
	AD	56.6	56.61	1.00
	K	109.3	109.7	1.00
19 PC, rec rad O3-only	Direct	25.33	25.34	1.00
	TL	25.59	25.61	1.00
	AD	25.6	25.61	1.00
	K	84.7	85.11	1.00
20 PC 6gas	Direct	56.6	56.61	1.00
	TL	56.6	56.61	1.00
	AD	56.6	56.61	1.00
	K	112.2	112.6	1.00
21 PC, rec rad 6gas	Direct	25.33	25.34	1.00
	TL	25.61	25.62	1.00
	AD	25.62	25.63	1.00
	K	87.56	87.97	1.00

Table 6 (continued from above): Memory test results.