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CRTM: LBLRTM v11.3 Install and Test

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1 Introduction

This document details the installation and testing of the LNFL v2.5 and LBLRTM v11.3 software with the HITRAN2004 AER v2.1 spectrosopic database on two systems: an Intel PC running Red Hat RHE4.0 linux and an IBM SP running AIX 5.3. All the original source code and datafiles were obtained from the AER, Inc. website: http://www.rtweb.aer.com.

Several example inputs and outputs are provided with the LBLRTM v11.3 distribution. In all cases, the tests were performed using both the locally generated `TAPE3` file (see section 3) and the one supplied by AER. All the comparisons that follow are for the generated `TAPE27` files only where the computed radiances were converted to brightness temperatures and then differenced with the same for the AER-supplied `TAPE27_ex` files.

2 Compilation

The compiler and compilation switches used for the two build systems are shown in table 2.1. Two executables were built: a single precision and a double precision version. For the latter build, compiler switches were used to promote the default floating point real and default integer types to double precision. As shown in table 2.1, two compilers were used in the testing on the linux system: gfortran and pgf95.

System	Compiler	Switches
Red Hat RHE4.0 linux	gfortran 4.4.0 (20081021)	-c -ffixed-form -fdefault-real-8† -fdefault-integer-8†
	PGI f95 7.2-4	-c -fast -r8† -i8†
IBM AIX 5.3	xlf95 10.01.0000.0006	-c -qarch=auto -qfixed=72 -qmaxmem=-1 -O2 -qrealsize=8† -qintsize=8†

Table 2.1: Switches for the compilers on the two systems on which LNFL v2.5 and LBLRTM v11.3 were tested. †These switches were only used for the double precision build for LBLRTM.

Note that the gfortran switches do not include any optimisation levels. Anomalous residuals occurred in one of the test cases when either the -O2 or -O3 switch was used when compiling the LBLRTM v11.3 source code with gfortran. Results from this optimised gfortran test case are shown in appendix A.

Also note that an earlier version of the IBM AIX compiler, v10.01.0000.0002, does not correctly compile LBLRTM in double precision mode when certain LBLRTM input options are used. For the sake of other user's sanity, results for that particular compiler version for the double precision build are shown separately in appendix B. This is a known bug in the IBM compiler and a bug report was previously filed with IBM when the issue was discovered during LBLRTM v9.3 builds.

3 TAPE3 input files

3.1 Local TAPE3

The TAPE5 input file used to generate a local TAPE3 file from the HITRAN2004 AER v2.1 spectroscopic database is shown in figure 3.1.

```
(PvD) 19-Jan-2000 LNFL; 7 mol; No rej; 0-20000cm-1
     0.000 20000.000
1111111
```

Figure 3.1: TAPE5 input to LNFL v2.5 for the local TAPE3 creation.

Only the first seven HITRAN absorbers were selected (H_2O, CO_2, O_3, N_2O, CO, CH_4, and O_2) and no lines were rejected. As indicated in figure 3.1, this LNFL input has been used since 2000. No LNFL TAPE5 was supplied with the LBLRTM distribution test cases. The TAPE6 logfile output from running LNFL v2.5 with the input of figure 3.1 is shown in figure 3.2. LBLRTM runs using this data for input will be labelled as a **Local** TAPE3 run.

```
(PvD) 19-Jan-2000 LNFL; 7 mol; No rej; 0-20000cm-1    V:  2.4  I 08/09/25  14:36:57
                    VMIN =    0.000000 CM-1,      VMAX =20000.000000 CM-1
                                          H2O  = 1
                                          CO2  = 1
                                           O3  = 1
                                          N2O  = 1
                                           CO  = 1
                                          CH4  = 1
                                           O2  = 1
         TAPE NO. = 3
         LOWEST LINE =     0.000010 CM-1,  HIGHEST LINE = 19996.646484 CM-1,
         TOTAL NUMBER OF LINES = 744590
                      COUPLED    NLTE   NEGATIVE   RESET     SUM LBLRTM      STRENGTH
      MOL     LINES    LINES    LINES      EPP      EPP       STRENGTHS      REJECTION
      H2O  =  63133        0        0     3259        0      9.0575E-19      0.000E+00
      CO2  =  60823    34114        0        0        0      5.7901E-20      0.000E+00
       O3  = 311481        0        0        0        0      7.7917E-20      0.000E+00
      N2O  =  47843        0        0        0        0      4.2666E-20      0.000E+00
       CO  =   4477        0        0        0        0      7.3883E-21      0.000E+00
      CH4  = 251440        0        0    43116        0      8.0356E-21      0.000E+00
       O2  =   5393       41        0        0        0      1.4374E-22      0.000E+00
                    NUMBER OF BLOCKS =3127
           TOTAL TIME =    70.416 TIME IN =     0.001 TIME OUT =    70.417
```

Figure 3.2: TAPE6 file produced by LNFL v2.5 for the local TAPE3 creation. Reformatted to fit on page.

3.2 LNFL TAPE3

The LNFL v2.5 distribution also comes with an example. The LNFL distribution TAPE5 input file shown in figure 3.3 was used to generate another local TAPE3 file from the HITRAN2004 AER v2.1 spectroscopic database.

All 39 HITRAN absorbers were selected in this case, but over a much smaller frequency range. The TAPE6 logfile output from running LNFL v2.5 with the input of figure 3.3 is shown in figure 3.4. LBLRTM runs using this data for input will be labelled as a **LNFL** TAPE3 run.

```
$ f100 format
   300.      3500.
1111111111111111111111111111111111111111    NBLK1 LNOUT
%
```

Figure 3.3: TAPE5 example input supplied with the LNFL v2.5 distribution.

3.3 AER TAPE3

The LBLRTM distribution examples came with a precomputed TAPE3 file. LBLRTM runs using this data for input will be labelled as a **AER** TAPE3 run.

```
$ f100 format                                       V:  2.4  I 08/10/17  15:08:24
                  VMIN =  300.000000 CM-1,      VMAX = 3500.000000 CM-1
 ** NOTE IFLG SET - LNOUT *****
  H2O = 1  CH4 = 1   NH3 = 1   HBR = 1   HOCL = 1  C2H2 = 1     H2S = 1    NO+ = 1
  CO2 = 1   O2 = 1  HNO3 = 1    HI = 1     N2 = 1  C2H6 = 1   HCOOH = 1   HOBr = 1
   O3 = 1   NO = 1    OH = 1   CLO = 1    HCN = 1   PH3 = 1     HO2 = 1   C2H4 = 1
  N2O = 1  SO2 = 1    HF = 1   OCS = 1  CH3CL = 1  COF2 = 1       O = 1  CH3OH = 1
   CO = 1  NO2 = 1   HCL = 1  H2CO = 1   H2O2 = 1   SF6 = 1  CLONO2 = 1
        TAPE NO. = 3
        LOWEST LINE =   300.006073 CM-1,  HIGHEST LINE =  3499.996826 CM-1,
        TOTAL NUMBER OF LINES =1276310
                    COUPLED    NLTE   NEGATIVE   RESET    SUM LBLRTM      STRENGTH
      MOL     LINES   LINES    LINES       EPP     EPP     STRENGTHS      REJECTION
      H2O  =  17027       0        0         0       0    2.7904E-20      0.000E+00
      CO2  =  41009   21566        0         0       0    5.7139E-20      0.000E+00
       O3  = 201777       0        0         0       0    1.6229E-20      0.000E+00
      N2O  =  37179       0        0         0       0    3.6643E-20      0.000E+00
       CO  =   1413       0        0         0       0    4.7091E-21      0.000E+00
      CH4  = 143925       0        0         0       0    7.7967E-21      0.000E+00
       O2  =    435       0        0         0       0    6.0967E-30      0.000E+00
       NO  =  42935       0        0         0       0    2.4633E-21      0.000E+00
      SO2  =  25575       0        0         0       0    3.4091E-20      0.000E+00
      NO2  =  71999       0        0         0       0    3.8055E-20      0.000E+00
      NH3  =  20536       0        0         0       0    2.6919E-20      0.000E+00
      HNO3 = 335929       0        0         0       0    1.1504E-19      0.000E+00
        OH =   9034       0        0         0       0    2.6736E-21      0.000E+00
        HF =     14       0        0         0       0    5.2310E-21      0.000E+00
      HCL  =    164       0        0         0       0    2.1819E-21      0.000E+00
      HBR  =    779       0        0         0       0    5.5844E-22      0.000E+00
       HI  =    410       0        0         0       0    8.4907E-24      0.000E+00
      CLO  =   2048       0        0         0       0    4.7073E-22      0.000E+00
      OCS  =  18442       0        0         0       0    6.0091E-20      0.000E+00
     H2CO  =   1161       0        0         0       0    7.0740E-21      0.000E+00
     HOCL  =   4986       0        0         0       0    6.6136E-21      0.000E+00
       N2  =    120       0        0         0       0    2.8663E-30      0.000E+00
      HCN  =   3795       0        0         0       0    1.9259E-20      0.000E+00
    CH3CL  =  18344       0        0         0       0    7.3480E-21      0.000E+00
     H2O2  =  59283       0        0         0       0    5.2845E-20      0.000E+00
     C2H2  =   3356       0        0         0       0    4.6654E-20      0.000E+00
     C2H6  =   5123       0        0         0       0    2.9869E-21      0.000E+00
      PH3  =  14839       0        0      3049       0    1.4900E-20      0.000E+00
     COF2  =  70601       0        0         0       0    8.7582E-20      0.000E+00
      SF6  =  22901       0        0         0       0    5.8896E-20      0.000E+00
      H2S  =   8529       0        0         0       0    1.9504E-22      0.000E+00
    HCOOH  =  18000       0        0         0       0    1.5922E-20      0.000E+00
      HO2  =  12929       0        0         0       0    4.1003E-21      0.000E+00
        O  =      0       0        0         0       0    0.0000E+00      0.000E+00
    CLONO2 =  32199       0        0         0       0    3.7076E-21      0.000E+00
      NO+  =   1206       0        0         0       0    1.1145E-21      0.000E+00
     HOBr  =     96       0        0         0       0    4.8612E-22      0.000E+00
     C2H4  =  12978       0        0      1393       0    1.5191E-20      0.000E+00
    CH3OH  =  15234       0        0       122       0    1.7336E-20      0.000E+00
                  NUMBER OF BLOCKS =5212
          TOTAL TIME =   115.996 TIME IN =     0.001 TIME OUT =   115.997
```

Figure 3.4: TAPE6 file produced by LNFL v2.5 for the local TAPE3 creation using the AER-supplied input file in the LNFL v2.5 distribution. Reformatted to fit on page.

4 Test Case: Built-in Atmosphere Upwelling

4.1 Double precision linux results

The double precision results for the linux/gfortran system for the built-in atmosphere test case are shown in figure 4.1. Residuals for LBLRTM runs using the local and LNFL `TAPE3` spectroscopic input files are shown. Results using the AER `TAPE3` file were identical to the LNFL results.

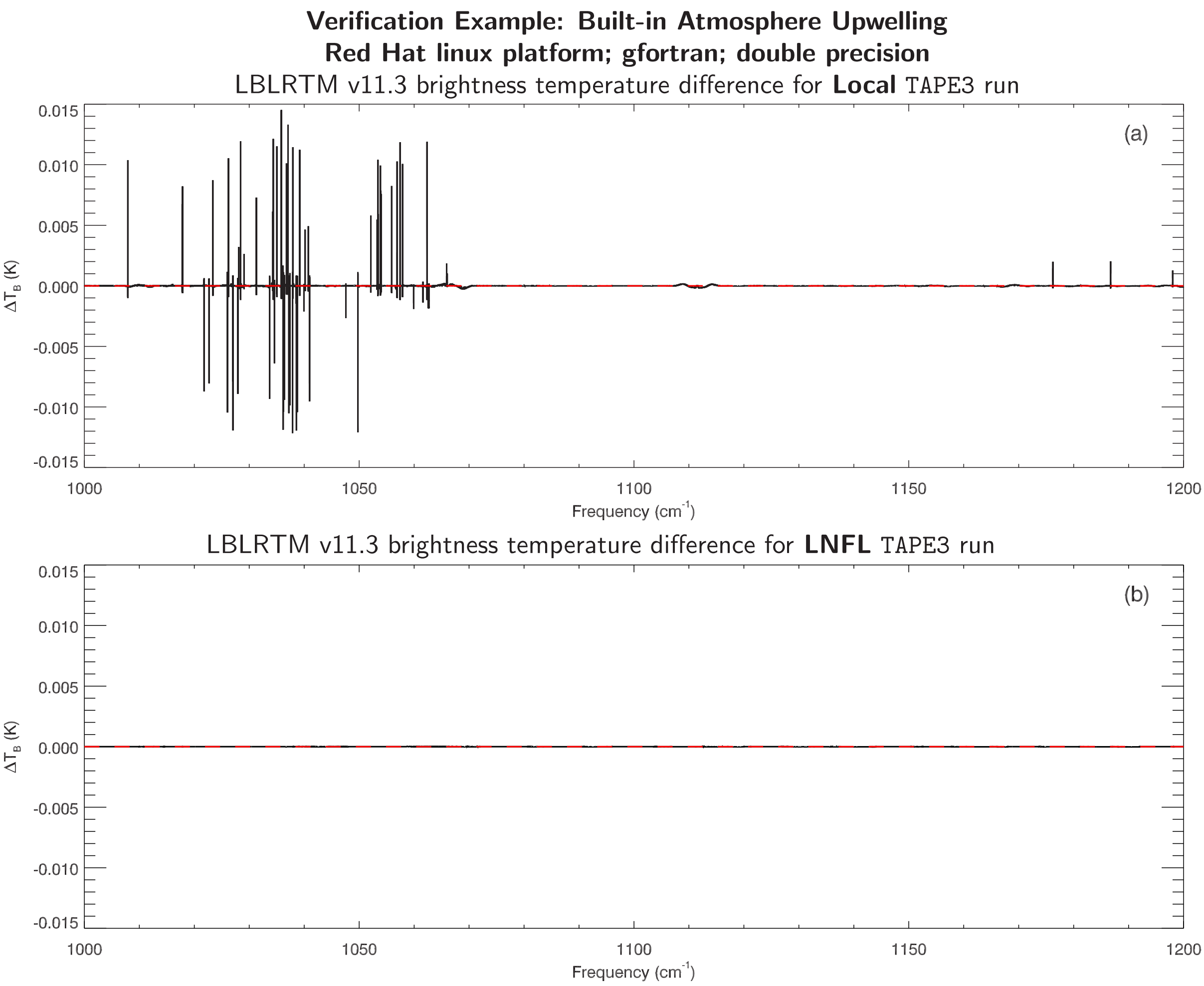

Figure 4.1: Built-in Atmosphere Test: Comparison of the AER-supplied `TAPE27_ex` output to the locally generated `TAPE27` output for the *double precision* version of LBLRTM v11.3 running on a Red Hat linux system using the gfortran compiler. **(a)** Using the little-endian `TAPE3` spectroscopic datafile generated from the local input shown in figure 3.1. **(b)** Using the little-endian `TAPE3` spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3. This result is identical to the same using the **AER** little-endian `TAPE3` spectroscopic datafile.

The anomaly seen in the optimised linux/gfortran results (see appendix A) was the main reason an additional compiler, the PGI one, was used. The double precision results for the linux/PGI system are effectively identical to the gfortran results shown in figure 4.1.

The main residuals in figure 4.1(a) are due to the differences in how the `TAPE3` files were generated; that is, fewer molecular species. A magnification of these individual line differences for the locally generated TAPE3 case is shown in figure 4.2. The character of the differences suggest a line width difference. This type of difference could be explained by to a diffent number of absorption lines (due to the different number of included absorbers in the TAPE3 files) being included in a line summation over a particular range of frequencies. That, however, is a speculative hypothesis and, since using similarly generated TAPE3 data makes those differences go away, not worthy of further investigation here.

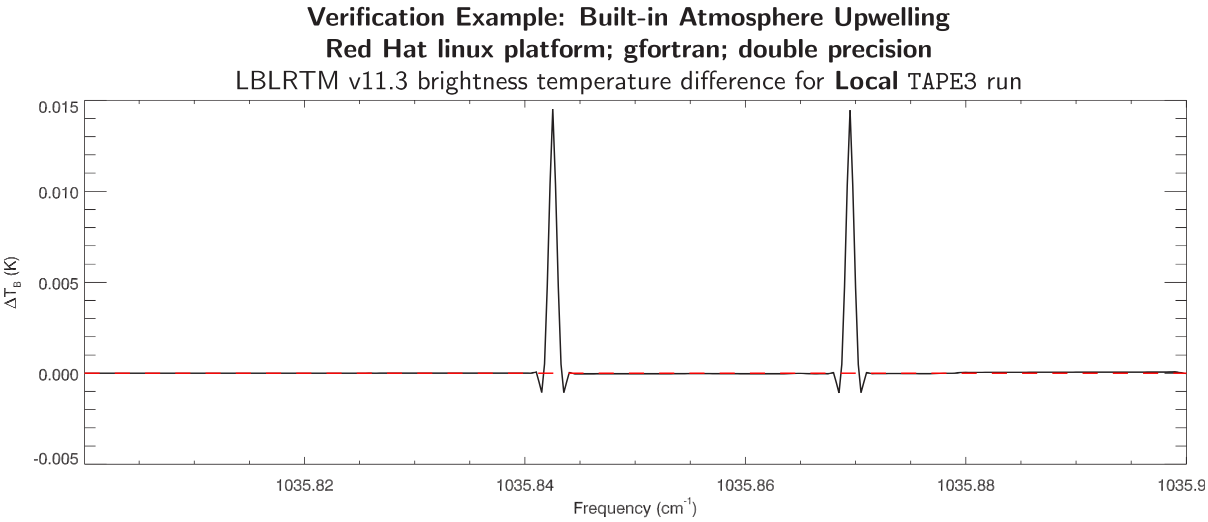

Figure 4.2: Built-in Atmosphere Test: A magnification of the 1035.8-1035.9cm^{-1} spectral region from figure 4.1(a) showing the typical residuals seen for the individual "lines" when TAPE3 inputs files containing different numbers of absorbers are used. The PGI compiler also produced the same result.

A feature of figure 4.1(b) is not visible at the y-axis scaling shown; a magnification of figure 4.1(b) is shown in figure 4.3. The periodicity of the residuals is quite evident – as is the residual line structure seen superimposed on the periodic differences – although it must be pointed out that the magnitudes of the residuals are very small.

4.2 Double precision AIX results

The double precision results for the AIX system for the built-in atmosphere test case are shown in figure 4.4.

Similar magnifications of figure 4.4 as seen in figures 4.2 and 4.3 show the IBM system produces the same residuals as the linux system.

4.3 Single precision results

The single precision results for both the linux and AIX systems for the built-in atmosphere test case are shown in figures 4.5 and 4.6 respectively. The two sets of results are effectively identical.

The size of the residuals are, however, slightly disconcerting. These residuals are determined from comparison between the AER-supplied double precision TAPE27_ex result and the locally generated TAPE27 result using a single precision build of LBLRTM v11.3.

So, what is the cause of the relatively large residuals when comparing the single precision calculations? Magnification of any of the panels of figures 4.5 or 4.6, as shown in figure 4.7, reveals the answer: a frequency shift.

Inspection of the TAPE27 (radiance output) and TAPE28 (temperature output) datafiles themselves reveals that the frequency shift is in the computed frequencies. Table 4.1 shows sections of computed frequency output from the AER-supplied TAPE28_ex file and that from the linux system single-precision calculation TAPE28 output file. As can be seen, the frequency grids are not the same so differenceing the two values highlights the frequency shift. The magnitude differences seen in the brightness temperatures may be quite reasonable for the frequency shift.

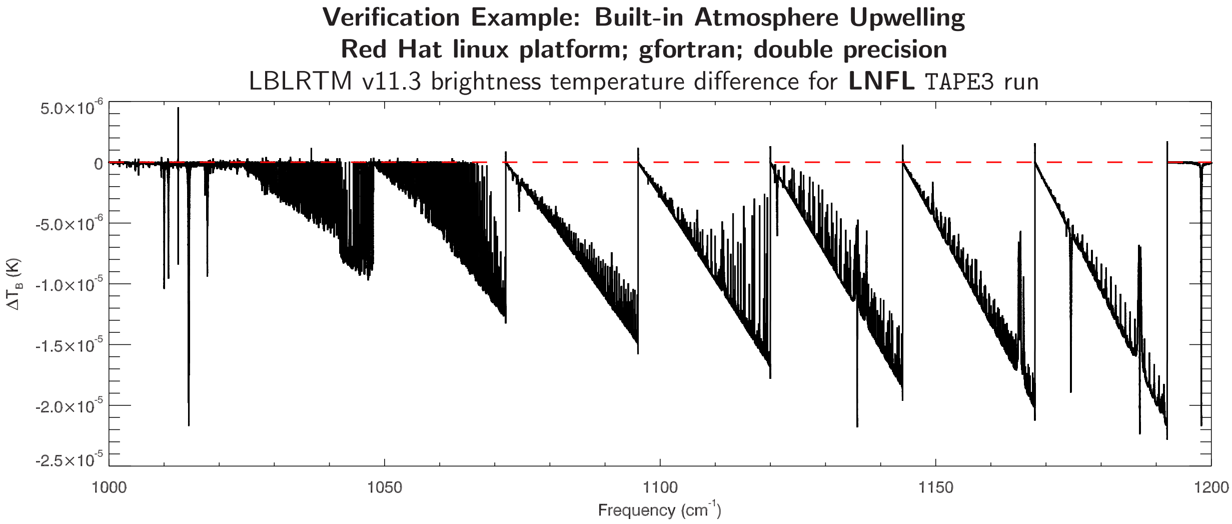

Figure 4.3: Built-in Atmosphere Test: A magnification of figure 4.1(b) showing the periodic residuals. This result is identical to the same using the **AER** little-endian `TAPE3` spectroscopic datafile. The PGI compiler also produced the same result.

AER `TAPE28_ex` (double precision)		**Local** `TAPE28` (single precision)	
Frequency (cm^{-1})	T_B (K)	**Frequency** (cm^{-1})	T_B (K)
1000.00000000	285.17976	1000.00000000	285.18686
1000.00024972	285.37625	1000.00024971	285.38333
1000.00049944	285.59329	1000.00049942	285.60040
1000.00074915	285.78922	1000.00074914	285.79636
...		...	
1099.99958543	291.95654	1099.99963348	291.95667
1099.99983515	291.95805	1099.99988322	291.95816
1100.00008487	291.95968	1100.00013296	291.95975
1100.00033458	291.96149	1100.00038269	291.96158
...		...	
1199.99917086	292.68271	1199.99912876	292.68265
1199.99942058	292.68505	1199.99937849	292.68506
1199.99967029	292.68725	1199.99962822	292.68732
1199.99992001	292.68910	1199.99987795	292.68921

Table 4.1: Built-in Atmosphere Test: Comparison of tabulated frequencies and brightness temperatures between the AER-supplied `TAPE28_ex` output file (calculated in double precision) and the local `TAPE28` output file (calculated in single precision). The difference in the frequencies, which should always be computed in double precision, is evident.

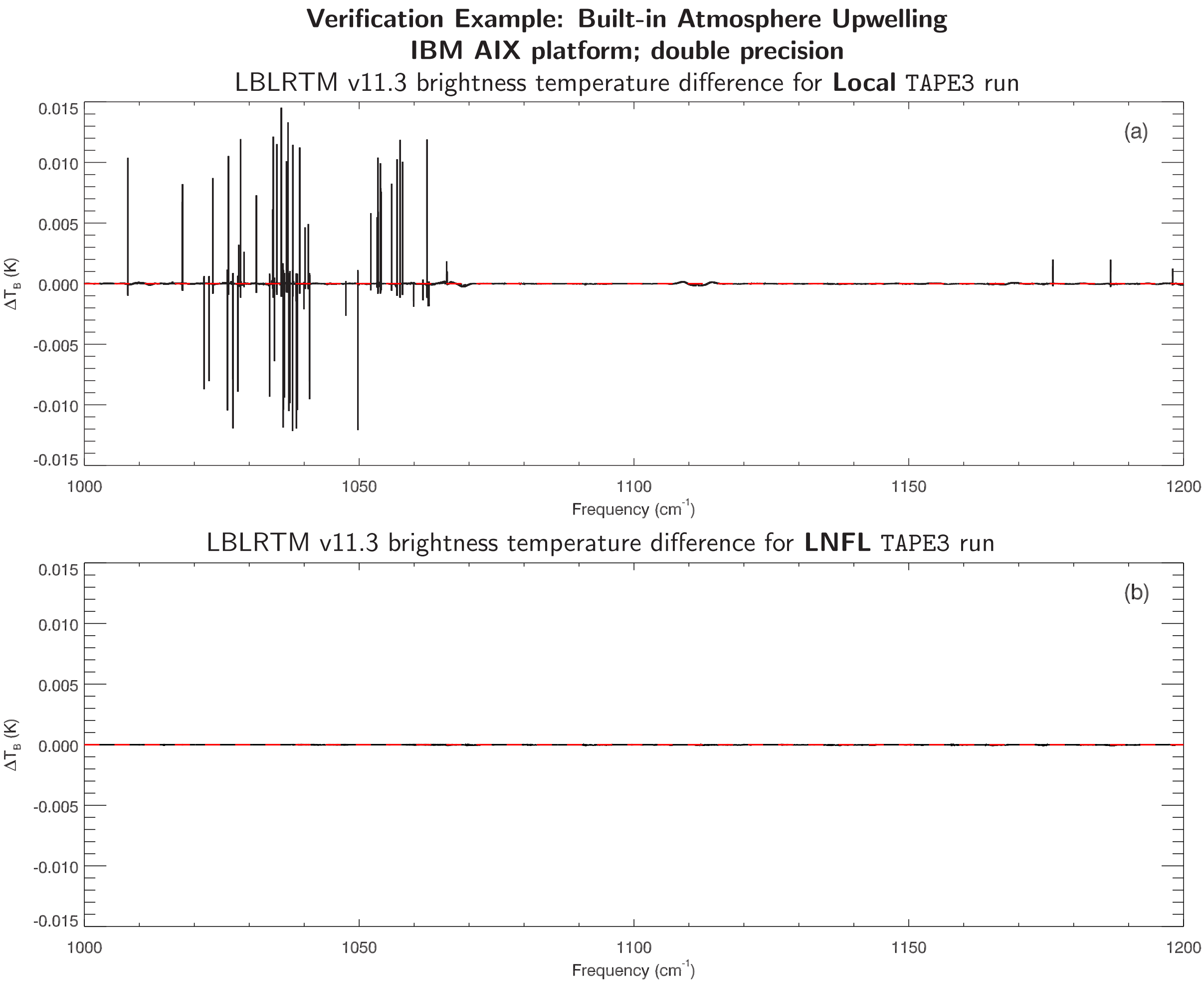

Figure 4.4: Built-in Atmosphere Test: Comparison of the AER-supplied TAPE27_ex output to the locally generated TAPE27 output for the *double precision* version of LBLRTM v11.3 running on an IBM AIX system. **(a)** Using the big-endian TAPE3 spectroscopic datafile generated from the local input shown in figure 3.1. **(b)** Using the big-endian TAPE3 spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3. This result is identical to the same using the **AER** big-endian TAPE3 spectroscopic datafile.

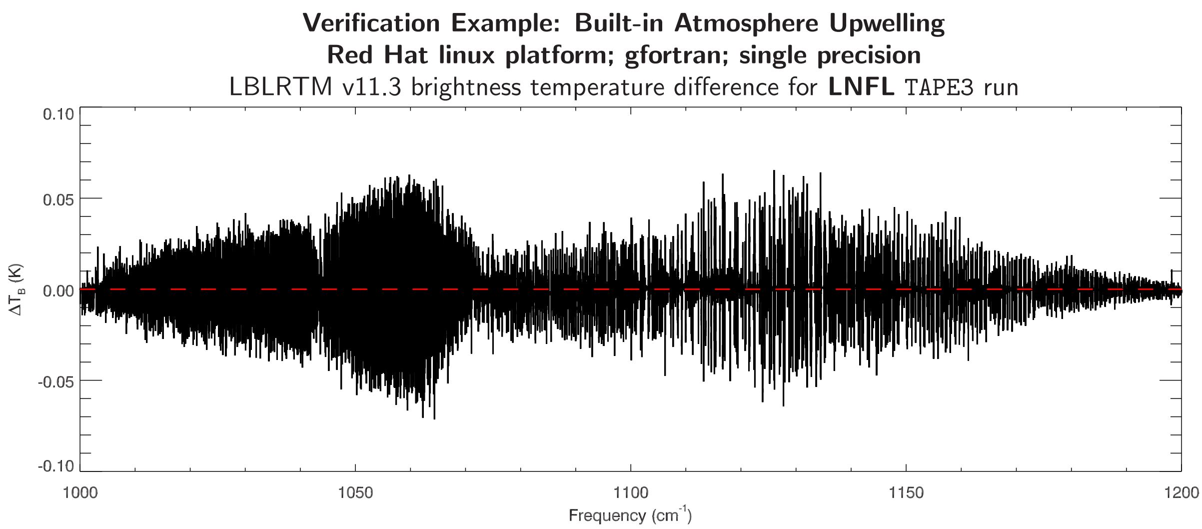

Figure 4.5: Built-in Atmosphere Test: Comparison of the AER-supplied TAPE27_ex output to the locally generated TAPE27 output for the *single precision* version of LBLRTM v11.3 running on a Red Hat linux system using the gfortran compiler. The little-endian TAPE3 spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3 was used. This result is the same as those produced using either the **Local** or **AER** little-endian TAPE3 spectroscopic datafile.

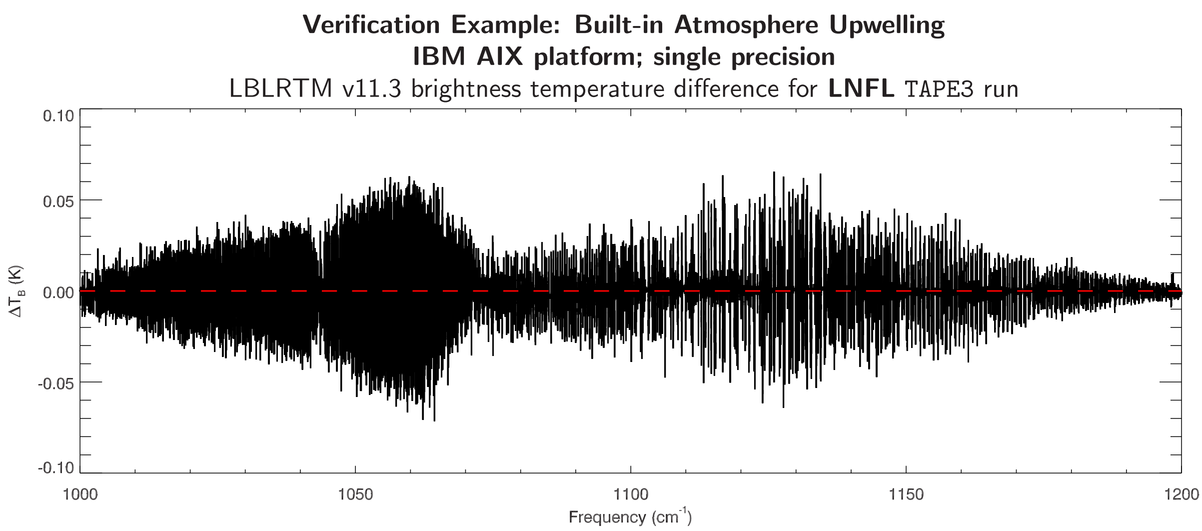

Figure 4.6: Built-in Atmosphere Test: Comparison of the AER-supplied TAPE27_ex output to the locally generated TAPE27 output for the *single precision* version of LBLRTM v11.3 running on an IBM AIX system. The big-endian TAPE3 spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3 was used.This result is the same as those produced using either the **Local** or **AER** big-endian TAPE3 spectroscopic datafile.

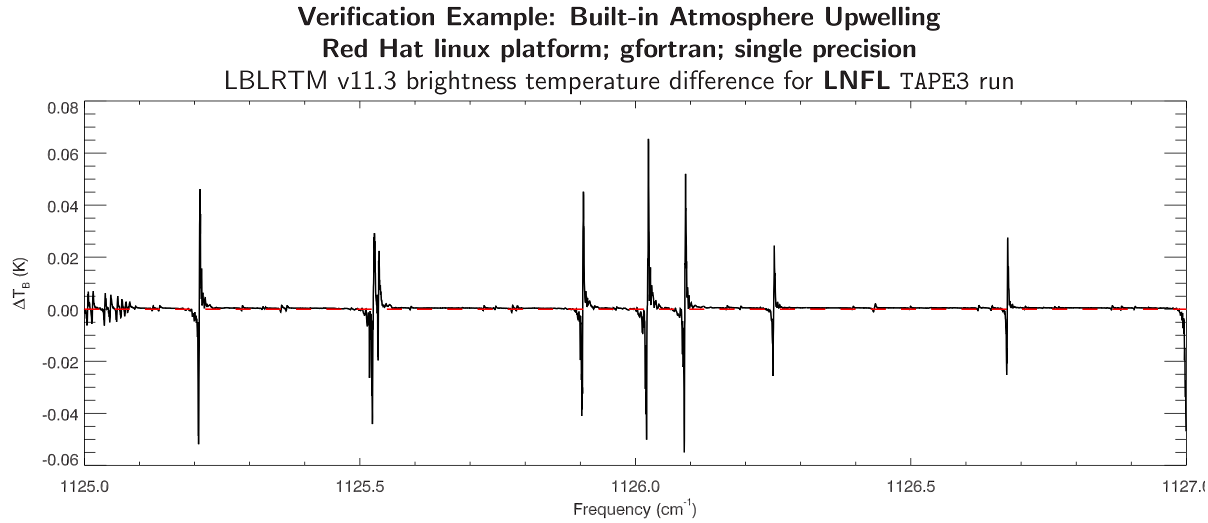

Figure 4.7: Built-in Atmosphere Test: A magnification of the 1125-1127cm^{-1} spectral region from figure 4.5(b) showing residuals with the characteristic shape due to a frequency shift. The PGI compiler also produced the same result, as did the IBM AIX tests.

This frequency shift was unexpected since the frequency variables in the LBLRTM source code are always typed as double precision regardless of the compilation switches – it is conceivable that at some point in the source code, an intermediate frequency calculation involves a default type floating point real variable or literal constant leading to a slight loss in precision for all subsequent calculations. The actual frequency shift spectrum between the double- and single-precision LBLRTM runs is shown in figure 4.8.

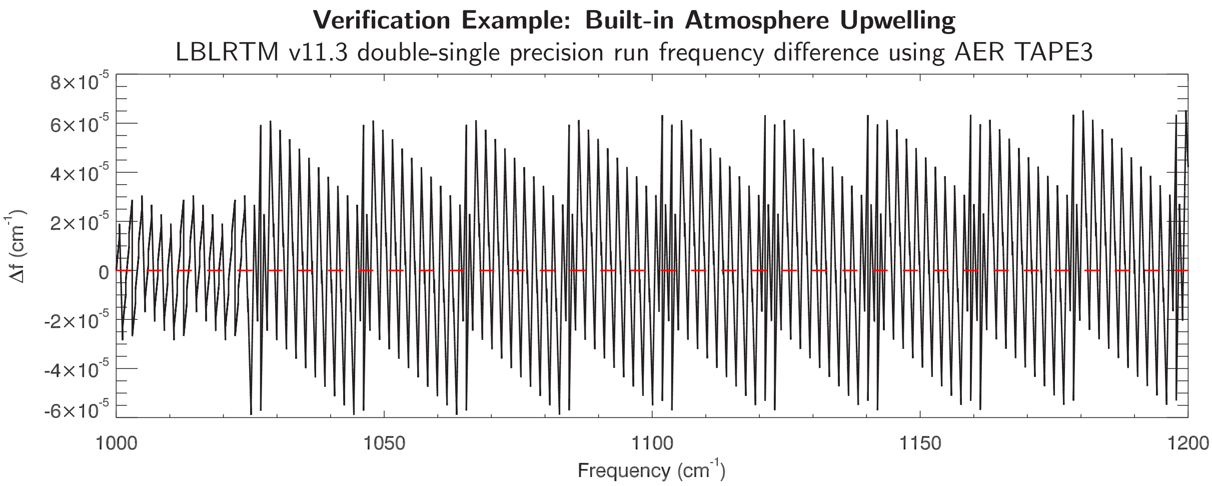

Figure 4.8: Built-in Atmosphere Test: The difference in the output `TAPE27` and `TAPE28` frequencies between a double- and single-precision LBLRTM v11.3 executable.

5 Test Case:User-defined Atmosphere Upwelling

The user-defined atmosphere test case is sightly different for that of the built-in atmosphere in that the `TAPE5` uses defined surface emissivities and reflectivities, includes CFC profile information, and invokes the FFT scanning function.

5.1 Double precision linux results

The double precision results for the linux/gfortran system for the user-defined atmosphere test case are shown in figure 5.1. Results using the AER `TAPE3` file were identical to the LNFL results. The linux/PGI runs produced identical results in all cases.

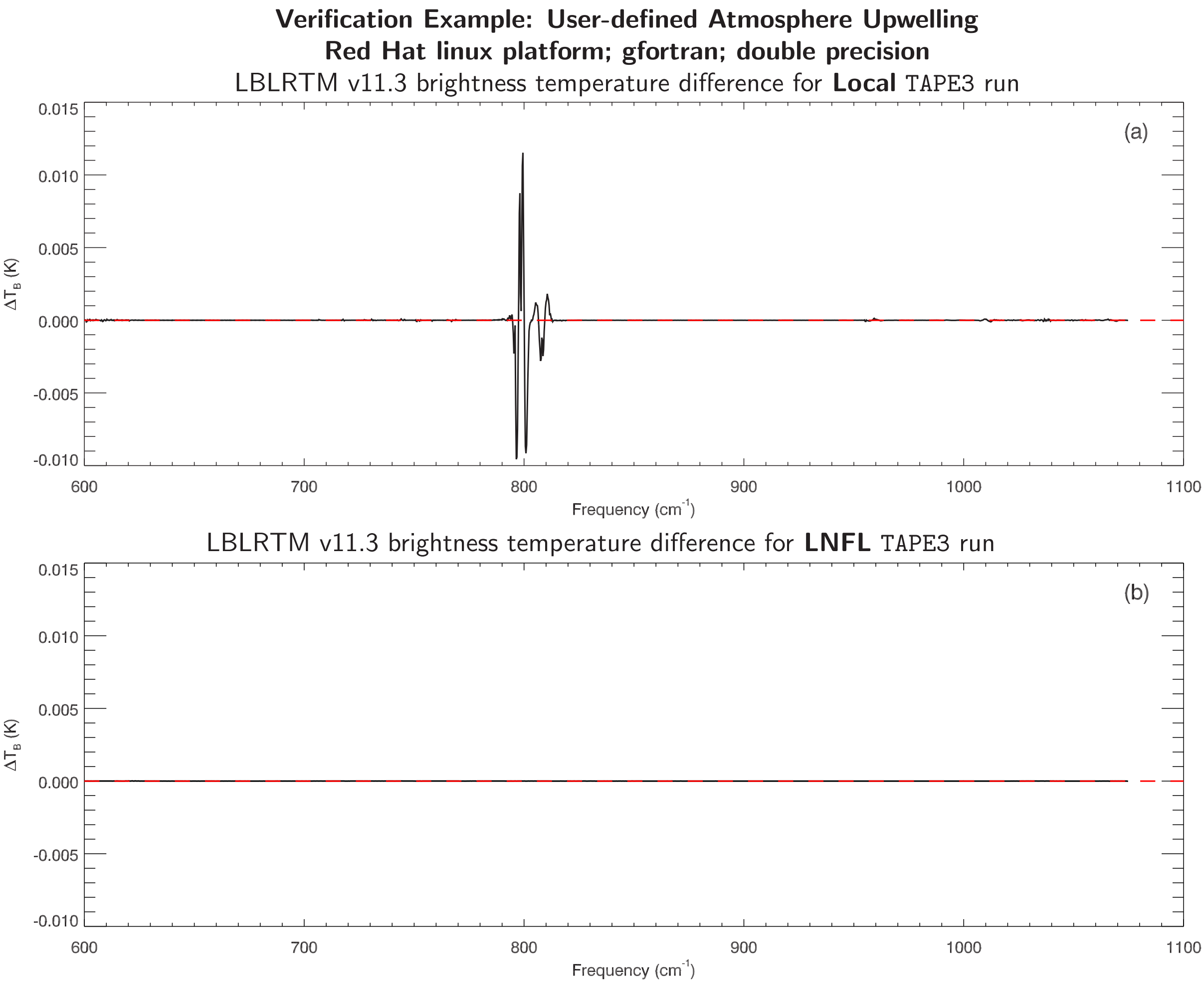

Figure 5.1: User-defined Atmosphere Test: Comparison of the AER-supplied `TAPE27_ex` output to the locally generated `TAPE27` output for the *double precision* version of LBLRTM v11.3 running on a Red Hat linux system using the gfortran compiler. **(a)** Using the little-endian `TAPE3` spectroscopic datafile generated from the local input shown in figure 3.1. **(b)** Using the little-endian `TAPE3` spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3. This result is identical to the same using the **AER** little-endian `TAPE3` spectroscopic datafile.

The spectral location of the main feature in the brightness temperature differences using the locally generated `TAPE3`, figure 5.1(a), is at approximately 800cm^{-1}. As with the built-in atmosphere test case, this residual is attributed to the different number of molecules in the two TAPE3 files since the LNFL TAPE3 run result in figure 5.1(b) does not contain the feature at 800cm^{-1}.

A magnification of the LNFL TAPE3 run result of figure 5.1(b) is shown in figure 5.2. As is evident, the remaining residuals are negligible.

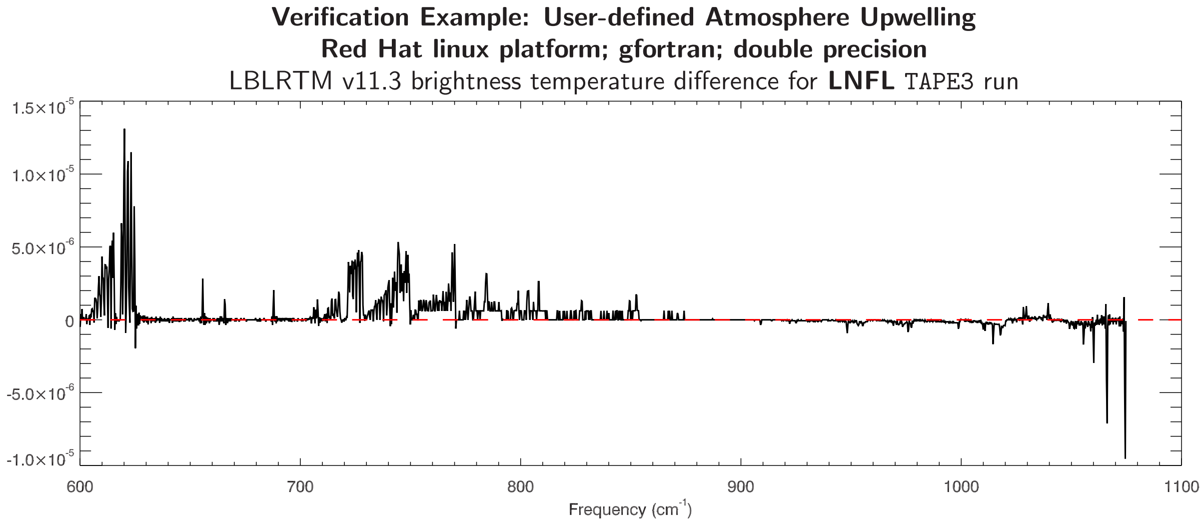

Figure 5.2: User-defined Atmosphere Test: A magnification of figure 5.1(b) showing the negligible residuals. This result is identical to the same using the **AER** big-endian TAPE3 spectroscopic datafile. The PGI compiler also produced the same result.

5.2 Double precision AIX results

The double precision results for the IBM AIX system for the user-defined atmosphere test case are shown in figure 5.3. Similar magnification of figure 5.3(b) as seen in figure 5.2 show the IBM system produces the same residuals as the linux system.

5.3 Single precision run results

The single precision results for both the linux and AIX systems for the user-supplied atmosphere test case are shown in figures 5.4 and 5.5 respectively.

The feature due to using the locally generated TAPE3 file is present at around 800cm^{-1} in both the linux and AIX runs. However, other than that, the two platforms yield very similar results. The character of the single precision residuals for this case are also different. Recall that the built-in atmosphere test case residuals for the single precision test case (see section 4.3) indicated there was a frequency shift in the output TAPE27 data files. That is not the case here. A magnification of figure 5.4(b) is shown in figure 5.6 for 700-770cm^{-1}, and in figure 5.7 for 900-1000cm^{-1}. There does appear to be some residual low spectral resolution feature in figure 5.7. It is not known what is causing this feature (CFC absorption differences?) but the magnitude is of the order of millikelvin so no further investigation will be undertaken.

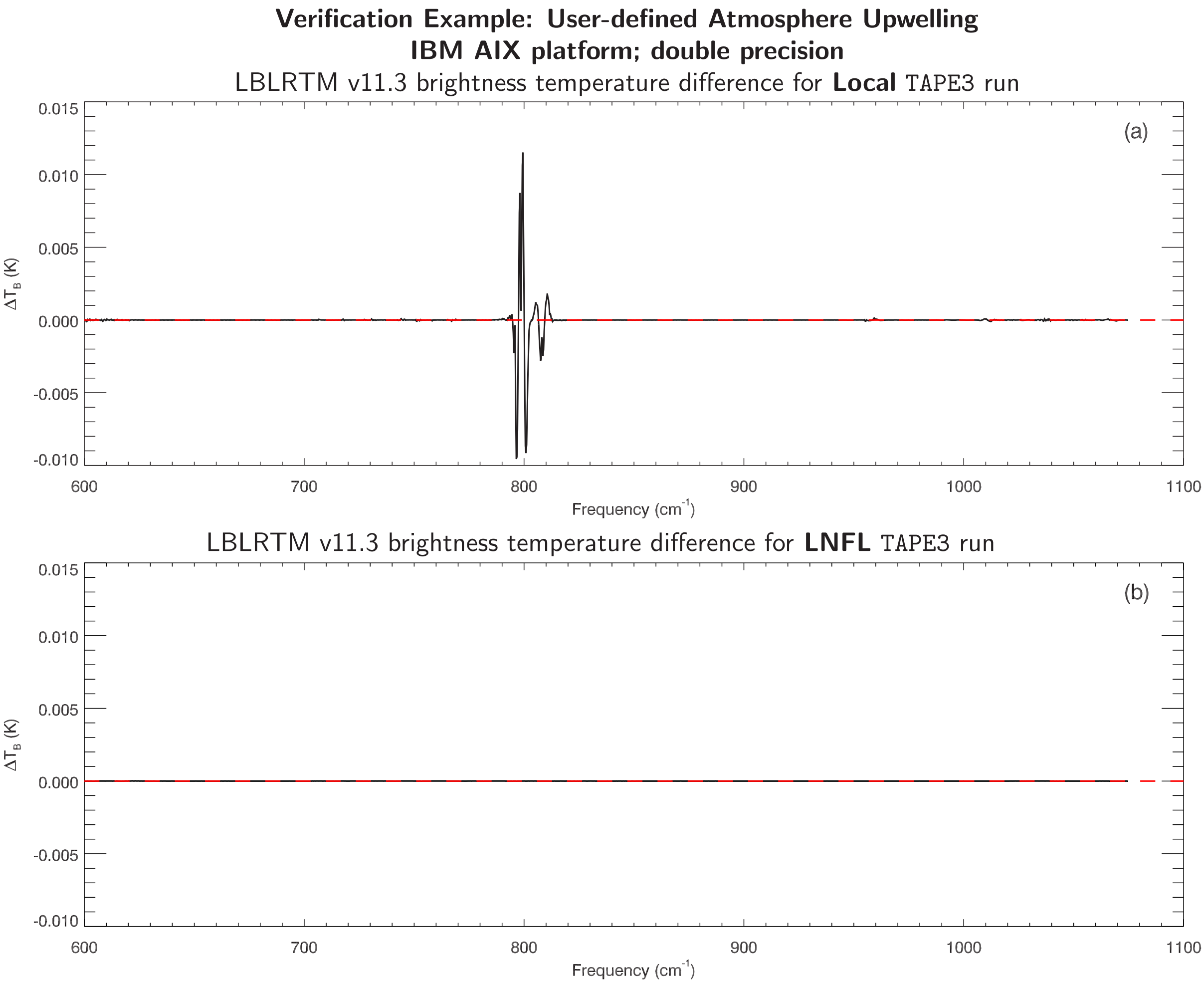

Figure 5.3: User-defined Atmosphere Test: Comparison of the AER-supplied `TAPE27_ex` output to the locally generated `TAPE27` output for the *double precision* version of LBLRTM v11.3 running on an IBM AIX system. **(a)** Using the big-endian `TAPE3` spectroscopic datafile generated from the local input shown in figure 3.1. **(b)** Using the big-endian `TAPE3` spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3. This result is identical to the same using the **AER** big-endian `TAPE3` spectroscopic datafile.

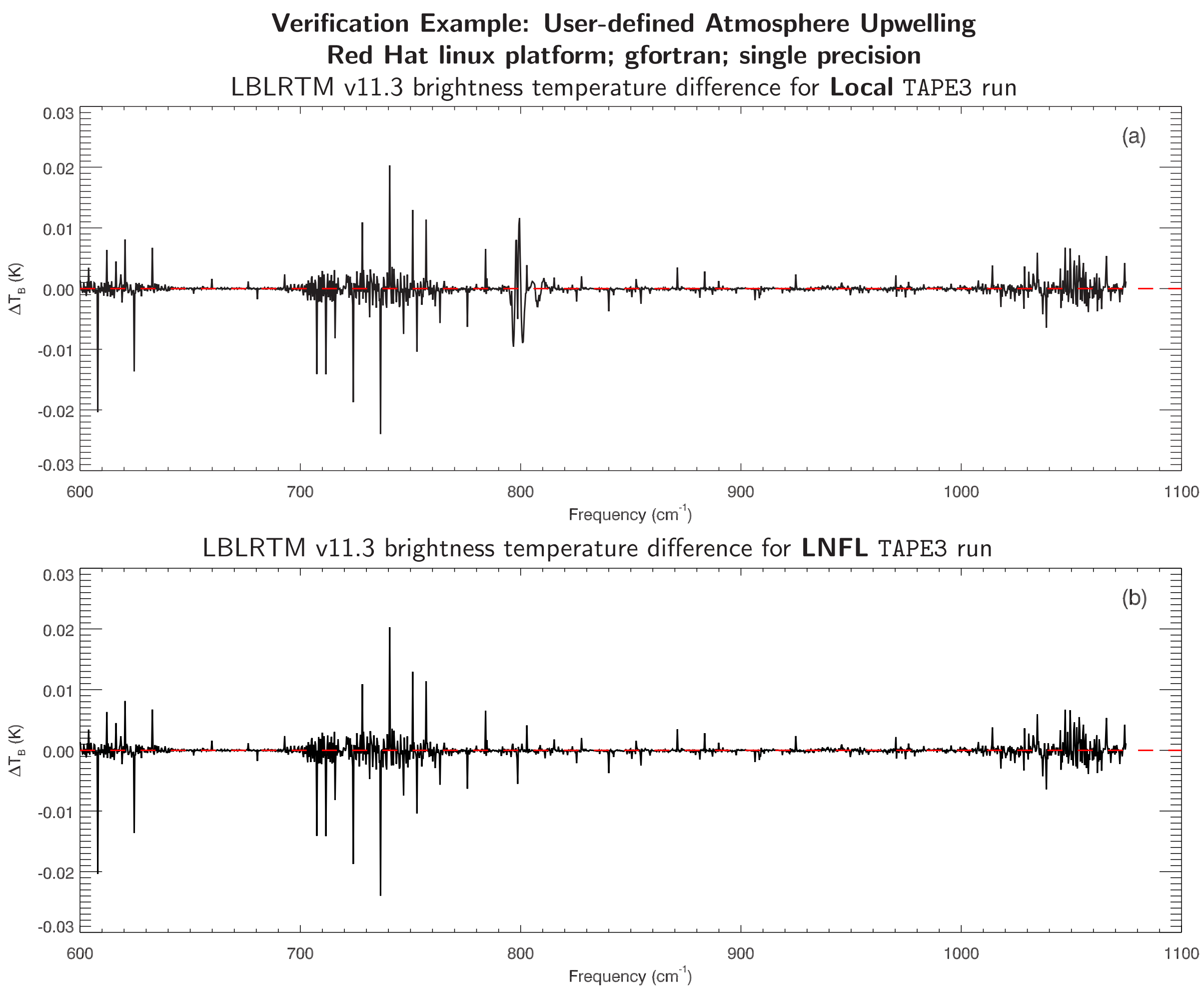

Figure 5.4: User-defined Atmosphere Test: Comparison of the AER-supplied TAPE27_ex output to the locally generated TAPE27 output for the *single precision* version of LBLRTM v11.3 running on a Red Hat linux system using the gfortran compiler. **(a)** Using the little-endian TAPE3 spectroscopic datafile generated from the local input shown in figure 3.1. **(b)** Using the little-endian TAPE3 spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3. This result is identical to the same using the **AER** little-endian TAPE3 spectroscopic datafile.

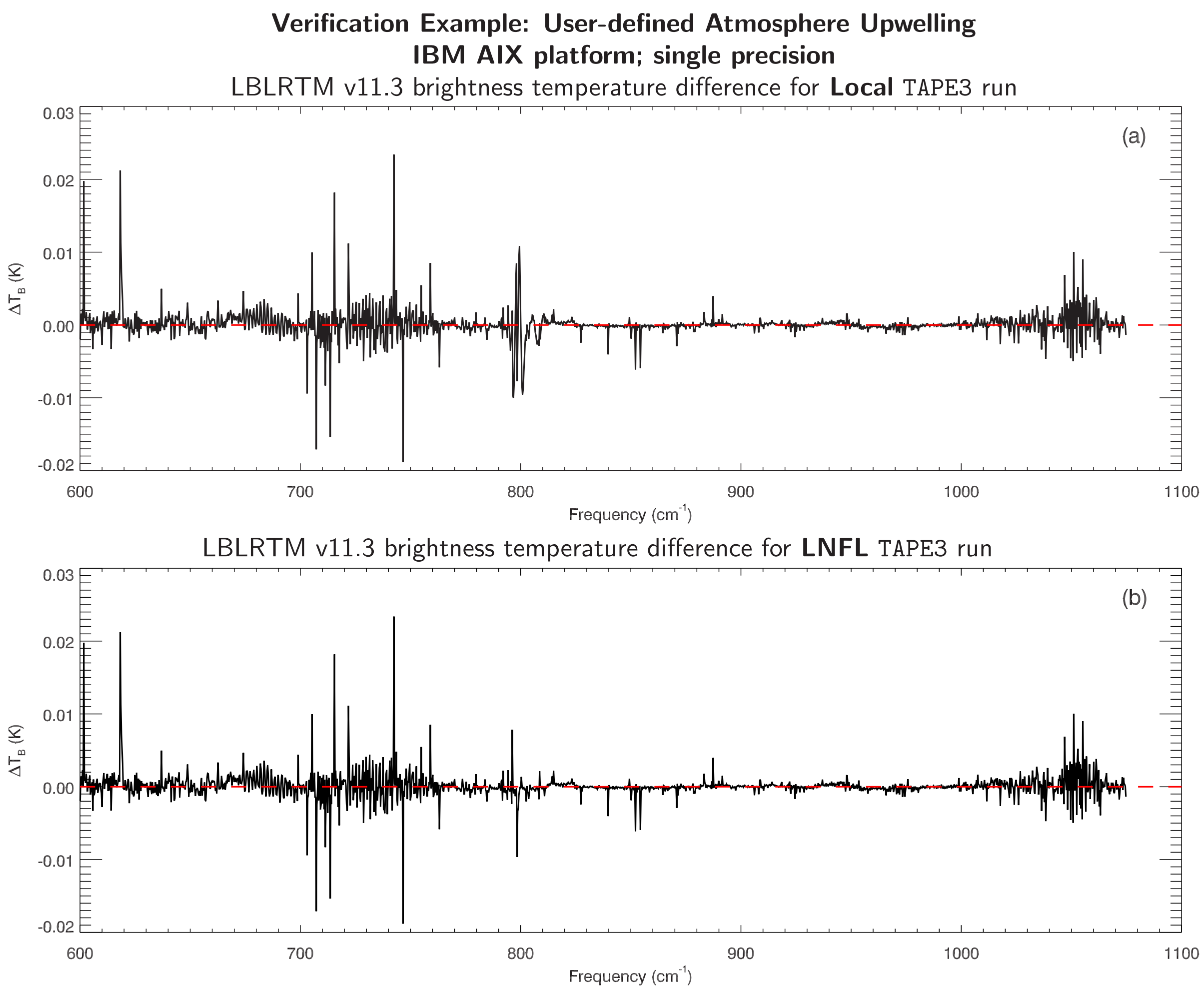

Figure 5.5: User-defined Atmosphere Test: Comparison of the AER-supplied TAPE27_ex output to the locally generated TAPE27 output for the *single precision* version of LBLRTM v11.3 running on an IBM AIX system. **(a)** Using the big-endian TAPE3 spectroscopic datafile generated from the local input shown in figure 3.1. **(b)** Using the big-endian TAPE3 spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3. This result is identical to the same using the **AER** big-endian TAPE3 spectroscopic datafile.

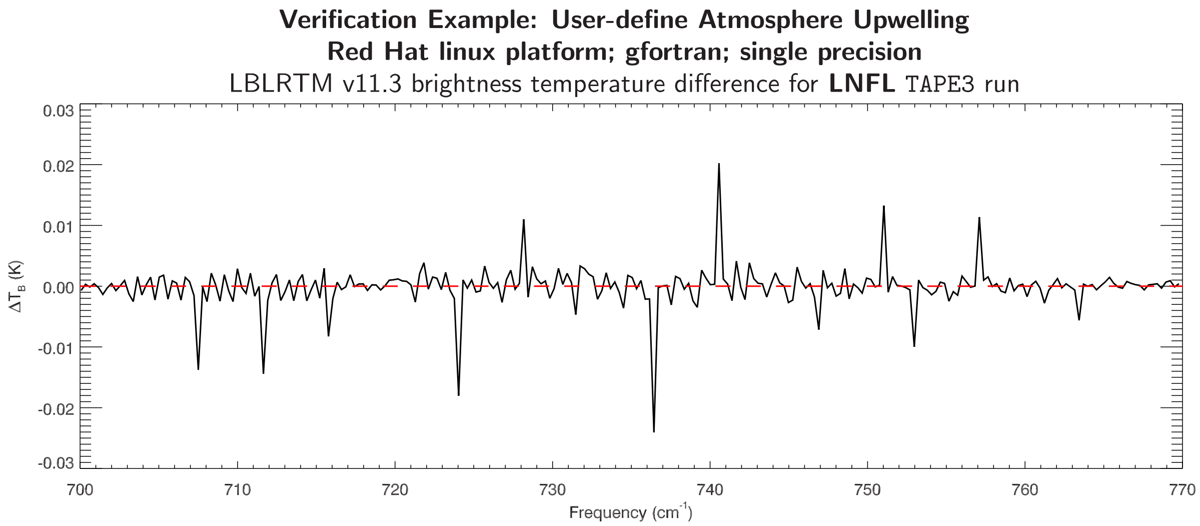

Figure 5.6: User-defined Atmosphere Test: A magnification of the 700-770cm^{-1} spectral region from figure 5.4(b). The character of the differences does not indicate a frequency shift (as seen in figure 4.7).

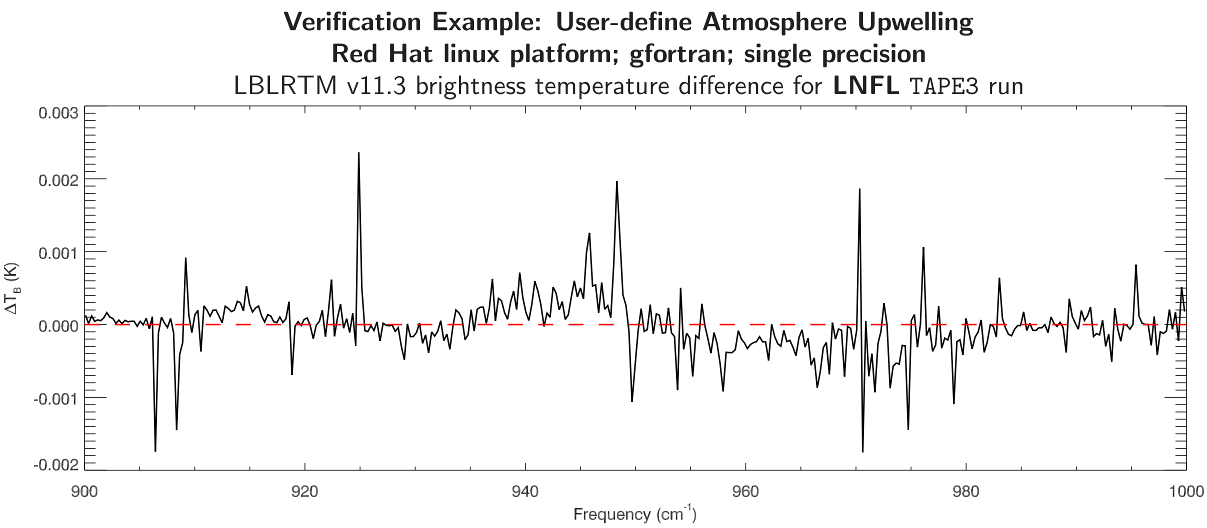

Figure 5.7: User-defined Atmosphere Test: A magnification of the 900-1000cm^{-1} spectral region from figure 5.4(b). The cause of the low spectral resolution feature is not known (CFC absorption differences?).

Acknowledgements

The LBLRTM software and associated data files are an integral part of our ability to use satellite radiances in the data assimilation systems at NCEP/EMC/JCSDA. So, thanks go to the people at AER, Inc. who provide and, importantly, maintain the LBLRTM source code and spectroscopic data inputs. Any list of inidividuals would be woefully short and incomplete but special thanks go to Jean-Luc Moncet, Vivienne Payne, and Mark Shephard of AER Inc., and Tony Clough of Clough Associates for their help.

A Anomalous Test Case Result with the gfortran Compiler

This section briefly details the results for the LBLRTM v11.3 built-in atmosphere test case when the gfortran v4.4.0(20081021) compiler is used with either the `-O2` or `-O3` optimisation switch. The anomalous LBLRTM v11.3 results occur for this compiler version in both the single and double precision builds, but the anomalous residuals in the single precision case are masked by the larger signal.

The double precision results for the linux/gfortran system with the optimisation switch set for the built-in atmosphere test case are shown in figure A.1. Residuals for LBLRTM runs using the local, LNFL, and AER `TAPE3` spectroscopic input files are shown.

The most obvious feature in the brightness temperature differences of figure A.1 is the "linear ramp" from 1000 to approximately 1025cm^{-1}. A magnification of this spectral region is shown in figure A.2. It is present regardless of which input spectroscopic `TAPE3` file is used. Additionally, after repeating the computations several times, it seems that the magnitude of this feature varies according to the compute load of the test platform. For example, the peak value of this feature at 1000cm^{-1} *for any of the `TAPE3` test runs* varied from -0.005 to -0.03K.

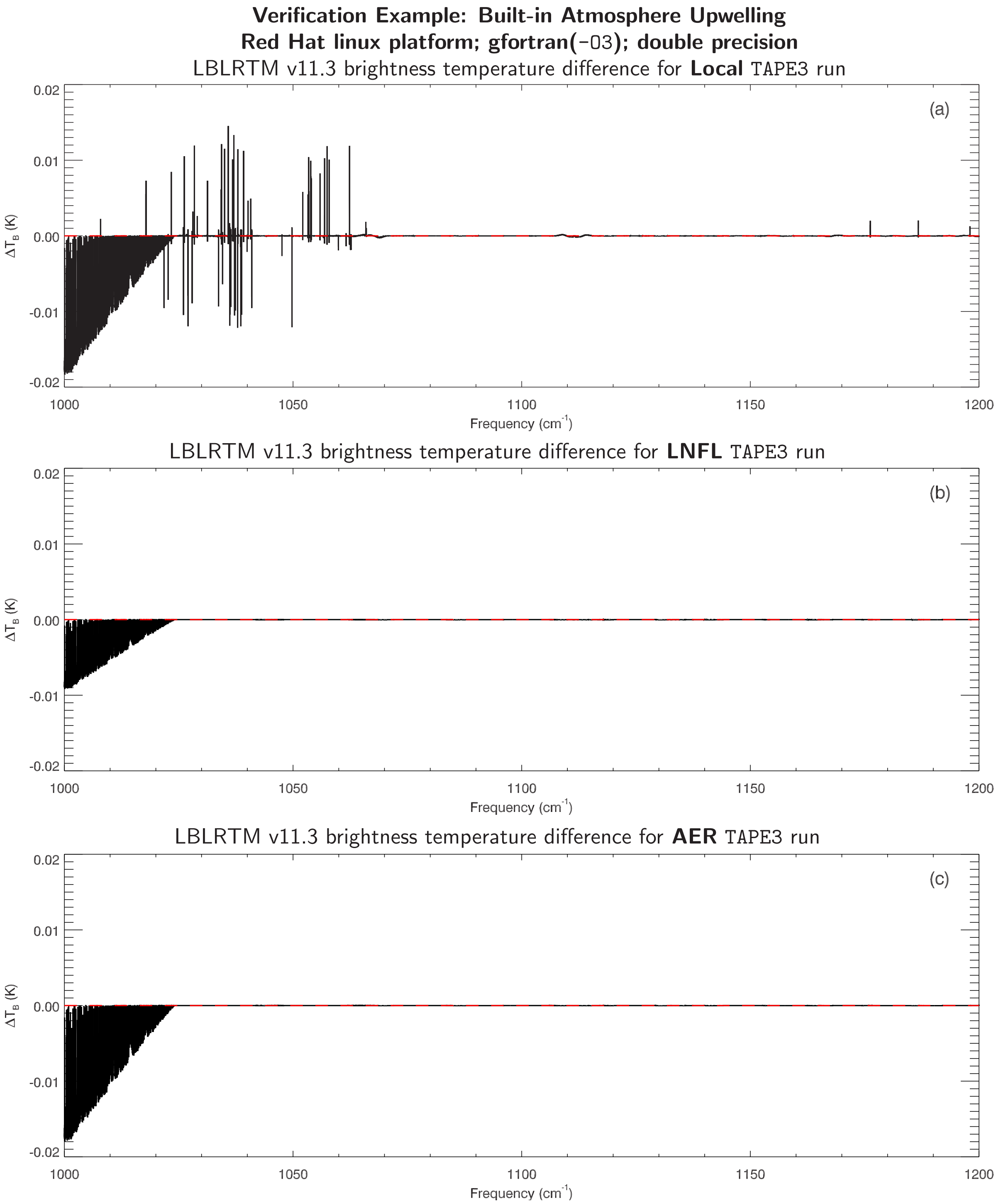

Figure A.1: Built-in Atmosphere Test: Comparison of the AER-supplied TAPE27_ex output to the locally generated TAPE27 output for the *double precision* version of LBLRTM v11.3 running on a Red Hat linux system using the gfortran compiler with an optimisation level of -O3. **(a)** Using the little-endian TAPE3 spectroscopic datafile generated from the local input shown in figure 3.1. **(b)** Using the little-endian TAPE3 spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3. **(c)** Using the AER-supplied little-endian TAPE3 spectroscopic datafile.

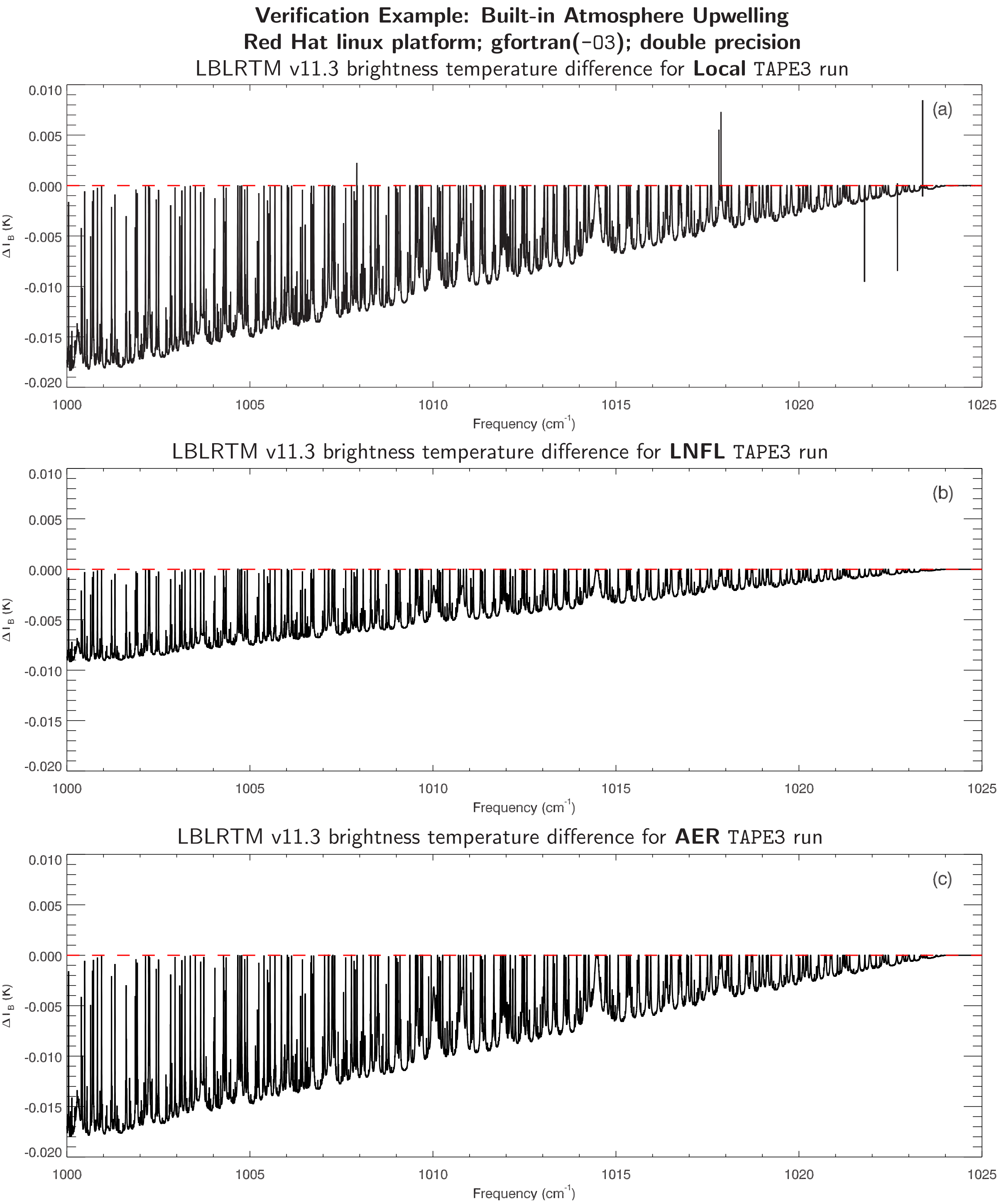

Figure A.2: Built-in Atmosphere Test: A magnification of the 1000-1025cm^{-1} spectral region from figure A.1. **(a)** Using the little-endian `TAPE3` spectroscopic datafile generated from the local input shown in figure 3.1. **(b)** Using the little-endian `TAPE3` spectroscopic datafile generated from the LNFL v2.5 distribution input shown in figure 3.3. **(c)** Using the AER-supplied little-endian `TAPE3` spectroscopic datafile.

B Anomalous Test Case Result with IBM Compiler

This section briefly details the results for the LBLRTM v11.3 user-defined atmosphere test case when the IBM AIX xlf95 v10.1.0000.0002 compiler is used (henceforth referred to as v10.1.0.2) . You can find out the version of your IBM compiler via the `-qversion` switch:

```
$ xlf95 -qversion
IBM XL Fortran Enterprise Edition V10.1 for AIX
Version: 10.01.0000.0002
```

The anomalous LBLRTM v11.3 results only occur for this compiler version and only for the double precision build – the single precision build does not appear to have any problem. Additionally, the problem also only occurs for the user-defined atmosphere test case; the built-in atmosphere test case produces expected results for all builds using the v10.1.0.2 AIX compiler. Thus, it is thought that the anomalous results stem from some sort of interaction between the double precision build and the use of the `SCAN` options - in this particular case the `FFTSCN` option, but similar anomalous results have been seen when the `SCNMRG` option has been used.

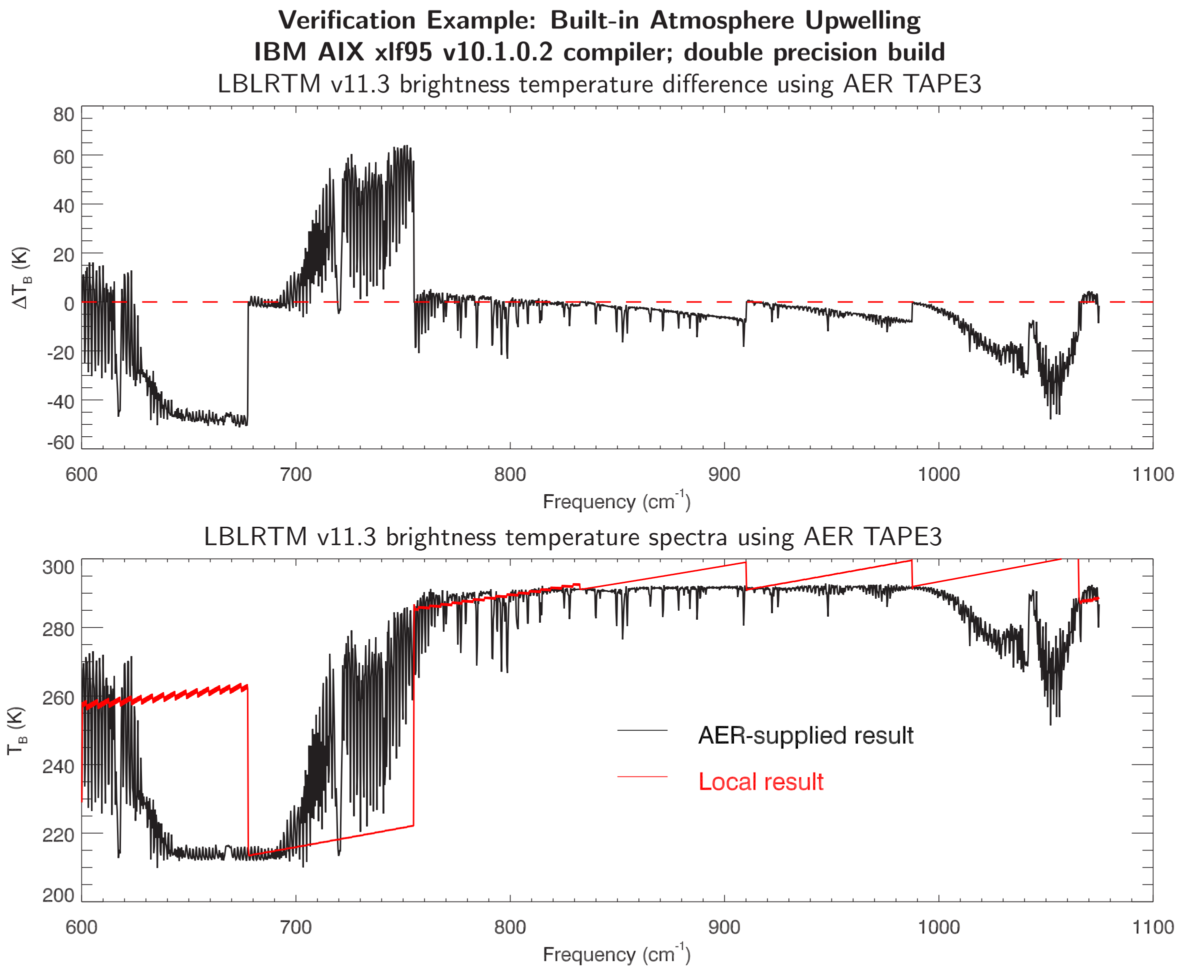

Figure B.1: Comparison of the AER-supplied `TAPE27_ex` output to the locally generated `TAPE27` output for the *double precision* version of LBLRTM v11.3 using the IBM AIX xlf 95 v10.1.0.2 compiler. The AER-supplied big-endian `TAPE3` spectroscopic datafile was used. **(Upper Panel)** Brightness temperature differences. **(Lower Panel)** Brightness temperature spectra. The locally generated result using the v10.1.0.2 compiler is clearly incorrect.