Sensitivity of WRF simulation to different code compiler version

Abstract

This evaluation compares results from WRF code built by different versions of Intel's ifort compiler. It has been shown that differences in model output using different fortran compiler do exist and in some situations like during convective weather can be significant. More research would be required in order to establish confident conclusions. Simulation accuracy has not been evaluated in this research.

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Introduction

Different compiler options are available to build WRF from source code [1]. For linux, three fortran compilers can be used, open source GNU Fortran (**gfortran**) [2], Intel Fortran Compiler (**ifort**) [3] and PGI Compilers **PGI** [4]. Depending on compiler choice, WRF execution speed will be different. gfortran will produce slowest code, while ifort code is usually fastest on Intel hardware, on AMD hardware PGI code wins performance benchmarks.

As we use Intel hardware in most if not all of our applications, Intel's ifort is our compiler of choice for several years. However during time, compiler has been updated with yearly major version increases and several minor increases in between. We were intersted in comparing WRF simulations of same case by using two different wrf.exe binaries, produced by different ifort compiler generation.

We were speculating that differences in simulated meteorological fields from code produced by different compiler version should be non-existent or at worst minimal and not statistically significant. However, as will be demonstrated in this paper, our testing reveal that differences are larger than we predicted.

Methods

4 different WRF runs were performed using ARW solver, over the same data produced from metgrid.exe program that was not rerun between WRF runs. Results from WRF runs were converted into grib2 format by UPP (unipost.exe) and cnvgrib programs and then analyzed in GrADS and with python.

Model domain consisted of single non-nested domain created by geogrid.exe program, spanning over 150x125 points with domain center at 45°N 15°E. Grid resolution was 9km and domain is prepared using unmodified GEOGRID.TBL.ARW default static datasets.

For initial and boundary conditions, CFS v2 [5] dataset has been used. Simulation start was at 06th August 2017 and simulation length was 24 hours. Adaptive time step was used.

All WPS and WRF programs used are version 4.0.3 and where built from completely unmodified source code. namelist.wps and namelist.input or any other configuration option was not changed between any of 4 runs. The only differences in runs were that two runs were performed using real.exe and wrf.exe compiled using Intel's **ifort 2019** and two runs were performed with code from **ifort 2016**.

Two runs were performed by using same code in order to rule out any possibility of result differences caused by any math rounding, lowered precision of floating point divisions, square root calculations (compiler options *no-prec-div*, *no-prec-sqrt*, …) or any other possible non value-safe code optimizations by compiler.

Code has been compiled statically and both has been executed on the same machine, inside identical environment. Compile-time dependencies (netcdf, libpng, jasper, …) were of the same versions, but ifort 2019 code has been compiled on linux Mint 19, whereas ifort 2016 code has been compiled on Centos 6 operating system. Different OS has been used in order to satisfy compatibility of installed Intel fortran/icc compilers with system gcc compilers.

Model setup was not optimized for simulation accuracy but aimed for simplicity and speed, as main objective of this study was to find possible differences between runs and not so much to verify simulation against measurements. With such goal, namelist.input template was set up with only most basic entries and options.

namelist.wps file contents:

```
&share
 wrf_core = 'ARW',
 max_dom = 1,
 start_date = '2017-08-06_00:00:00', '2017-08-06_00:00:00', '2017-08-06_00:00:00',
 end_date = '2017-08-07_00:00:00', '2017-08-07_00:00:00', '2017-08-07_00:00:00',
 interval_seconds = 21600,
 io_form_geogrid = 2,
/

&geogrid
 parent_id         =   1,    1,    2,
 parent_grid_ratio =   1,    3,    3,
 i_parent_start    =   1,   45,   45,
 j_parent_start    =   1,   32,   34,
 e_we              =  150,  127, 118,
 e_sn              =  125,  109, 100,
 geog_data_res = 'default'
 dx = 9000,
 dy = 9000,
 map_proj = 'lambert',
 ref_lat   =  45.00,
 ref_lon   =  15.00,
 truelat1  =  45.00,
 truelat2  =  45.00,
 stand_lon =  15.00,
 geog_data_path = '/home/arw/AY/GEOG4/',
 opt_geogrid_tbl_path = '.'
/

&ungrib
 out_format = 'WPS',
 prefix = 'FILE',
/

&metgrid
 fg_name   =  'FILE'
 io_form_metgrid = 2,
 opt_metgrid_tbl_path = '.'
 constants_name = './TAVGSFC'
/
```

namelist.input file contents:

```
&time_control
 !------------------- START/END -------------------------
 start_year                   = 2017, 2017, 2017,
 start_month                  = 08, 08, 08,
 start_day                    = 06, 06, 06,
 start_hour                   = 00, 00, 00,
 start_minute                 = 00, 00, 00,
 start_second                 = 00, 00, 00,
 end_year                     = 2017, 2017, 2017,
 end_month                    = 08, 08, 08,
 end_day                      = 07, 07, 07,
 end_hour                     = 00, 00, 00,
 end_minute                   = 00, 00, 00,
 end_second                   = 00, 00, 00,
 !------------------- INPUT -----------------------------
 interval_seconds             = 21600,
 !input_from_file              = .true., .true., .true.,
 !fine_input_stream             = 0, 0, 0,
 !io_form_input                 = 2,
 !io_form_boundary              = 2,
 !------------------- OUTPUT ----------------------------
 history_interval             = 60, 60, 60,
 adjust_output_times          = .true.,
 frames_per_outfile           = 1, 1, 1,
 io_form_history              = 2,
 /


 &domains
 !------------------- FIXED TIME STEP -------------------
 time_step                    = 54,
 !------------------- ADAPTIVE TIME STEP ----------------
 use_adaptive_time_step       = .true.,
 step_to_output_time          = .true.,
 target_cfl                   = 1.10, 1.10, 1.10,
 target_hcfl                  = 0.80, 0.80, 0.80,
 max_step_increase_pct        = 5, 51, 51,
 starting_time_step           = 27, 9, 3,
```

```
max_time_step                    = 108, 36, 12,
min_time_step                    = 27, 9, 3,
!adaptation_domain                = 1,
!-------------------- DOMAIN -----------------------------
s_we                             = 1, 1, 1,
e_we                             = 150, 127, 118,
s_sn                             = 1, 1, 1,
e_sn                             = 125, 109, 100,
s_vert                           = 1, 1, 1,
e_vert                           = 40, 40, 40,
p_top_requested                  = 5000,
dx                               = 9000, 3000, 1000,
dy                               = 9000, 3000, 1000,
!-------------------- REAL -------------------------------
num_metgrid_levels               = 33,
num_metgrid_soil_levels          = 4,
!-------------------- NESTING ----------------------------
grid_id                          = 1, 2, 3,
max_dom                          = 1,
parent_id                        = 0, 1, 2,
i_parent_start                   = 1, 45, 45,
j_parent_start                   = 1, 32, 34,
parent_grid_ratio                = 1, 3, 3,
parent_time_step_ratio           = 1, 3, 3,
!-------------------- MISC -------------------------------
smooth_cg_topo                   = .true.,
/


&physics
!
mp_physics                       = 4, 4, 4,
ra_lw_physics                    = 1, 1, 1,
ra_sw_physics                    = 1, 1, 1,
sf_sfclay_physics                = 1, 1, 1,
sf_surface_physics               = 2, 2, 2,
bl_pbl_physics                   = 1, 1, 1,
cu_physics                       = 11, 0, 0,
!
!
!
! PHYSICS OPTIONS:
!
!-------------------- MICROPHYSICS -----------------------
do_radar_ref                     = 1,
!-------------------- RADIATION --------------------------
radt                             = 10, 10, 10,
swint_opt                        = 1,
!-------------------- SURFACE LAYER ----------------------
!
!-------------------- LSM --------------------------------
num_soil_layers                  = 4,
num_land_cat                     = 21,
!-------------------- PBL --------------------------------
bldt                             = 0, 0, 0,
!-------------------- CUMULUS ----------------------------
cudt                             = 0,
!-------------------- MISC -------------------------------
!
/


&dynamics
!
!-------------------- DIFFUSION/TURBULENCE ---------------
diff_opt                         = 1, 1, 1,
km_opt                           = 4, 4, 4,
!-------------------- DAMPING ----------------------------
w_damping                        = 1,
damp_opt                         = 3,
epssm                            = 0.5, 0.5, 0.5,
!-------------------- ADVECTION --------------------------
use_theta_m                      = 0,
use_q_diabatic                   = 0,
!-------------------- MISC -------------------------------
!
/


&bdy_control
spec_bdy_width                   = 5,
spec_zone                        = 1,
relax_zone                       = 4,
specified                        = .true., .false., .false.,
nested                           = .false., .true., .true.,
/


&namelist_quilt
nio_tasks_per_group              = 0,
nio_groups                       = 1,
/
```

Results

Comparing simulation results from two runs of same compiler code, no differences has been found. The simulated meteorological fields in grib2 files were byte-identical between two ifort 2016 and between two ifort 2019 runs.

Contrary to that, outputs from 2016 and 2019 runs were not identical, and some differences between them are presented below. On figures 1-6, temperature at 2m and MSLP values are extracted for 6 locations within region (Rijeka, Zagreb, Split, Zadar, Rovinj and Osijek). Figures 7-15 display differences in several meteorological field at the time of last simulation hour (24 hours after model initialization) when the differences are generally found to be largest.

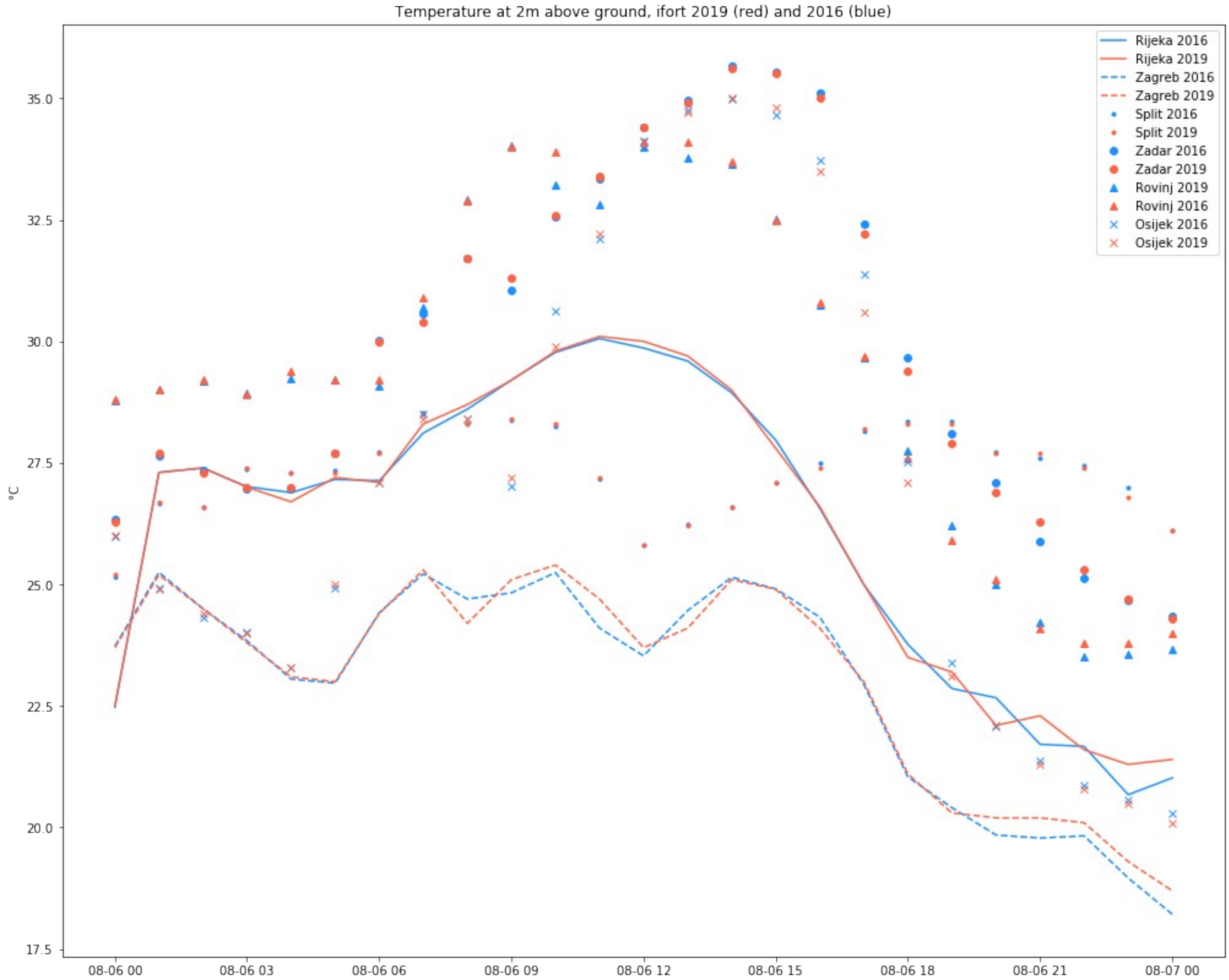

Figure 1: Temperature at 2m above ground comparision for Rijeka, Zagreb, Split, Zadar, Rovinj and Osijek using both compilers

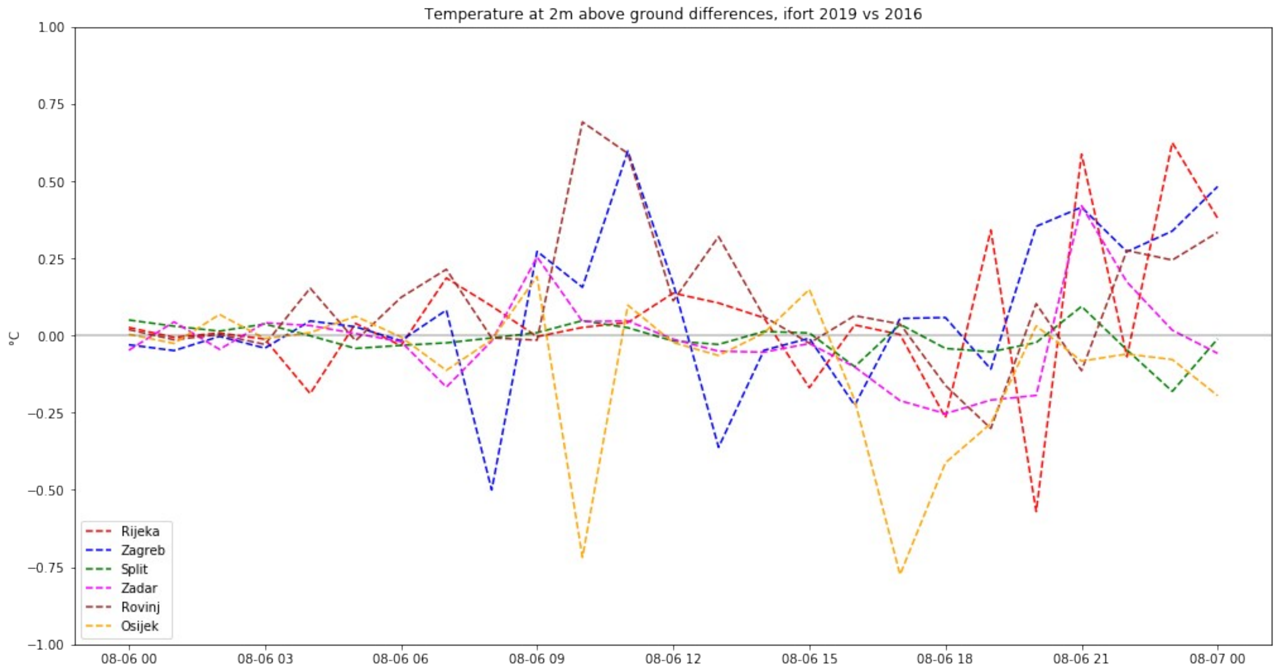

Figure 2: Temperature at 2m above ground difference between ifort 2019 and ifort 2016 runs for Rijeka, Zagreb, Split, Zadar, Rovinj and Osijek

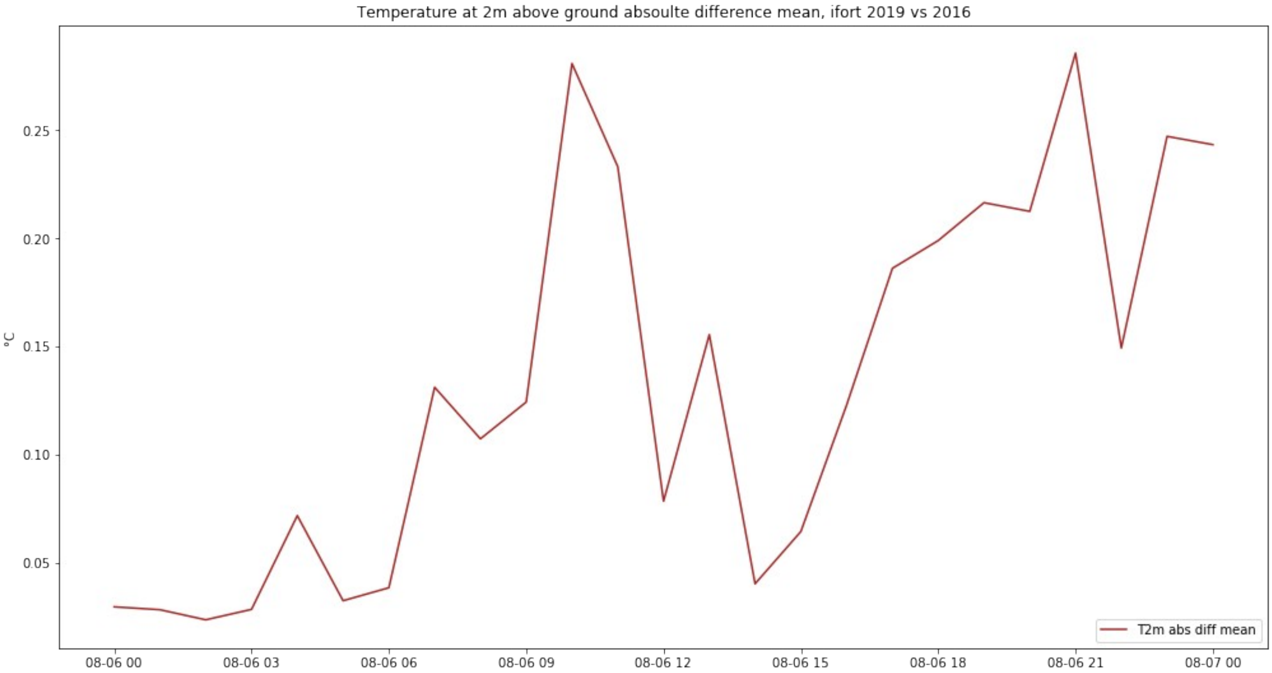

Figure 3: Mean value of absolute temperature at 2m above ground difference for Rijeka, Zagreb, Split, Zadar, Rovinj and Osijek

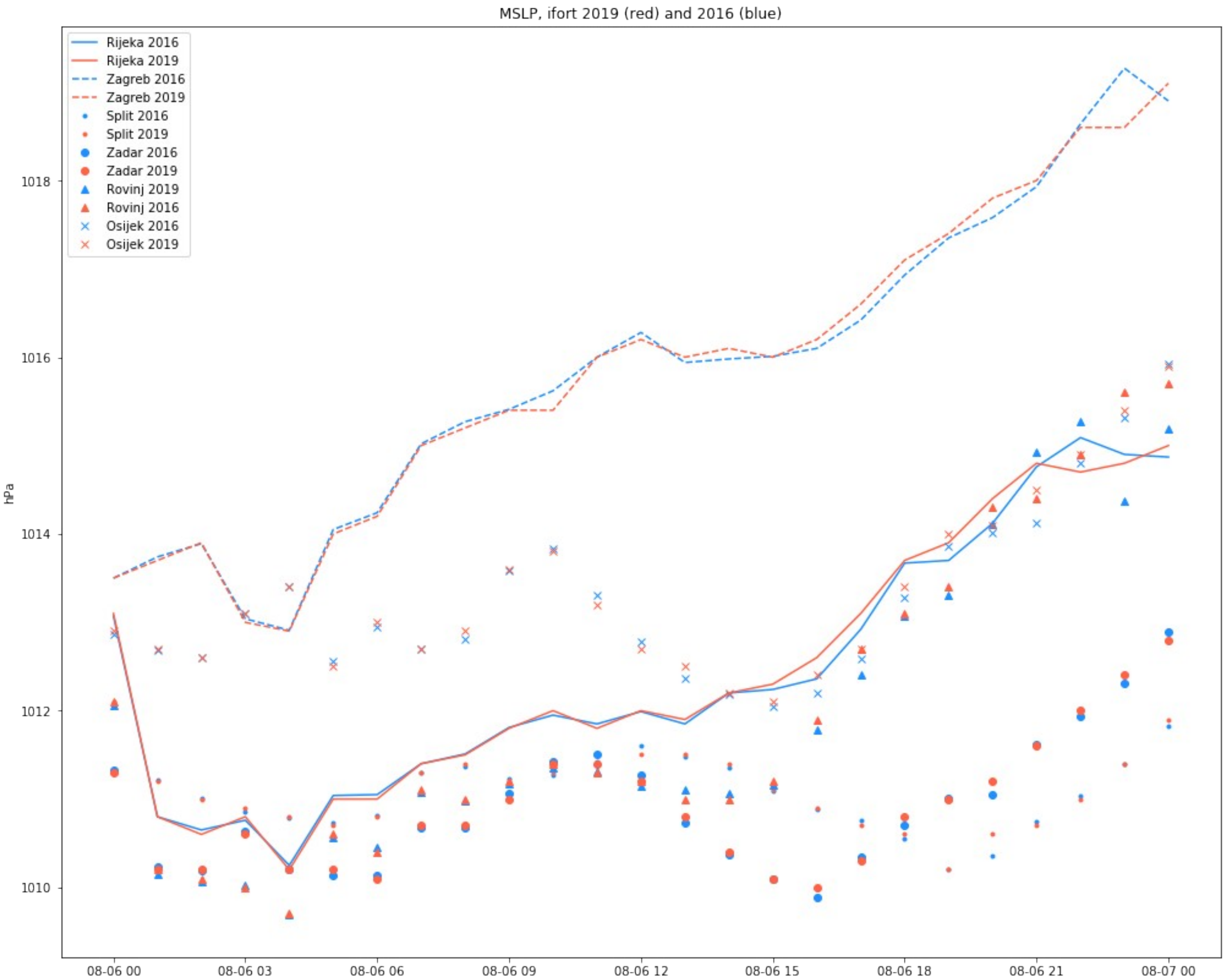

Figure 4: Mean sea level pressure comparision for Rijeka, Zagreb, Split, Zadar, Rovinj and Osijek using both compilers

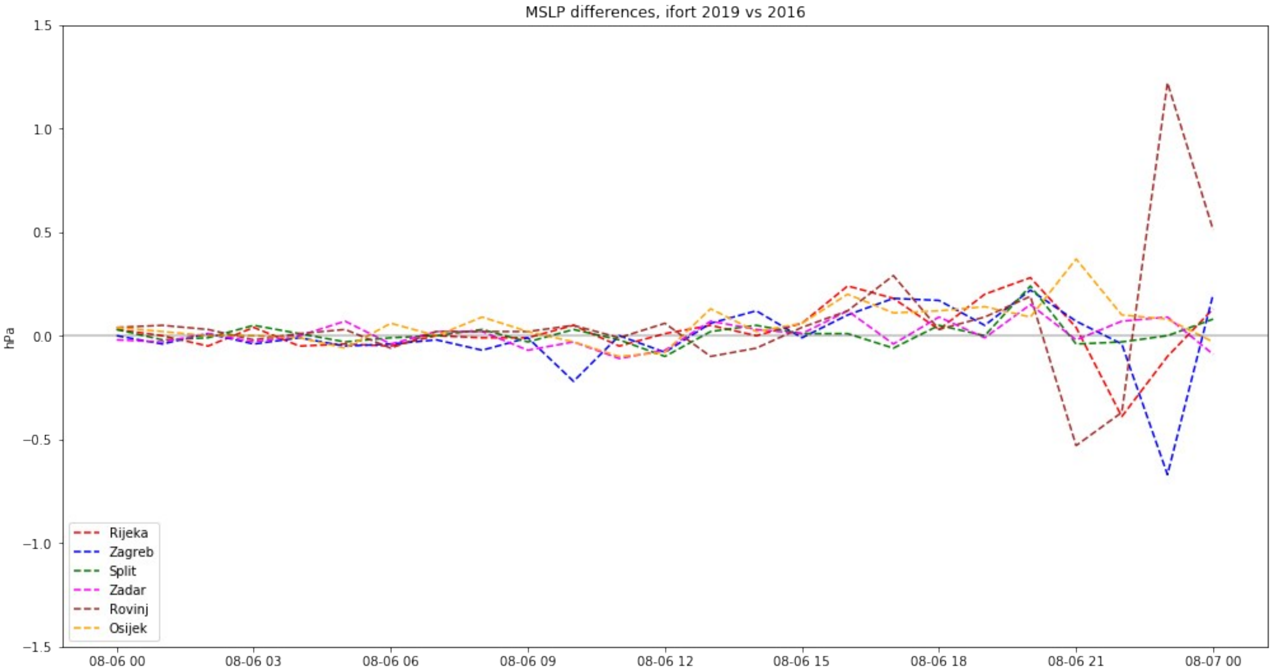

Figure 5: Mean sea level pressure difference between ifort 2019 and ifort 2016 runs for Rijeka, Zagreb, Split, Zadar, Rovinj and Osijek

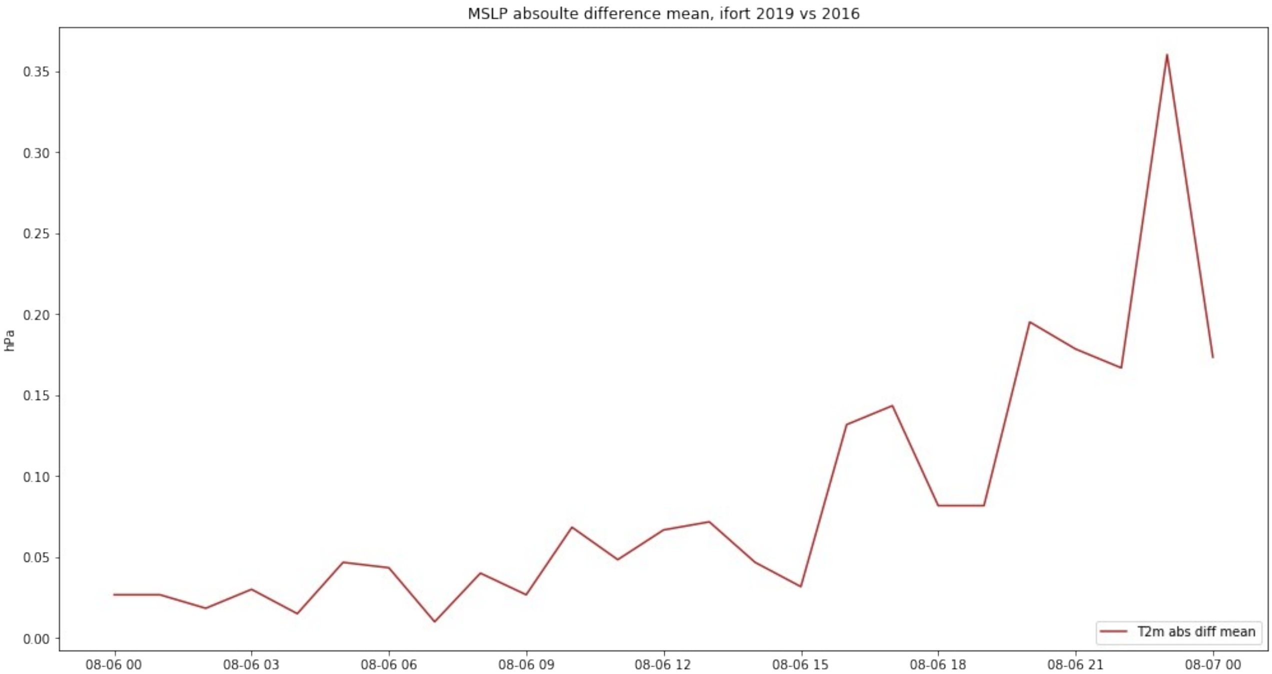

Figure 6: Mean value of absolute mean sea level pressure difference for Rijeka, Zagreb, Split, Zadar, Rovinj and Osijek

It has been found that the differences in meteorological fields produced by WRF code build by different compiler does exist and generally increases with time. The most notable differences are found near areas with active convective processes (ex. Northern Adriatic Sea, south/west of Istria, at the end of simulation period). The large increase in results difference is notable in MSLP plot for Rovinj and Zagreb (Figure 5, brown and blue lines), that are locations closest to convective weather at the end of simulation period.

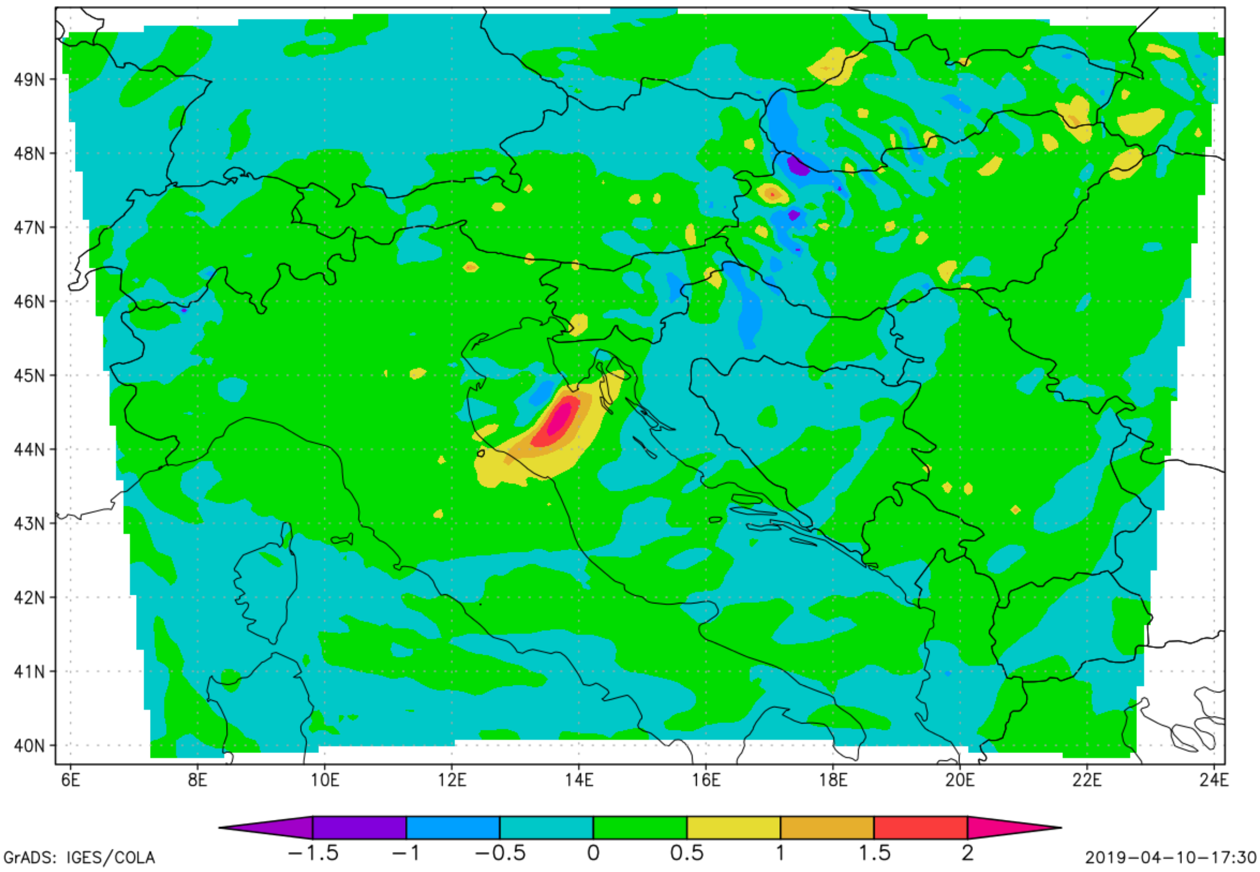

Figure 7: Mean sea level pressure difference over domain, 24h after model initialization (hPa)

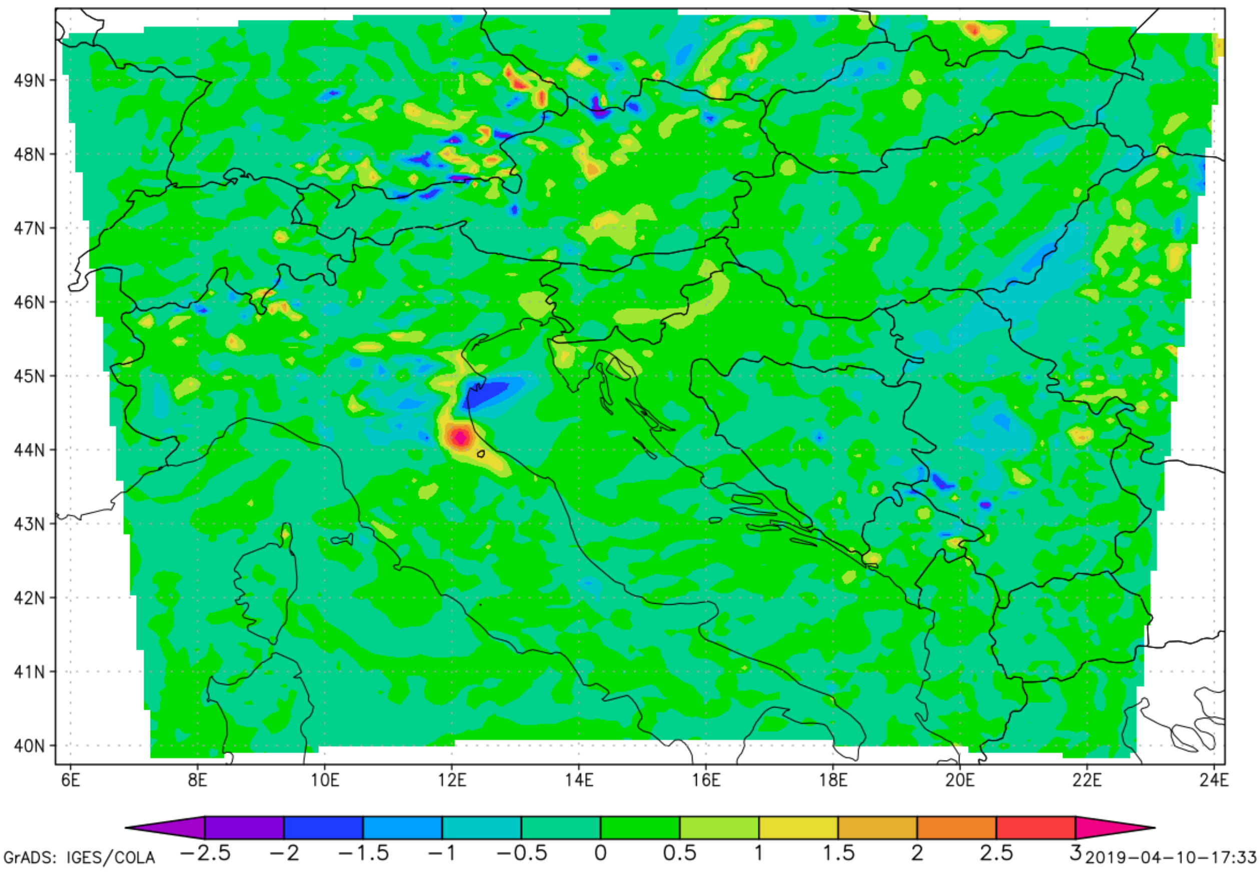

Figure 8: Temperature at 2m above ground difference over domain, 24h after model initialization (°C)

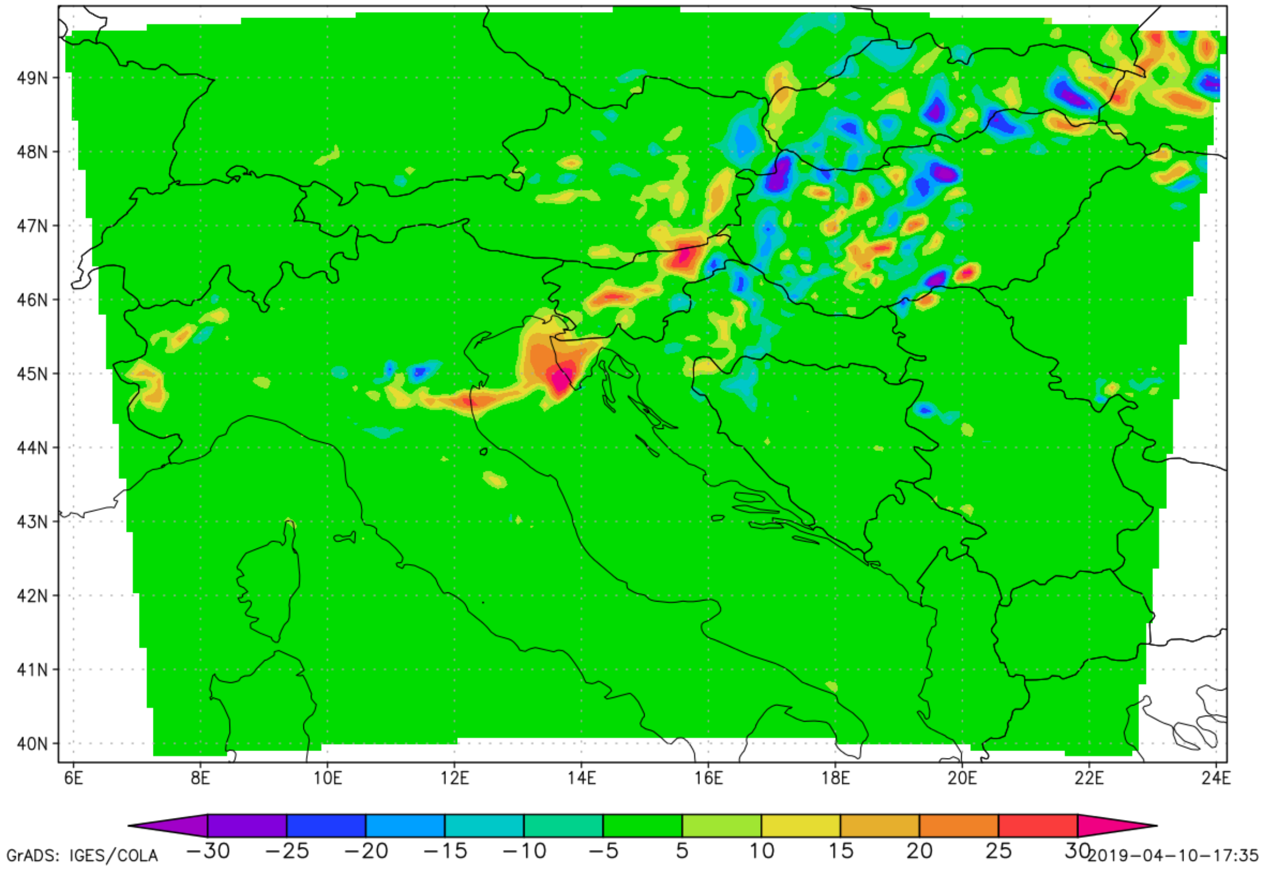

Figure 9: Composite radar reflectivity difference over domain, 24h after model initialization (dBZ)

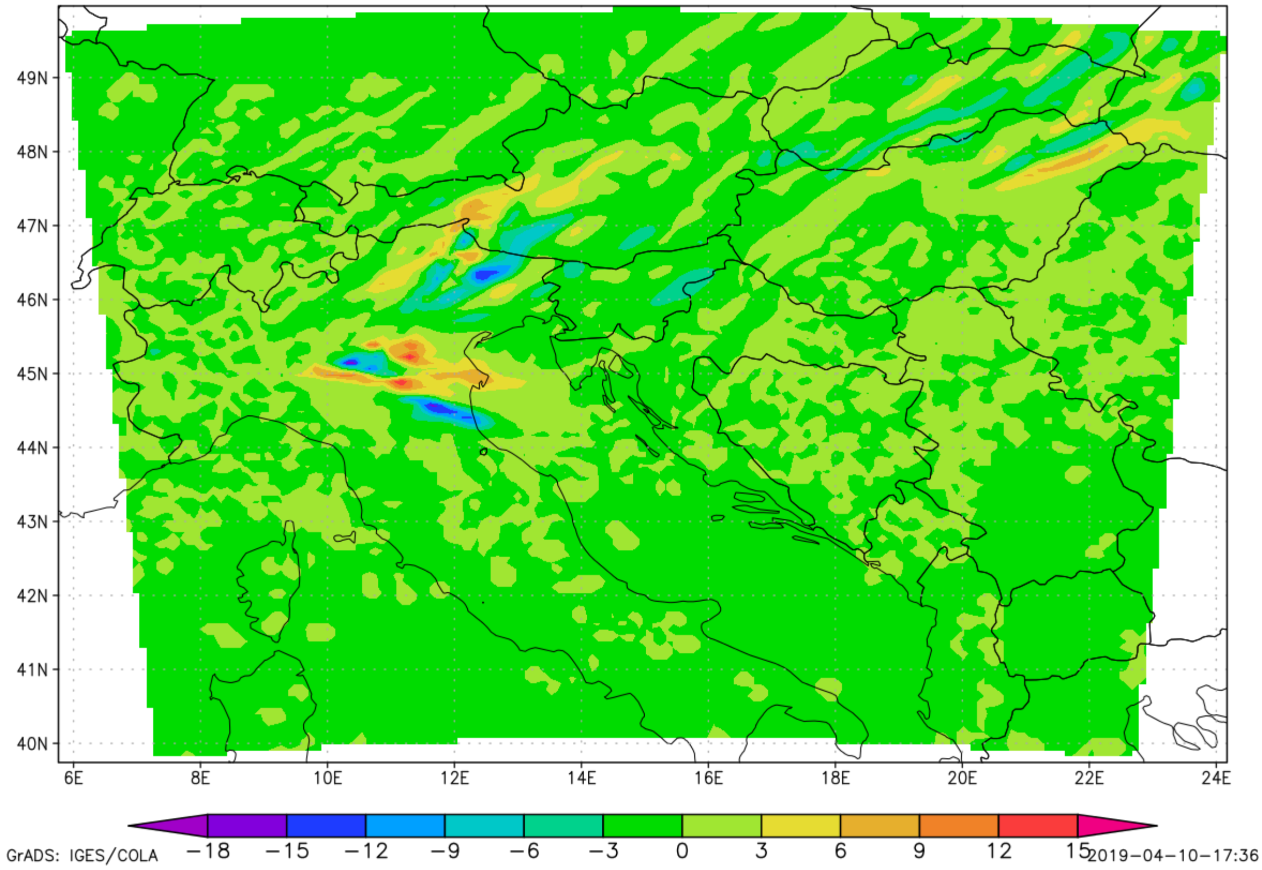

Figure 10: Total accumulated precipitation amount from model start, difference over domain, 24h after model initialization (mm)

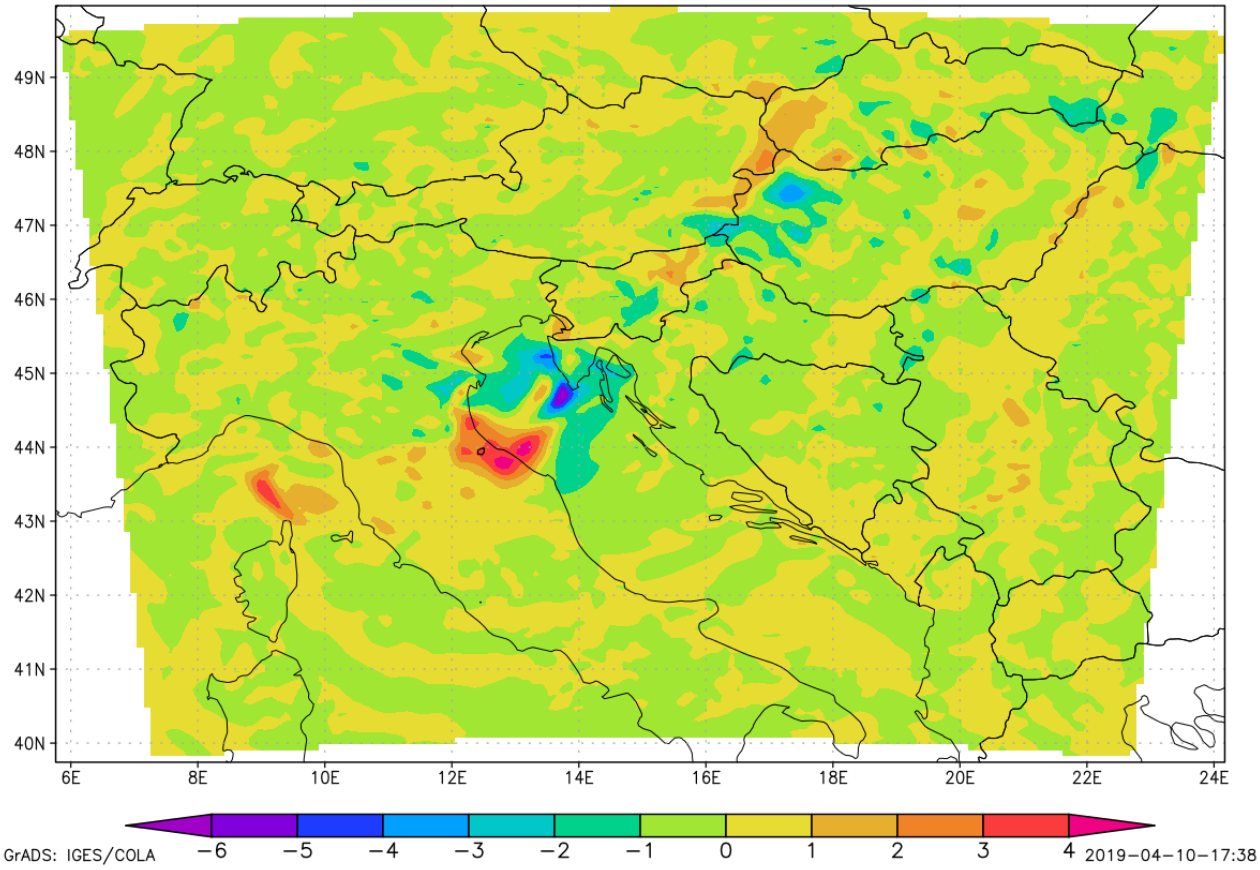

Figure 11: Wind speed at 10m above ground difference over domain, 24h after model initialization (m/s)

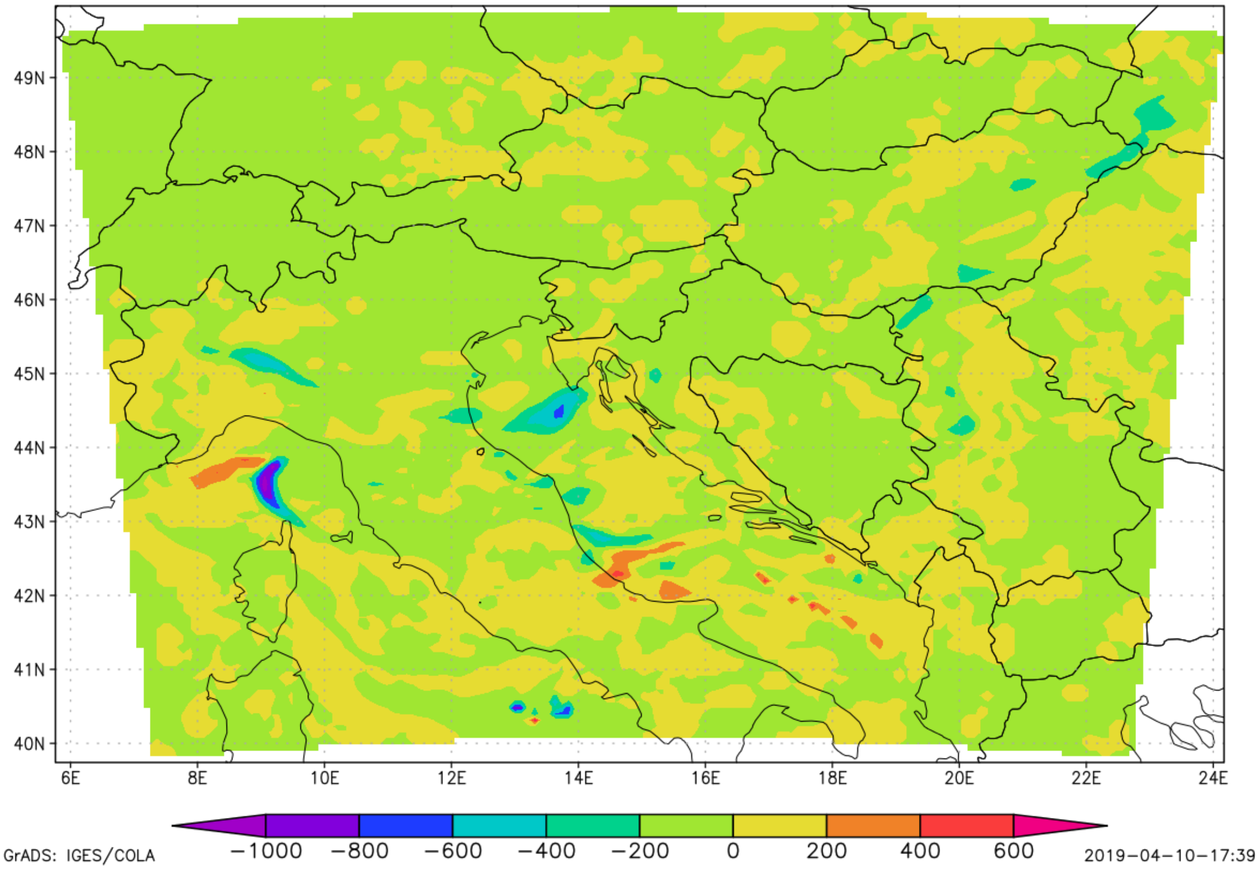

Figure 12: MLCAPE difference over domain, 24h after model initialization (J/kg)

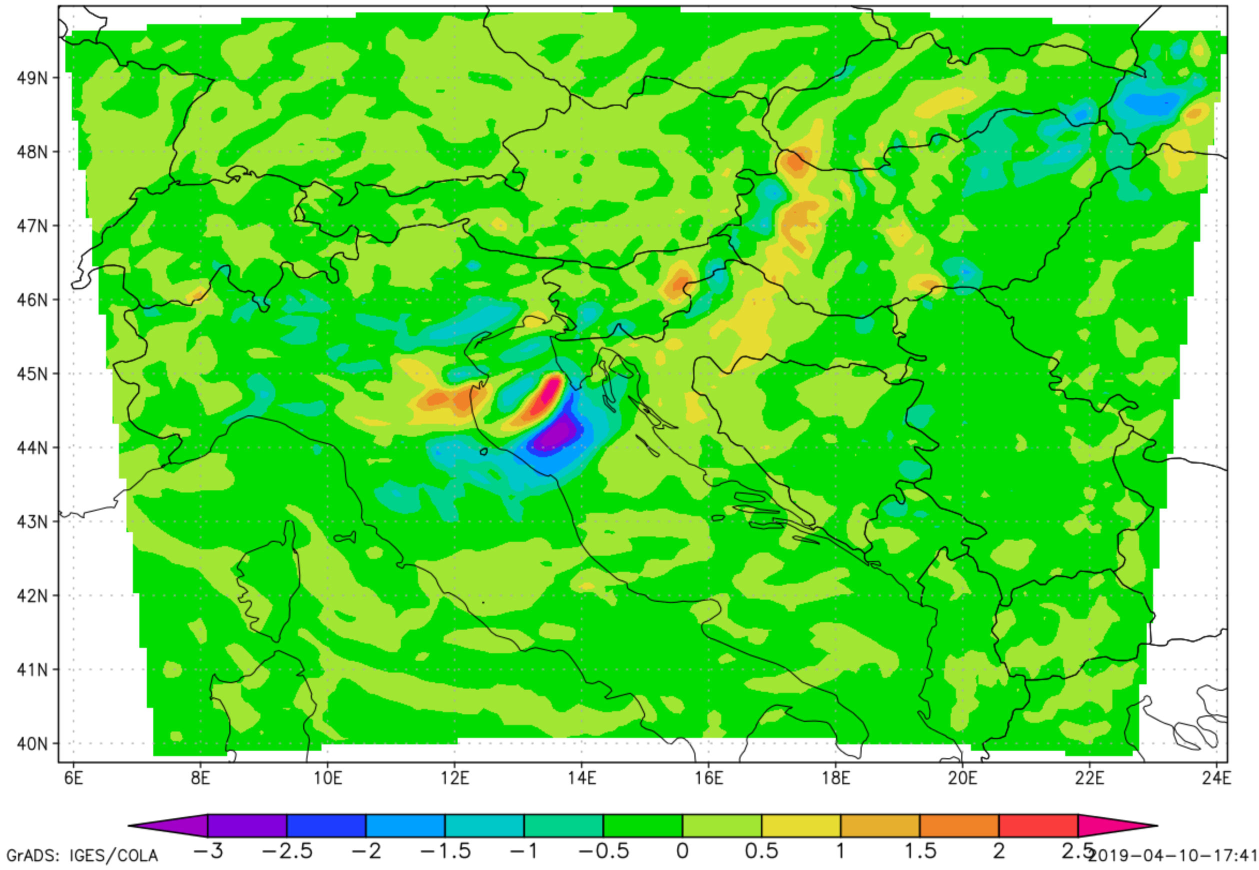

Figure 13: Temperature at 850hPa difference over domain, 24h after model initialization (°C)

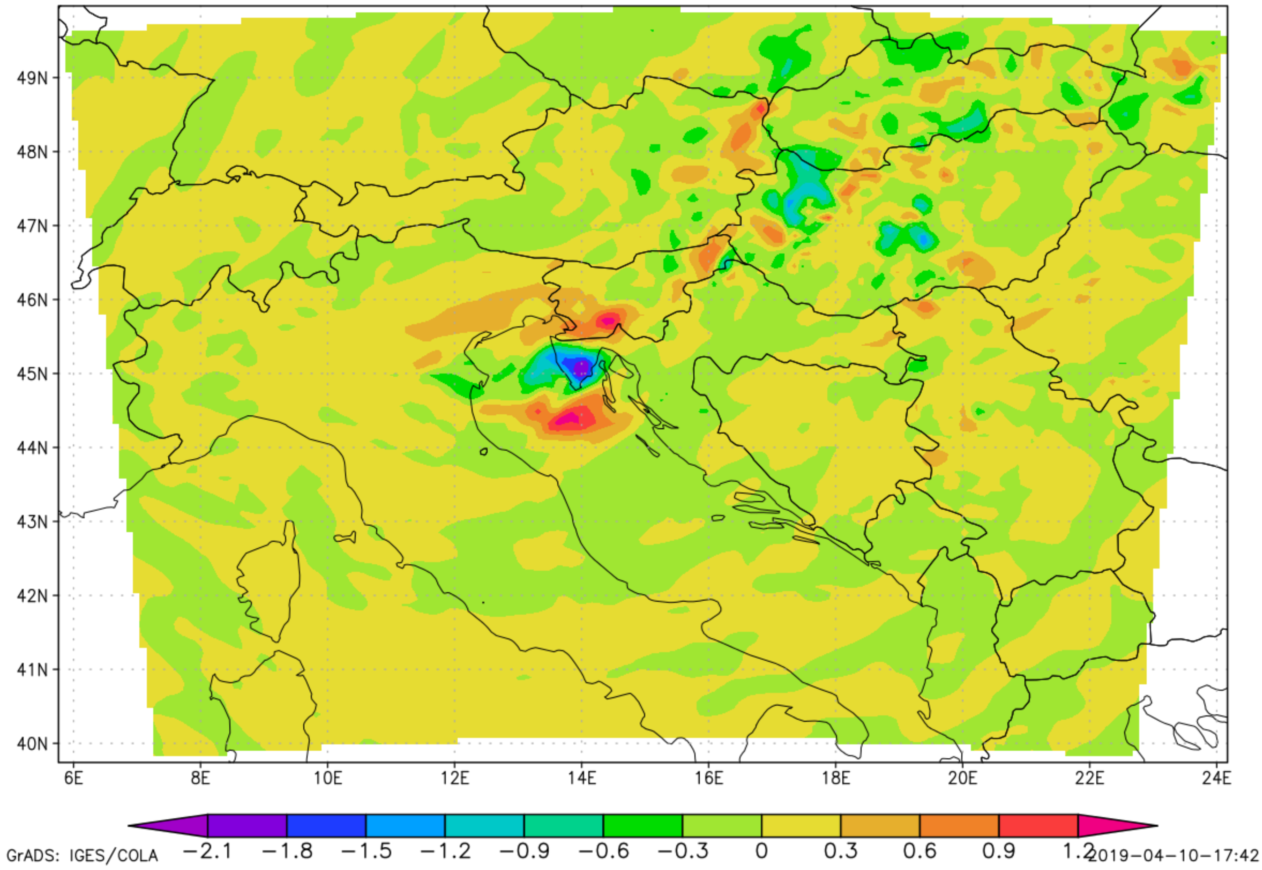

Figure 14: Temperature at 500hPa difference over domain, 24h after model initialization (°C)

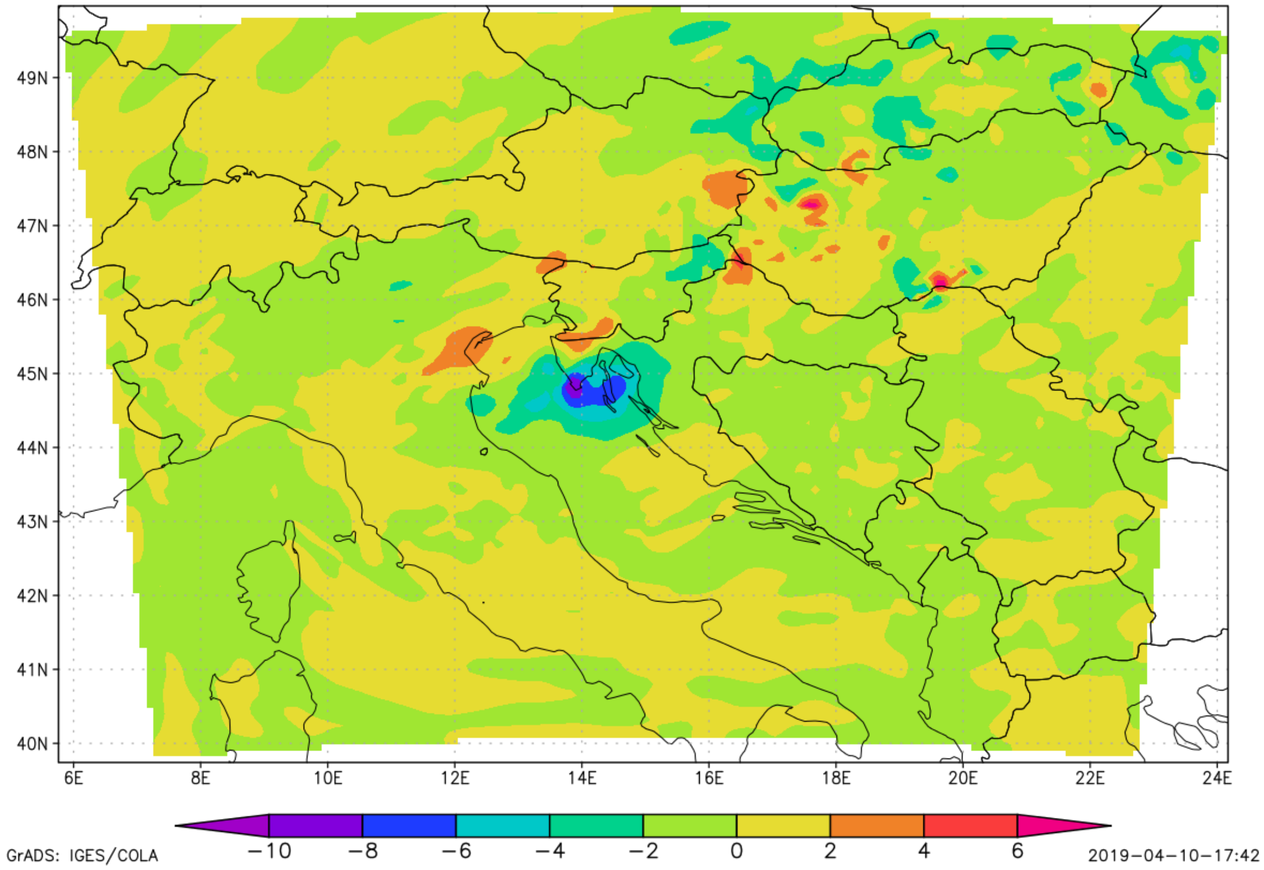

Figure 15: Geopotential height at 500hPa difference over domain, 24h after model initialization (m)

Discussion and conclusions

In this evaluation has been found that WRF model did not calculated the same meteorological solution when code has been compiled using different fortran compiler version. The differences was generally small in magnitude, but seem to increase with time, so it could be expected that differences would be larger for longer simulation periods. Also from the data, it could be expected that especially large differences are probable in convective situations.

Within the limits of this evaluation, model solution accuracy could not be determined. The results were not compared against measurements, and even if they were, the differences shown could be of mostly random nature, so probably very large sample of evaluations during long period of time that includes various weather types should be performed in attempt to evaluate solution accuracy against measurements and draw any statistically valid conclusion about that with confidence. For now, we are only sure that diffrences do exist.

Furthermore, as already mentioned, different fortran compilers exist that can build the code. It would be interesting to expand the evaluation using gfortran and PGI compilers along with Intel’s ifort. Also, for model accuracy assessments, model setup should probably be different and include more complex physical parametrizations, finer grid distance and other more advanced options aimed at accuracy instead of performance.

As practical recommendation to users, not much could be concluded at this point, having very limited amount of data, but users should be aware that differences do exist and in some cases it could be good idea to try more than one code built by different compiler if default run does not produce expected results in terms of accuracy or quality in general.

References

1. WRF, Weather Research and Forecasting model. Skamarock, W. C., J. B. Klemp, J. Dudhia, D. O. Gill, Z. Liu, J. Berner, W. Wang, J. G. Powers, M. G. Duda, D. M. Barker, and X.-Y. Huang, 2019: A Description of the Advanced Research WRF Version 4. *NCAR Tech. Note NCAR/TN-556+STR*, 145 pp.
doi:10.5065/1dfh-6p97

2. GNU Fortran. https://gcc.gnu.org/fortran/

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5. CFS v2. Saha, S., et al. 2011, updated daily. *NCEP Climate Forecast System Version 2 (CFSv2) 6-hourly Products*. Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory. https://doi.org/10.5065/D61C1TXF.

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