REQUEST FOR A SPECIAL PROJECT 2024–2026

MEMBER STATE: CROATIA

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Project Title: Implementation of a new method for eddy diffusivity parameterizations in WRF-Chem model

To make changes to an existing project please submit an amended version of the original form.)

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP** …………..	
Starting year: (A project can have a duration of up to 3 years, agreed at the beginning of the project.)	2024	
Would you accept support for 1 year only, if necessary?	YES ☒	NO ☐

Computer resources required for project year:		**2024**	**2025**	**2026**
High Performance Computing Facility	[SBU]	20 000 000	20 000 000	25 000 000
Accumulated data storage (total archive volume)[2]	[GB]	3000	5000	7000

EWC resources required for project year:		**2024**	**2025**	**2026**
Number of vCPUs	[#]	/	/	/
Total memory	[GB]	/	/	/
Storage	[GB]	/	/	/
Number of vGPUs[3]	[#]	/	/	/

Continue overleaf.

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[1] The Principal Investigator will act as contact person for this Special Project and, in particular, will be asked to register the project, provide annual progress reports of the project's activities, etc.

[2] These figures refer to data archived in ECFS and MARS. If e.g. you archive x GB in year one and y GB in year two and don't delete anything you need to request x + y GB for the second project year etc.

[3] The number of vGPU is referred to the equivalent number of virtualized vGPUs with 8GB memory.

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Extended abstract

1) Introduction

The intensity of vertical mixing and representation of fluxes is of the highest importance in model simulations. In comparison of different planetary boundary layer (PBL) schemes in numerical weather prediction (NWP) Weather Research and Forecast (WRF) model (Hu et al., 2010) it is identified that differences among the schemes are predominantly due to differences in vertical mixing strength and entrainment of air from above the PBL. Deficiencies in mixing representation are identified in the performance of schemes in statically stable conditions as during night-time eddy viscosity declines near the surface when all the schemes tend to produce large low-level wind shear (Hu et al., 2013).

In weather, climate and air quality models, the vertical mixing by turbulent fluxes is usually parameterized in terms of K-theory or higher-order closures (Troen and Mahrt, 1986). Although simple approach, the K-theory is nowadays still widely applied in PBL schemes in meteorological and atmospheric chemistry simulations (Hu et al., 2019). The application of K-theory in models mainly differs in the formulation of local or non-local eddy diffusivity, K(z) for momentum (Km) and heat (Kh). One of the well-known first-order nonlocal scheme commonly used in WRF model simulations is the Yonsei University (Hong et al., 2006) PBL (YSU PBL) scheme. It is shown that YSU PBL scheme captures well the PBL structure (Yang et al., 2019) and it increases boundary layer mixing in the thermally induced free convection regime and decreases it in the mechanically induced forced convection regime due to the inclusion of nonlocal momentum mixing (Hu et al, 2010).

2) Materials and methods

Gradually-varying function for K(z) is introduced to generalize the classical analytical solution for the Ekman layer flow using the WKB method (Grisogono and Oerlemans, 2002). Since there is no explicit relation between the PBL profiles and K(z), a solution which generalizes the third order (O'Brien, 1970) polynomial is defined between a constant K value and a numerically derived solution of the Ekman profile (Grisogono, 1995). The approach to parameterize K(z), both for momentum and scalar (Km and Kh), is firstly developed and applied for stable stratification (Jeričevič and Večenaj, 2009; Jeričević et al., 2012). It is based on a generalized linear-exponentially decaying function scheme combining a linear term (which dominates near the surface) with an exponential decay (e.g., Grisogono and Oerlemans, 2002):

$$K(z) = (K_{\max} e^{1/2} / z_{\max}) z \exp\left[-0.5(z / z_{\max})^2\right], \tag{1}$$

where is the height of K(z) maximum value ( ).

Following previous work, here for convective conditions, generalized linear exponential function is in the same form as used for stable conditions, however main challenge is in defining height and intensity of maximum vertical diffusion for both heat and momentum.

As K(z) is a theoretical value that describes the extent of vertical mixing in the PBL, it cannot be directly measured and needs to be evaluated either from measurements or LES profiles. Here we used LESNIC model (Large Eddy Simulation Nansen Centre Improved Code), (e.g. Esau, 2004; Zilintkievich et al, 2006) in order to calculate fluxes used to determine the coefficients for the new exponential approach of Km and Kh parameterization in the different convective conditions (accounting for non-local mixing and the impact of the entrainment layer).

By calculating the exponential curve (equation 1) to the non-local methods for Kh_LESE and Km_LESE empirical coefficients are determined for every LES run (in total, 17 different runs). Averaged empirical coefficients are shown in Table 1.

Table 1. Empirical coefficients for maximum of *K(z)* and its height, $C_u(K_{h,m})$ and $C(z_{\max})$ respectively, both for momentum and heat turbulent transport, with the corresponding standard deviations σ, used for determination of *K(z)* profiles with the exponential equation approach for statically stable and unstable conditions in LES model.

	Statically stable		Statically unstable	
	$C_s(K)\pm\sigma$	$C(z_{\max})\pm\sigma$	$C_u(K)\pm\sigma$	$C(z_{\max})\pm\sigma$
K_m	0.045 ± 0.02	0.32 ± 0.16	0.018 ± 0.010	0.33 ± 0.27
K_h	0.051 ± 0.02	0.21 ± 0.08	0.067 ± 0.005	0.30 ± 0.04

Based on derived empirical coefficients shown in Table 1 the analytical Km and Kh profiles are calculated for each LES run which is further implemented in the YSU PBL scheme.

3) WRF modelling

The first, initial simulation with WRF model was performed for period from 19 to 22 February 2012 in order to evaluate the modeling performance of newly proposed analytical scheme in YSU PBL scheme within the PBL (modified scheme). Results of the model were compared against mast-mounted measurements over complex terrain within the PBL. The comparison of the time series 10 minute averaged wind speed from default (blue) and modified (red) WRF model against measurements (at e.g. 40 m height; green) is shown in Figure 1. The modeling performance differs at each altitute which can be seen as well on statistical intercomparison (Figure 2). In comparison of timeseries of measurements versus modeling values, more agreement with measurements is present in lower altitudes in case with modified version (red color, Figure 2). On the same altitudes the peak values which occur in default version were reduced to a measurement magnitude in modified version. At 40 m altitude, the BIAS is significantly lower in case with modified version in respect to the default WRF version. Both NMSE and RMSE were decreased, while IOA was higher in case with modified version. The correlation coefficient was to small extent reduced in case with modified version which can be due to a higher variability, and mismatch of peak measurement values. Based on all results (not shown here) the absolute value of BIAS in the case with the modified version increases with height, contrary to BIAS of the default version. Going to higher altitudes (40 to 200 m), the performance of default WRF version slowly increased in terms of reduced BIAS, NMSE, increased IOA and correlation coefficient. The better performance was obtained with modified version for all statistical measures on all altitudes except for the BIAS on the 200m height.

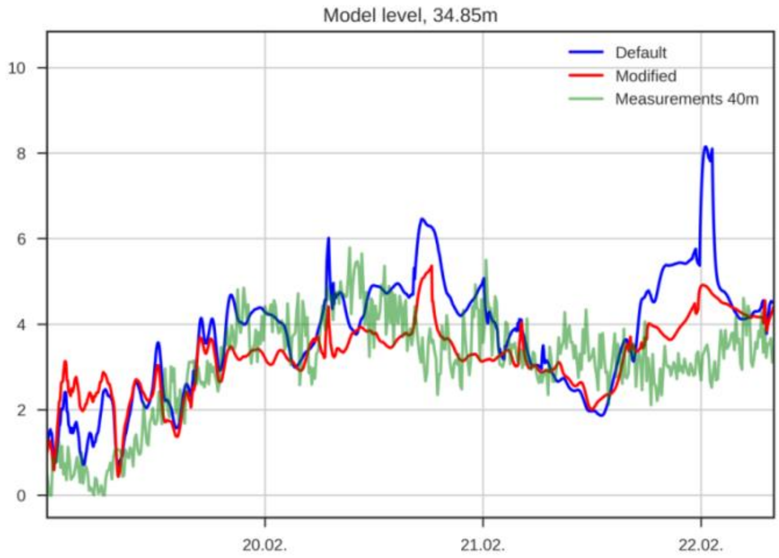

Figure 1. Time series of default (blue), modified WRF (red) and measured (green) 10 minute avereged wind speed in respect to the height of mast (40m shown here).

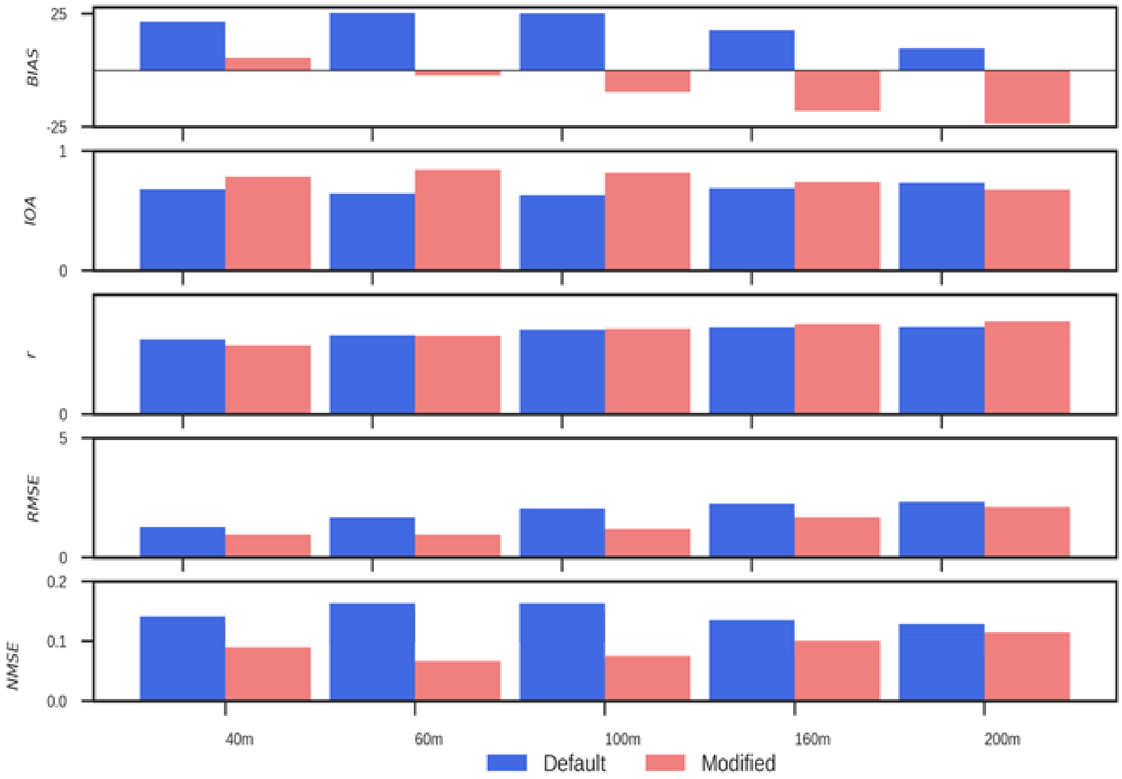

Figure 2. Intercomparison of the applied statistical measures (BIAS, IOA, r, RMSE, NMSE,) between measured and modelled wind speed with respect to the station height.

4) Proposed work

Further work will include simulations with WRF-Chem model (WRF with chemistry module) over same domain as shown in this summary. The main motivation of proposed work are interesting preliminary results from WRF only simulations - increase of modeling performance over altitudes up to 180m in terms of wind speed. The results indicate possible solution to addressed problems in the previous conducted research (Gašparac et al., 2020), e.g. overestimation of surface wind speed led to an underestimation of the PM10 concentrations in the WRF-Chem simulations. This was as well recognized in the other related referenced papers in the Gašparac et al., 2020.

The proposed work will encompass following phases (roughly phase per year):

I) Sensitivity analysis with modified YSU scheme (model validation against surface, mast mounted measurements and airborne measurements from Methane2GO project lead by DLR). Estimated HPCE: 20 000 000 SBU (based on previous simulations), needed storage: 3TB. Control simulations will be done on coarse resolution (1 domain only; ~ 18km horizontal resolution), while focused on 2-3 nested domain simulations over Croatia, reaching high vertical (for airborne concentrations validation) and horizontal resolution (desired resolution bellow 7km).

II) Implementation of more accurate emission inventory (data fusing with local emission inventories). Estimated HPCE: 20 000 000 SBU (nested simulations over specific areas where local emission inventory is available, e.g. Slavonski brod; preliminary estimation of simulation resolution: ~ 500m), needed storage: 2TB.

III) Sensitivity analysis with different chemical parameterization (one of the guidelines from Gašparac et al. 2020) in order to validate results of the modified WRF-Chem simulations against measurements of various polutants, eg. NOx, SOx, PM. Estimated HPCE: 25 000 000 SBU (separate nested simulations for gaseous and aerosol pollutants; expected setup as in 1 phase). needed storage: 2TB. Increase in SBU usage is due to separate simulations for gaseous and aerosol compounds.

SBU usage is estimated based on previous simulations. Simulation duration for all phases up to 10 days (with spin up time). Max usage of CPU per simulation 450, max CPU time ~ 1.5 days.

Proposed work is for research purposes only.

5) References

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