NAME-PPM
MD14/1(1)

Porting of NAME 4.8 Fortran 77 to Fortran 90/95 (NAME 5.0)

Matthew Hort

9 March 2001

1 Summary

To facilitate the integration of the current NAME code into the NAME-PPM model the porting of the NAME 4.8 Fortran 77 code to Fortran 90/95, to be called NAME 5.0, has been undertaken. In addition it is hoped that this ported code will be adopted as the operational code within the atmospheric dispersion group and there by ease the further integration of current and future changes/additions to NAME into NAME-PPM. This note briefly reports on significant changes to the code and compiler options as well as performance and validation tests that have been carried out by the author.

2 Compilers, compilers and more compilers

Currently NAME is compiled using the HP Fortran77 compiler, here after referred to as HP_F77. This is the office standard compiler on the HP system. Name-PPM is being written using Fortran 90. Currently on the HP system the only F90 compiler available is the NAG Fortran 90 compiler (NAG_F90). However, the iminante upgrade of the HP Unix operating system will see the arrival of the NAG Fortran 95 (NAG_F95) and HP Fortran 90 (HP_F90) compilers. Within this work all these compilers have been used and the resulting executables tested for performance.

It should be noted that the F90 and F95 compilers are being operated in fixed format mode i.e., Fortran 77 layout conventions e.g., continuation line marks, line lengths, etc. This occurs automatically provided that the Fortran files end in .f. Further, the current NAG_F95 compiler is not the latest version which will only become available once the HP UNIX upgrade takes place.

Table 1 lists the compilers and the options that have been used as standard. The options: +es, -132, +extend_source allow lines of greater than 72 characters to be compiled; -On, +On indicate level of optimisation; -NInnn the maximum number of continuation lines. The -K option proved necessary for the HP_F90 compiler to produce code that would run with the global met grid. The use of */ after the -I option just indicates the local path above the inclib directory. Further options used under F77 were not required by the newer compilers. The option -w used with the NAG compiler suppressed warning messages of which there were a significant number under this compiler.

Compiler	Options
HP_F77	+O2 +es +E1 -I */inclib.2001 -K +Onolimit -o NAME2001.exe NAME2001.f
NAG_F90/F95	-O2 -132 -NI65 -w -I*/inclib.2001/ -o NAME2001.exe NAME2001.f
HP_F90	+O2 +extend_source -I*/inclib.2001/ -K -o NAME2001.exe NAME2001.f

Table 1: Standard compiler options.

3 Code Changes

The transfer of NAME from F77 to F90 was carried out under the NAG_F90 compiler. This compiler adheres to a very strict implementation of the F90 standard and it is therefore expected that the code should prove far more portable as a result. The following sections provide a brief description of the errors/problems found and the implemented solution.

3.1 NAG_F90 compilation problems

Problem Number of continuation lines in GRIDDEF exceeded default value for compiler.
Solution Compiler option.

Problem $HP9000_800 INTRINSICS ON.
Solution Commented out.

Problem Common Block DATA statements in main code.
Solution Moved into BLOCK DATA PROGRAM UNIT at start of main code.

Problem Operands to .EQ. operator are of type LOGICAL. .EQ. is not a permissible logical operator.
Solution .EQV. substituted for .EQ.

Problem Array subscripts of type REAL.
Solution Subscripts set correctly to INTEGER.

Problem FLOAT used to convert integer to real. Not standard Fortran.
Solution Substituted for REAL.

Problem Arguments in reference to WCOEFF and WEQTOLL are not arrays. In the previously mentioned routines these arguments are arrays.
Solution Arguments in calling routines converted from scalar to array of size (1).

Problem Intrinsic subroutines DATE and TIME not standard Fortran.
Solution Replaced by the intrinsic subroutine DATE_AND_TIME, as already used by PC version of code.

Problem External function SYSTEM in READFF does not seem to be supported under NAG_F90.
Solution NAG_F90: Commented out. An equivalent command which requires f90_unix_proc to be used does exist under NAG_F95 compiler.
Solution HP_F90. Supports system function, command left in.

Problem Intrinsic functions GRAN and RAND not standard Fortran.
Solution New functions GRANNUM and RANDNUM written (By Alistair). These use the 'standard' F90 intrinsic subroutine RANDOM_ NUMBER to generate a Gaussian and normal random number respectively. The seed for the subroutine RANDOM_ NUMBER is set at the start and recorded at the end of each run using the intrinsic subroutine RANDOM_SEED located in name.f.

Problem Tab spacing used at some locations in code.
Solution Replaced with spaces.

Problem REAL*8 not standard.
Solution Replaced with DOUBLE PRECISION.

Problem INTEGER*2 used.
Solution Replaced with INTEGER(2)

Problem NAMELIST syntax error.
Solution Syntax changed.

Problem Subroutine GENTSRS.f. ISPEC used in IF test causing error.
Solution Alistair provided change to code.

Problem Output buffer overflow occurring at UPDATE file write.
Solution RECL statement used to allow larger fields to be written; RECL = 10**9. Not needed under HP_F90.

3.2 NAG_F95 and HP_F90 compilation problems

Problem READFFE, logical write command 1L not accepted.
Solution Standard syntax should be L1.

4 Results/Run Time Comparisons

This section will present run time results for several runs of differing particle numbers and release duration. Further, standard graphical output will be presented as verification that the different model compilations are doing the same thing.

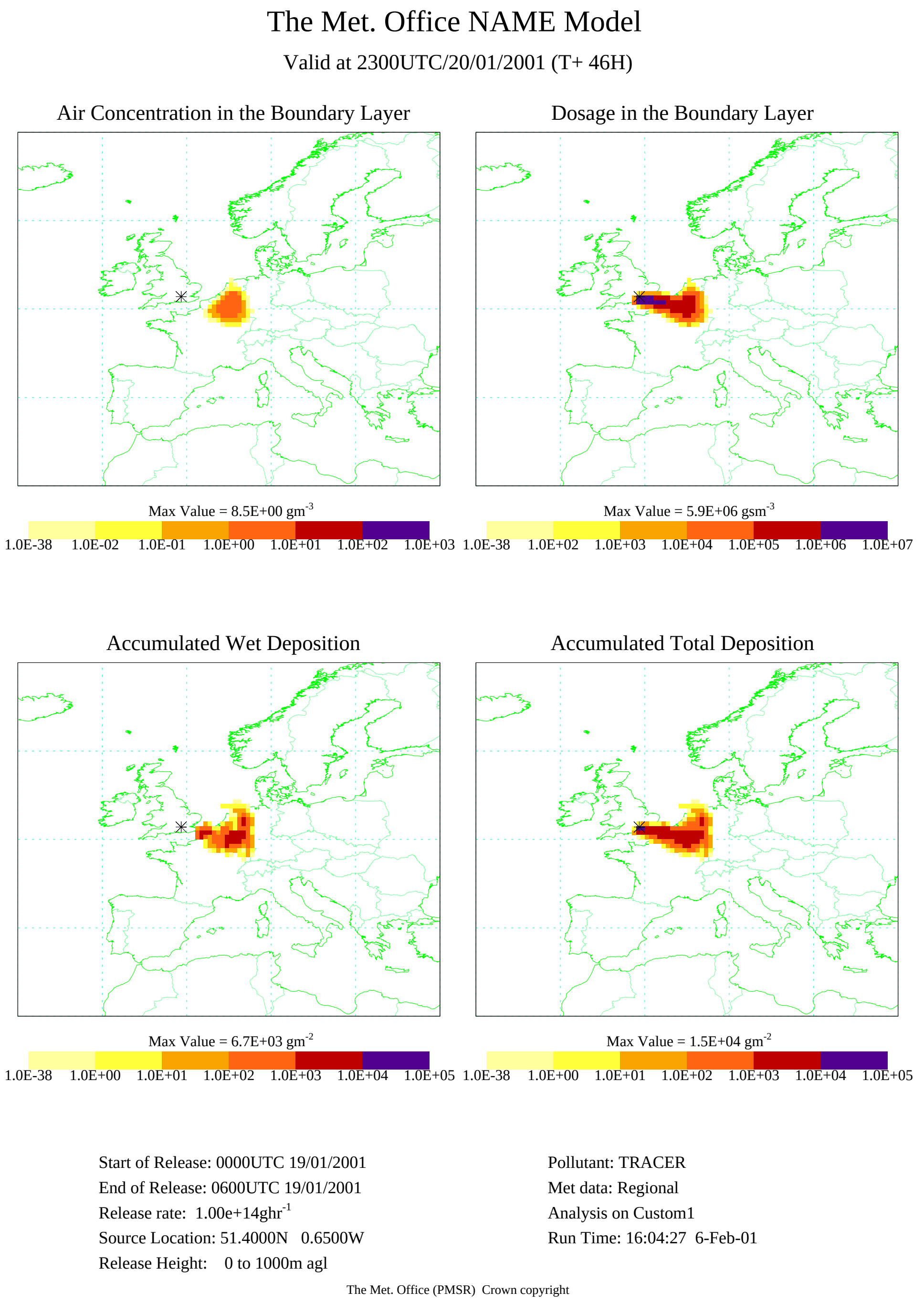
Table 2 lists results from two 47 hour runs conducted using the regional grid. All runs were conducted on the HP UX11 test machine DEVEL01. All run time changes are stated as the change relative to the HP_F77 i.e., the current standard, run time. We can clearly see the performance benefits of the HP_F90 compiled code over the NAG_F95 code and the current HP_F77 code. Runs using the NAG_F90 compiler were conducted on FR1140. These runs showed this compiler to be far worse than even the NAG_F95, producing run time that were a factor of 1.5 greater than the HP_F77 code.

Setup: 2000 particles; 3 hour release.		
Compiler	Run Time (sec)	Run Time Change
HP_F77	59.6	
NAG_F95	75.0	26% increase
HP_F90	36.3	39% decrease
Setup: 10000 particles; 6 hour release.		
Compiler	Run Time (sec)	Run Time Change
HP_F77	501.8	
NAG_F95	603.9	20% increase
HP_F90	286.6	43% decrease

Table 2: Run time comparison. 47 hour run on the regional grid.

Further test were carried out using the global met grid to ensure that no problems existed for larger jobs. Running using these settings highlighted a problem with the HP_F90 compiled code which produced a memory error at the start of a run. This was fixed by using the -K option when compiling, as indicated in Section 2, although the exact reasoning for this is not understood. Run times for these runs showed that using global met resulted in an insignificant increase in run time.

Figures 1 to 3 present standard graphical output from NAME. These figures were generated from data from the indicated compiled code. Each run extended for 47 hours and consisted of a six hour release of 2000 particles per hour. The regional met grid was used in all three runs.

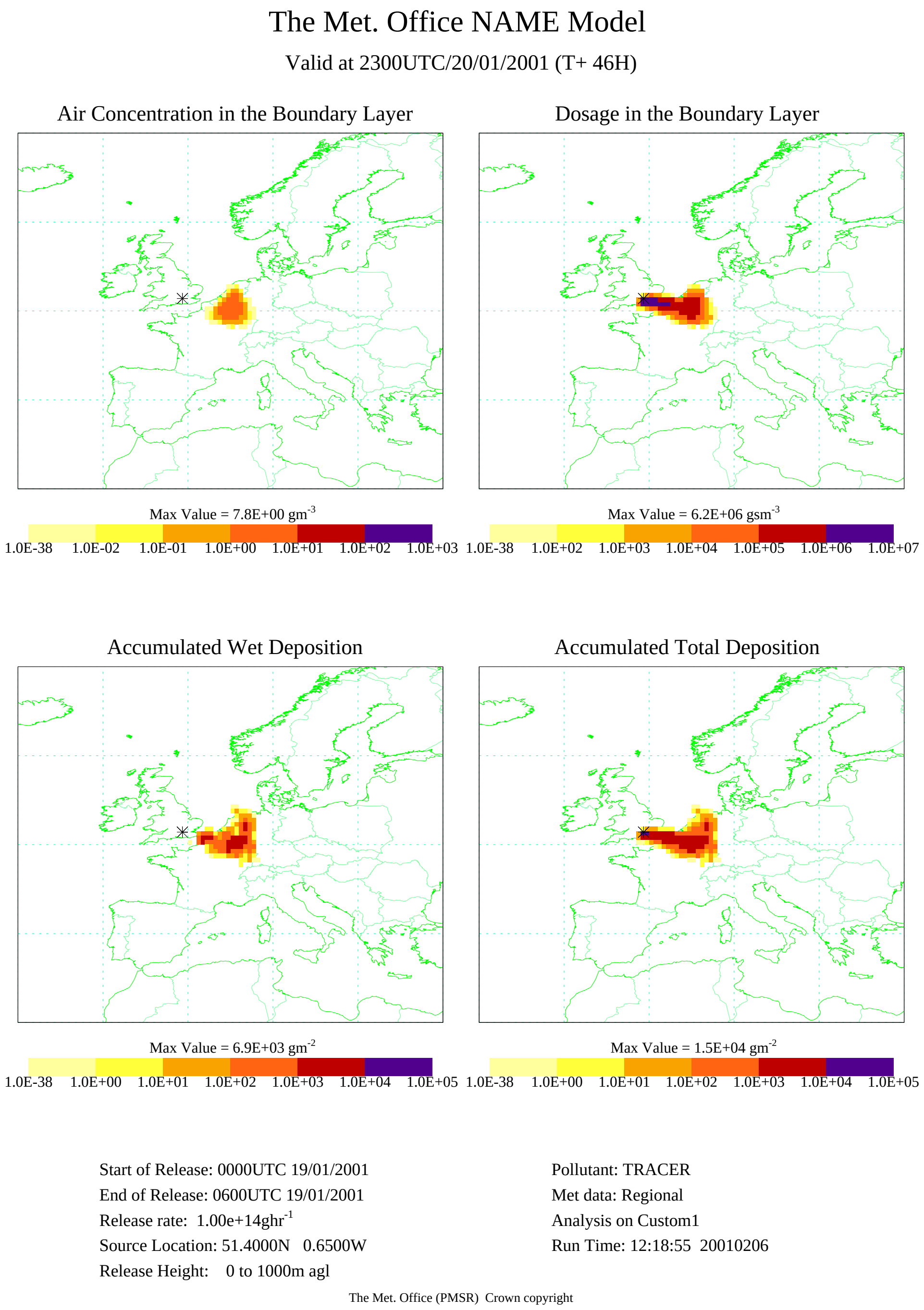

The Met. Office NAME Model
Valid at 2300UTC/20/01/2001 (T+ 46H)
Air Concentration in the Boundary Layer
Max Value = 8.5E+00 gm-3
1.0E-38 1.0E-02 1.0E-01 1.0E+00 1.0E+01 1.0E+02 1.0E+03
Dosage in the Boundary Layer
Max Value = 5.9E+06 gsm-3
1.0E-38 1.0E+02 1.0E+03 1.0E+04 1.0E+05 1.0E+06 1.0E+07
Accumulated Wet Deposition
Max Value = 6.7E+03 gm-2
1.0E-38 1.0E+00 1.0E+01 1.0E+02 1.0E+03 1.0E+04 1.0E+05
Accumulated Total Deposition
Max Value = 1.5E+04 gm-2
1.0E-38 1.0E+00 1.0E+01 1.0E+02 1.0E+03 1.0E+04 1.0E+05

Start of Release: 0000UTC 19/01/2001
End of Release: 0600UTC 19/01/2001
Release rate: 1.00e+14ghr-1
Source Location: 51.4000N 0.6500W
Release Height: 0 to 1000m agl

Pollutant: TRACER
Met data: Regional
Analysis on Custom1
Run Time: 16:04:27 6-Feb-01

The Met. Office (PMSR) Crown copyright

Figure 1: Output at T046 from HP_F77 compiled code.

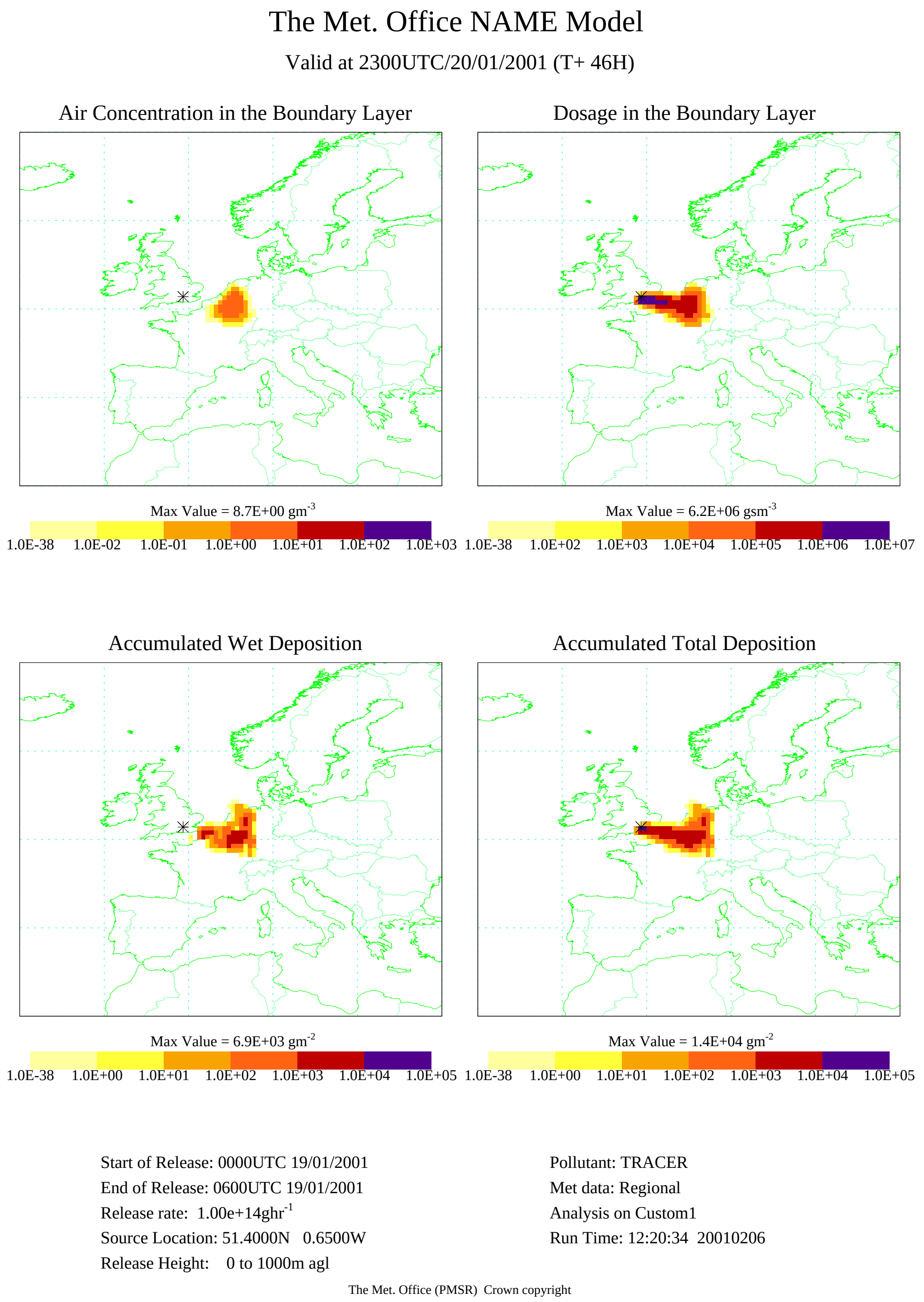

The Met. Office NAME Model
Valid at 2300UTC/20/01/2001 (T+ 46H)
Air Concentration in the Boundary Layer
Dosage in the Boundary Layer
Max Value = 7.8E+00 gm-3
1.0E-38 1.0E-02 1.0E-01 1.0E+00 1.0E+01 1.0E+02 1.0E+03
Max Value = 6.2E+06 gsm-3
1.0E-38 1.0E+02 1.0E+03 1.0E+04 1.0E+05 1.0E+06 1.0E+07
Accumulated Wet Deposition
Accumulated Total Deposition
Max Value = 6.9E+03 gm-2
1.0E-38 1.0E+00 1.0E+01 1.0E+02 1.0E+03 1.0E+04 1.0E+05
Max Value = 1.5E+04 gm-2
1.0E-38 1.0E+00 1.0E+01 1.0E+02 1.0E+03 1.0E+04 1.0E+05

Start of Release: 0000UTC 19/01/2001
End of Release: 0600UTC 19/01/2001
Release rate: 1.00e+14ghr^{-1}
Source Location: 51.4000N 0.6500W
Release Height: 0 to 1000m agl

Pollutant: TRACER
Met data: Regional
Analysis on Custom1
Run Time: 12:18:55 20010206

The Met. Office (PMSR) Crown copyright

Figure 2: Output at T046 from HP_F90 compiled code.


The Met. Office NAME Model
Valid at 2300UTC/20/01/2001 (T+ 46H)
Air Concentration in the Boundary Layer
Max Value = 8.7E+00 gm-3
1.0E-38 1.0E-02 1.0E-01 1.0E+00 1.0E+01 1.0E+02 1.0E+03
Dosage in the Boundary Layer
Max Value = 6.2E+06 gsm-3
1.0E-38 1.0E+02 1.0E+03 1.0E+04 1.0E+05 1.0E+06 1.0E+07
Accumulated Wet Deposition
Max Value = 6.9E+03 gm-2
1.0E-38 1.0E+00 1.0E+01 1.0E+02 1.0E+03 1.0E+04 1.0E+05
Accumulated Total Deposition
Max Value = 1.4E+04 gm-2
1.0E-38 1.0E+00 1.0E+01 1.0E+02 1.0E+03 1.0E+04 1.0E+05

Start of Release: 0000UTC 19/01/2001
End of Release: 0600UTC 19/01/2001
Release rate: 1.00e+14ghr^{-1}
Source Location: 51.4000N 0.6500W
Release Height: 0 to 1000m agl

Pollutant: TRACER
Met data: Regional
Analysis on Custom1
Run Time: 12:20:34 20010206

The Met. Office (PMSR) Crown copyright

Figure 3: Output at T046 from NAG_F95 compiled code.