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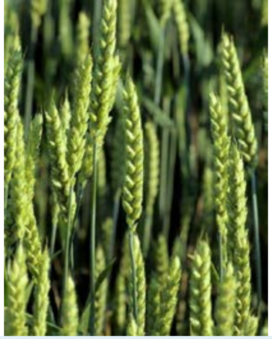


Performance, accuracy and bit-reproducibility aspects in handling transcendental functions with Cray and Intel compilers for the Met Office Unified Model

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Acknowledgements to

Dr. Martyn Corden (Intel), Dr. Zhang Zhang (Intel), Dr. Martin Dix (CSIRO)

Some requirements for meteorological applications

- **Performance**
  - **vectorisation**
  - **human factor: time spent to achieve a certain level in the performance gain**
- **Accuracy**
  - **single & double precision in weather forecasting models**
- **Results bit-reproducibility**

Note: all above mentioned aspects are applied for handling transcendental functions in an application and will be discussed in the presentation

Vector processing: Fortran compiler options related to the architecture

- **Intel compiler:** -x*code* for specific processor architecture
  - AVX – Intel Xeon processor E3/E5 and E3/E5/E7 v2 family
  - CORE-AVX2 - Intel Xeon processor E3/E5/E7 v3, v4 family
  - CORE-AVX512 – Intel Xeon Processor Scalable Family
  - Host – architecture on which the code is compiled

- **Cray compiler:** -h cpu=*target_system*

Compiler options set via modules on our XC-40 systems are

Module	Cray compiler	Intel compiler
craype-sandybridge	-hcpu=sandybridge	-mavx
craype-haswell	-hcpu=haswell	-xCORE-AVX2
craype-broadwell	-hcpu=broadwell	-xCORE-AVX2

Results bit-reproducibility

- Means getting identical results on a job rerun
- Benefits: useful in testing, debugging, tracking down code bugs or numerical instability
- Numerical implementation of UM includes a setting which provides results bit-reproducibility using different number of threads for the same horizontal decomposition

Rerun bit-reproducibility

- Intel Fortran compiler => need to specify

  `-fp-model precise`

  - may effect vectorisation of loops for some transcendental functions called within the loops

Note: below

- any reference to a compiler means Fortran compiler
- `-fp-model precise` is used in the Intel compiler case

- Cray compiler : results bit-reproducibility may depend on
  `-h flex_mp=`*`level`*

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Accuracy in calculation of transcendental functions

➢ **Accuracy is measured in terms of ULP**
(unit in the last place or unit of least precision)

- **accuracy for Cray CCE math libraries is controlled by `–hfpN` option**

Intel compiler		Cray compiler		
`default`	`-fp-model precise`	`-hfp0|-hfp1|-hfp2`	`-hfp3`	`-hfp4`
4 ULP	0.6 ULP	1.3 ULP	2.6 ULP	4 ULP

Note: `–hfp4` is used to compile the majority of UM files

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Vectorisation information for some transcendental functions in loops

With the Cray compiler and the Intel compiler with -fp-model precise, loops are

- **vectorised with SQRT, SIN, COS, EXP**
- **NOT vectorised with ASIN, ACOS, ATAN**

	Power (x^y)	ALOG	ALOG10	TANH	ATAN2
Cray compiler	Yes	Yes	No	No	Yes
Intel compiler	No	No	No	Yes	No

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Can loops for all transcendental functions be vectorised?

- Cray compiler: NO (as far as I know)
- Intel compiler: YES in two ways
  - `-fast-transcendentals -fimf-precision=<value>`

    `<value> = high | medium | low`

    high - 1 ULP, used in this presentation

    medium - 4 ULP, also tested with very similar performance

    low – not used

  - Intel Math Kernel Library (MKL) library using vector math library (the error usually is <0.75 ULP with high accuracy)

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Environment for implementation

- **Hardware**
  - Cray XC-40 (Terra), Intel Xeon E5-2690 v3, 2.6 GHz
    136 nodes with 24 cores/node (3264 cores)

- **Software**
  - Intel compiler v17.0.1.132
  - Cray cce 8.4.5
  - Cray MPICH 7.3.2
  - MPI_WTIME – for time measurements

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UM job description

- UM10.7 sources (Feb 2017)
- N768L70 (1532x1152x70 grid size) global model
- 24 hour (192 time steps) forecast with switched off I/O to tune computational capability of the model sources
- run configuration: 16x30 - horizontal decomposition with 2 threads on 960 cores
  - elapsed time for the job is 920-950 sec

Note: the job was used within the OpenMP coverage improvement collaboration project with the Met Office for UM10.4-10.8 releases

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Example: departure_point_eta_mod.F90

Subroutine includes 8 three-level nested loops:

```
DO k = 1, model_levels
  DO j = udims%j_start, udims%j_end
    DO i = udims%i_start, udims%i_end
. . .
      z_d = SQRT(1.0 - x_d**2 - y_d**2)

      depart_xi1(i,j,k) = xi1_u(i) +                               &
                          ATAN2(x_d,z_d*csxi2_p(j)-y_d*snxi2_p(j))
      depart_xi2(i,j,k) = ASIN(y_d*csxi2_p(j)+z_d*snxi2_p(j))
      depart_xi3(i,j,k) = eta_rho_levels(k) - timestep*w_a
    END DO
  END DO
END DO
```

Cray compiler loopmark output for the loop

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Loopmark output with `-rm` compiler option

```
251.  + M m----------<     DO k = 1, model_levels
252.  + M m 3--------<       DO j = udims%j_start, udims%j_end
253.    M m 3 Vp-----<         DO i = udims%i_start, udims%i_end
. . .
276.    M m 3 Vp                 z_d = SQRT(1.0 - x_d**2 - y_d**2)
277.    M m 3 Vp
278.    M m 3 Vp                 depart_xi1(i,j,k) = xi1_u(i) +                     &
279.    M m 3 Vp                                     ATAN2(x_d,z_d*csxi2_p(j)-y_d*snxi2_p(j))
280.    M m 3 Vp                 depart_xi2(i,j,k) = ASIN(y_d*csxi2_p(j)+z_d*snxi2_p(j))
281.    M m 3 Vp                 depart_xi3(i,j,k) = eta_rho_levels(k) - timestep*w_a
282.    M m 3 Vp----->         END DO
283.    M m 3-------->       END DO
284.    M m---------->     END DO

 A loop starting at line 253 was partially vectorized.
```

Comments:

- the inner loop is only partially vectorised
- the loopmark output does not provide details on what is not vectorised

Intel compiler diagnostic for the loop

```
-fp-model precise -qopt-report=5 -qopt-report-phase=vec
```

LOOP BEGIN at <path>/departure_point_eta_mod.F90(253,9)
remark #15382: vectorization support: call to function atan2 cannot be vectorized [<path>/departure_point_eta_mod.F90(279,31)]
remark #15382: vectorization support: call to function asin cannot be vectorized [<path>/departure_point_eta_mod.F90(280,31)]
remark #15344: loop was not vectorized: vector dependence prevents vectorization
LOOP END

```
-fp-model precise -fast-transcendentals -fimf-precision=high
   -qopt-report=5 -qopt-report-phase=vec
```

LOOP BEGIN at <path>/departure_point_eta_mod.F90(253,9)
. . .
remark #15305: vectorization support: vector length 4
remark #15309: vectorization support: normalized vectorization overhead 0.303
remark #15300: LOOP WAS VECTORIZED
remark #15476: scalar cost: 413
remark #15477: vector cost: 107.250
remark #15478: estimated potential speedup: 3.690
remark #15482: vectorized math library calls: 2
LOOP END

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Time measurements for departure_point_eta_mod loops

$$T = \left(\sum_{i=0}^{479} t_i\right) \Big/ 480$$ – average time taken by MPI process

t_i – total time for all 8 loops taken by MPI process with rank #*i* (the job is run on 480 MPI processes)

Compilation options for departure_point_eta_mod.F90

Cray compiler:

```
-hcpu=haswell -O3 -hvector3 -hscalar3
-hfp4 -hcache3 -haggress -hnocontiguous
–hconcurrent -hflex_mp=default
```

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Time measurements for departure_point_eta_mod loops (cont #2)

Intel compiler

STANDARD

`-align array64byte -qopenmp -O3 -fp-model precise -xavx` (1)

FAST_TRANS

`(1) "+" -fast-transcendentals -fimf-precision=high` (2)

FAST_TRANS+AVX2

`(2) with replacement –xavx => -xCORE-AVX2` (3)

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Time measurements for departure_point_eta_mod loops (cont #3)

Cray	Intel		
	STANDARD	FAST_TRANS	FAST_TRANS+AVX2
49.7 sec	**63.1 sec**	**29.8 sec**	**28.4 sec**

Conclusions:

- **usage of `-fast-transcendentals -fimf-precision=high` reduces the elapsed time by over 2 times**
- **the shortest elapsed time with the Intel compiler is 1.75 times better than with the Cray compiler**
- **minor speed up from AVX2**

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Usage of MKL in UM

Frequently called transcendental functions in the UM sources are managed by the following procedure:

```
SUBROUTINE exp_v(n,x,y)
. . .
#if defined(MKL)
CALL vdexp(n, x, y)
#else
DO i=1, n
  y(i) = EXP(x(i))
END DO
#endif
END SUBROUTINE exp_v
```

Similar routines are available in UM for

EXP, SQRT, LOG, SIN, COS, ASIN, ACOS, . . .

Performance results with Intel compiler

Build #1: STANDARD optimised build

Build #2: FAST_TRANS build for all model files

Build #3: FAST_TRANS build for all model files "+" pre-processor options are set to use the MKL library (-DMKL)

STANDARD	FAST_TRANS	FAST_TRANS + MKL
918 sec	874 sec	877 sec

Conclusions:

- **fast-transcendentals provide a reduction in the elapsed time for the job by ~5% with a relatively minor effort**
- **MKL has no additional benefit**

Performance results comparison for Intel and Cray compilers

Using the same run environment

Intel compiler => 874 sec

Cray compiler => 952 sec

with Cray compiler options set at the Met Office with enabled inter-procedural optimisation

Conclusion:

- **elapsed time with the Intel compiler is 9% better than with the Cray compiler**

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Conclusions

- Intel compiler
  - using fast-transcendentals and MKL library
    - vectorisation of some loops is improved
    - relatively good performance gains can be achieved
      - factor of 2 speed-up for SL departure point calculations loops
      - 5% improvement for full model
    - relatively minor effort required

- Cray compiler
  - at this stage it is not clear on whether a similar performance benefits are achievable with the compiler

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THANK YOU