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Uncertainty in Terrestrial Water Cycle Simulations

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TerrSysMP has been exploited to advance our understanding of terrestrial water cycle, by conducting km-scale simulations from field scale to continental scale at the massively parallel supercomputing environment of the Jülich Supercomputing Centre (JSC). The numerical simulations have led to quantification of uncertainties in the simulated terrestrial water cycle in terms of grid-scale representation of heterogeneity and bio-geophysical parameterisations. Ensemble simulations are thus prerequisite to quantify the uncertainty in the terrestrial water cycle, which then could also be utilised for data assimilation to improve prediction.

1 Introduction

The Terrestrial Systems Modelling Platform (TerrSysMP or TSMP)[1] with upgrade to OASIS3-MCT coupler for km-scale continental simulations in massively parallel supercomputing environments[2] has aided in advancing our understanding of the terrestrial water cycle including process related to *e. g.* vegetation and groundwater atmosphere connections.[1, 3–6] In an additional effort, Uebel *et al.*[7] extended TerrSysMP to simulate the terrestrial carbon cycle by including biogenic and anthropogenic CO_2 sources, however its use is currently limited due to non-readily available initial and lateral boundary conditions for CO_2. In the case of the terrestrial water cycle, Shrestha *et al.*[1] showed the presence of strong linkages between integrated surface water and groundwater dynamics (*e. g.* surface runoff with redistribution, groundwater abstraction) and atmospheric boundary layer (ABL) evolution. Their study further demonstrated the importance of hyper-resolution ($<$ 1 km) for coupled simulation with the inclusion of groundwater models. Rahman *et al.*[3] demonstrated that groundwater table dynamics do affect atmospheric boundary layer height, convective available potential energy, and precipitation via the coupling with land surface soil moisture and energy fluxes for convective events over Western Germany. Keune *et al.*[4] also showed that the inclusion of a physically-based groundwater model significantly impacts the simulation of the land surface-atmosphere processes at the continental scale over Europe. However, uncertainty in the modelled groundwater-vegetation-atmosphere feedbacks might persist when different atmospheric and land surface models are used, due to differences in modelled surface energy flux partitioning and precipitation patterns as shown by Sulis *et al.*[5] Besides, the inclusion of new physical processes does not often result in the expected improvement in predictions,[6] which is partly due to uncertainty in vegetation parameters[8] and the relative wet bias introduced with the inclusion of groundwater due to the lack of adequate resolution (often limited by computational burden over large regional domains[9]).

The modularity of TSMP has also allowed some flexibility to conduct land-atmosphere feedback experiments without including the explicit groundwater model[7, 8, 10, 11] or catchment hydrology simulations with offline atmospheric forcing.[9, 12, 13] The above studies have further advanced our understanding in terms of modelled pathways of evapotranspiration, grid resolution dependency of boundary layer mixing and surface energy flux partitioning, constituting roadmaps where further work is essential to improve the predictions by applying more physically based processes in our models.

In addition, the development of TSMP interface with modular data assimilation (DA) tools (*i. e.* applicable to any selected component models) has opened doors to improve model predictions, generate re-analysis data and investigate joint state parameter updates and model structural errors.[14–17] Kurtz *et al.*[14] implemented the DA interface for the hydrological component of TSMP with the Parallel Data Assimilation Framework (PDAF) which facilitates DA simulations at km-scale resolutions over regional domains, making efficient use of massively parallel supercomputing environments. Shrestha *et al.*[15] exploited PDAF for a DA of soil moisture (using 256 ensemble members) with the soil parameters to tune the rooting depth distribution and improve the simulated soil moisture variance and surface energy flux partitioning for a grassland site in Germany. Naz *et al.*[17] explored the potential of assimilating satellite soil moisture observations to produce downscaled and improved high-resolution soil moisture and runoff simulations at the continental scale. Their study showed general improvements in runoff over the continental scale, although also for some regions degraded performance was observed.

In the last 5 years, TSMP has evolved into a state-of-the-art terrestrial model to predict and quantify uncertainties in the terrestrial water cycle in terms of grid-scale representation of heterogeneity and bio-geophysical parameterisations from field scale to regional domains, exploiting the high-performance computing resources at JSC. In this work, we briefly report on simulations with TSMP performed on JURECA over western Germany to investigate:

1. groundwater modulation of the atmosphere at seasonal scales
2. effect of grid resolution on pathways of evapotranspiration
3. atmospheric boundary layer (ABL) schemes for hyper-resolution runs
4. weakly coupled data assimilation using the newly implemented DA interface with DART (Data Assimilation Research Testbed)[18] for all component models

2 Groundwater Modulation of Atmosphere under Seasonal Scales

In this study we evaluate the impact of increasing the complexity of subsurface-land surface physical processes on the performance of the numerical weather prediction model

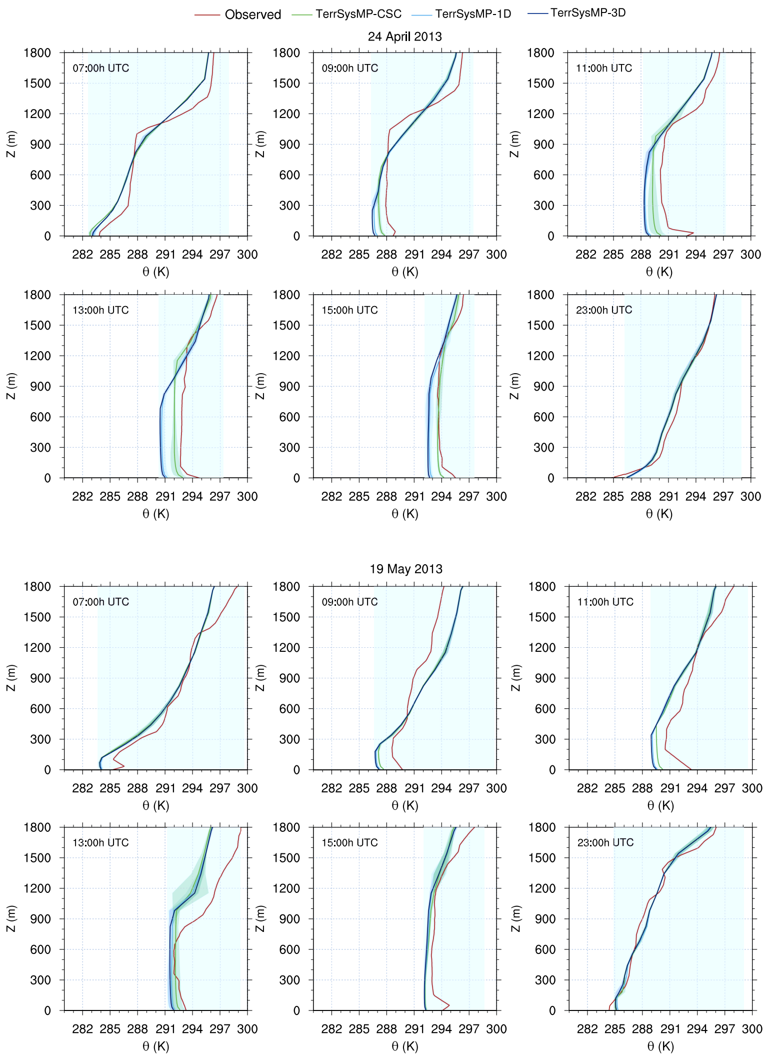

Figure 1. Observed and simulated vertical profiles of potential temperature at KITcube observatory. Shaded areas indicate the spatial variability ($\pm 2\sigma$) of model simulations around (± 4 km) the measurement point (Source: Sulis *et al.*, 2018[6]).

COSMO.[19] To this aim, mesoscale simulation experiments with three configurations of COSMO embedded in TSMP are carried out for a two month period over a domain located in western Germany. The configurations include the operational standalone COSMO model (TSMP-CSC), COSMO coupled with a more complex land surface parameterisation linking carbon fluxes with photosynthesis and stomatal resistance and with a 1D hydrological model (TSMP-1D), and the latter configuration augmented with a 3D groundwater model (TSMP-3D). The evaluation is performed using a wide array of atmospheric, land surface energy balance, and subsurface observations during the High Definition Clouds and Precipitation for advancing Climate Prediction (HD(CP)^2) Observational Prototype Experiment (HOPE) between April and May 2013.[20]

Fig. 1 shows the comparison of the vertical profiles of potential temperature for the three model configurations and observations for different times of the day during two intense observation periods (April 24 and May 19, 2013). On April 24 the simulated profiles are cooler than the observations especially in the TSMP-1D and -3D configurations by a few degrees between 09:00 UTC and 13:00 UTC. Around 15:00 UTC, when the land surface and the atmosphere are strongly coupled, TSMP-CSC matches the well-mixed observed temperature profile, while both TSMP-1D and -3D simulations show a cold bias of about 2 K. On May 19, the three configurations simulate the observed contrasting boundary layer evolution between dry and wet conditions, with the latter characterised by a slower temperature response and a shallower inversion between 09:00 and 13:00 UTC. At 15:00 UTC all models simulate similar vertical profiles. The contrasting response between the three model configurations can be explained as follows. Under relatively dry conditions (April 24, 2013), the warmer vertical profiles of atmospheric temperature, and hence higher ABL, simulated by TerrSysMP-CSC are controlled by the larger sensible heat contribution at the land surface, which is due to the higher soil temperature (results not shown). On the contrary, under relatively wet conditions (May 19, 2013), differences between the three model configurations are largely attenuated in the simulation of soil temperature, which again explains the similar energy partitioning at the land surface and diurnal evolution of the ABL height.

3 Grid Resolution Effects on Pathways of Evapotranspiration

Evaporation (E) and plant transpiration (T) contributes to the total terrestrial evapotranspiration (ET). In this study, we use the hydrological component of TSMP for a central European mid-latitude climate regime (Inde catchment, Germany) to examine the impact of the horizontal grid resolution on the model simulated water fluxes with a particular emphasis on the uncertainty of T/ET model estimates.[15] The simulations are conducted for a relatively wet and dry year at four different grid resolutions (120, 240, 480 and 960 m).

Coarsening of the grid resolution shifts the frequency distribution of groundwater table depth for both years towards shallower depths. For both years, T does not change much (not shown here) while E increases with the increase in available soil moisture for evaporation at the surface due to grid coarsening. This increases ET and thereby decreases T/ET ratio, with the amplitude depending upon the local vegetation cover and the dry/wet year (decrease in T/ET with grid-coarsening being higher for the wet year). Fig. 2 shows the scaling behaviour of T/ET for different vegetation types with coarsening of the grid resolution. For the wet year T/ET decreases between 10 to 14 % for crops and 10 to 11 % for trees; for the dry year, its decrease is around 10 % for the crops and 4 to 6 % for trees. In terms of domain average, T/ET decreases by around 5 % and 8 % for the dry and wet year respectively.[15]

4 ABL Schemes for Hyper-Resolution Runs

An ensemble of 32 idealised and 17 real data simulations were conducted with TSMP over diurnal scales. The study investigates convectively induced secondary circulations in

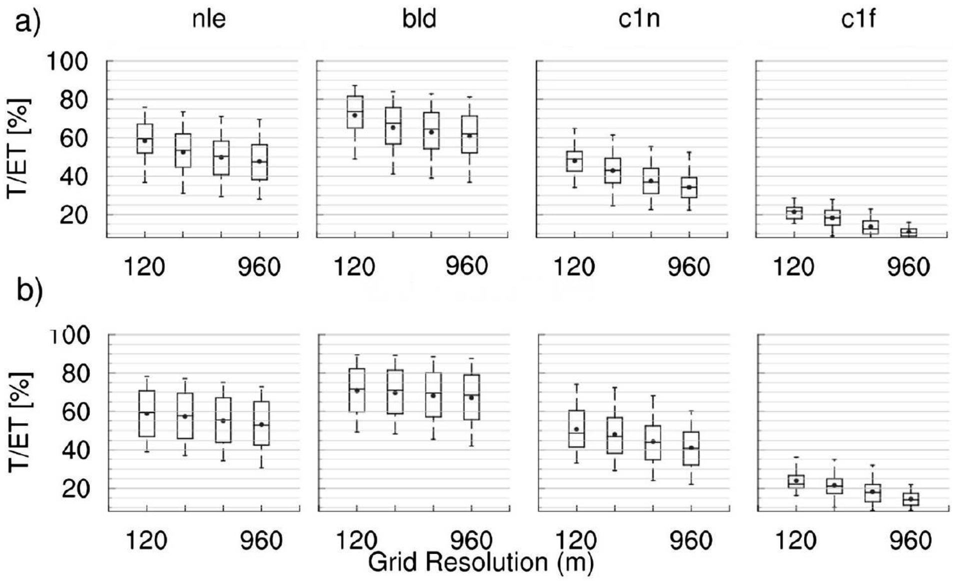

Figure 2. Scaling behaviour of T/ET with grid resolution for a) wet year (2009) and b) dry year (2011). The columns show the Plant Functional Types (PFTs) agricultural crops (c1f), agricultural crops with constant low LAI as substitute for urban areas (c1n), broadleaf deciduous tree (bld), and evergreen needle-leaf trees (nle). The box plot and the whiskers show the mean (solid markers), median, 5, 25, 75 and 95th percentile (Source: Shrestha *et al.*[15]).

response to varying grid spacings (Δx) within the turbulent grey zone (O(1 km)) for atmospheric boundary layer (ABL) schemes typically used in the numerical weather prediction.

The setup used large eddy simulation as benchmark runs for sensitivity simulations with varying turbulent mixing length scale and grid resolution, all located within the turbulent grey zone. The grid spacing of the land surface model, and thus its heterogeneity, is kept at $\Delta_x = 200\,\mathrm{m}$ for all runs to remove any uncertainty in the simulated results due to land surface heterogeneity at different spatial scales.

The model run with the finest resolution $\Delta_x = 200\,\mathrm{m}$, $l_\infty = 70\,\mathrm{m}$ is able to produce a vertical profile similar to the reference LES run (Fig. 3). While coarser simulations ($\Delta_x \geq 1000\,\mathrm{m}$) for the same asymptotic turbulent mixing lengthscale result in a stronger superadiabatic layer, as the model is not able to effectively remove heat from the surface by the ABL parameterisation. Due to the super-adibatic layer, artificial secondary circulation is triggered in the model. Increasing the asymptotic turbulent mixing lengthscale l_∞ to much larger values for the coarser grid spacings effectively removes the energy from the surface and attenuates the artificial secondary circulations.

Thus, the turbulent mixing length scales used in the ABL scheme can be tuned to suppress model generated convectively induced secondary circulations, while the non-resolved turbulence dealt with by the ABL scheme effectively propagates the surface fluxes into the ABL and sustains reasonable ABL profiles.

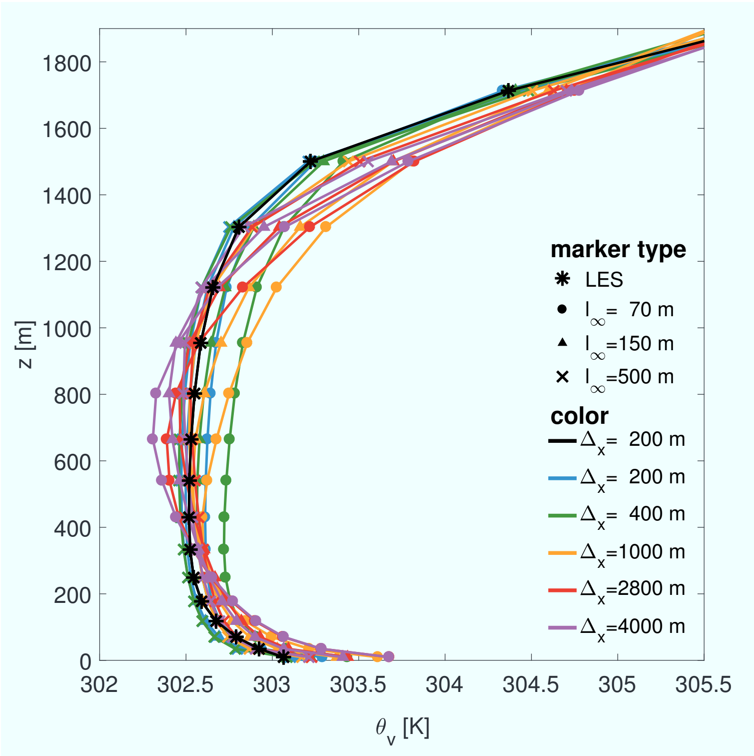

Figure 3. Domainaveraged vertical profile of virtual potential temperature on 25 July 2012 at 13:00 UTC for different grid spacings (Δ_x) and asymptotic turbulent mixing lengthscales (l_∞) (Source: Poll *et al.*[10]).

5 Weakly Coupled Data Assimilation (WCDA) with TerrSysMP-DART Interface

In a weakly coupled data assimilation experiment (WCDA), the models are tightly coupled and the DA only impacts the system that is directly responsible for the observations (*e. g.* assimilation of air temperature does not impact soil moisture directly or *vice versa*). WCDA is conducted for a semi-idealised setup with a horizontally homogeneous vegetated land surface and soil texture using the TerrSysMP-DART interface. DART is an open source ensemble data assimilation framework developed by the National Center for Atmospheric Research. DART provides data assimilation capability without changing the model code and already supports assimilation with COSMO and CLM. Assimilation support for ParFlow with DART was added along with software infrastructure for all component models required by TSMP.

The soil moisture is initialised horizontally homogeneous with a relative soil moisture content, $S_w = 0.11$ for the root zone, with ground water table at 3 m depth. Five types of simulations are performed with this idealised setup, which are summarised in Tab. 1. 48 ensemble members were generated by perturbing atmospheric boundary layer (ABL) temperature (below 850 hPa) and leaf area index (LAI) with a random uniform distribution.

1. Perfect Model Run to produce synthetic observations:	PM
2. Open Loop Run	OL
3. Weakly Coupled Data Assimilation with COSMO (ABL temperature)	$WCDA_{cos}$
4. Weakly Coupled Data Assimilation with CLM (Soil Temperature)	$WCDA_{clm}$
5. Weakly Coupled Data Assimilation with ParFlow (Soil Moisture)	$WCDA_{pfl}$

Table 1. Data Assimilation Experiments. OL and $WCDA$ runs are conducted with 48 ensemble members.

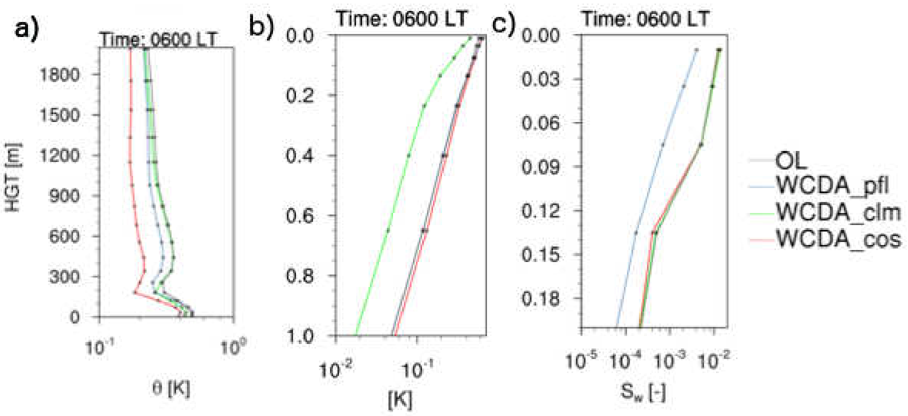

Figure 4. Diurnal evolution of the mean absolute error (MAE) of a) ABL potential temperature, b) soil temperature and c) soil moisture for the ensemble means. The vertical profiles at 0600 LT are temporally averaged for the entire period of simulation.

14 day simulations were conducted with DA at 00:00 UTC everyday for 10 different spatial locations at multiple heights, to examine its impact on diurnal scale evolution of the land surface states and the boundary layer.

Fig. 4 shows the time-averaged response of mean absolute error (MAE) for the ABL temperature, soil temperature and soil moisture with 6 hour lead forecast. Preliminary results indicate that the direct assimilation of boundary layer temperature results in the least MAE for $WCDA_{cos}$, whereas the assimilation of soil temperature and soil moisture also indirectly reduces the MAE for the $WCDA_{clm}$ and $WCDA_{pfl}$ relative to the open loop run. The direct assimilation of soil temperature and soil humidity also improves the MAE for $WCDA_{clm}$ and $WCDA_{pfl}$ respectively. But, the assimilation of soil moisture does not show any improvement in soil temperature and *vice versa*. Also, the assimilation of the ABL temperature shows no improvement in the surface soil moisture or temperature.

6 Concluding Remarks

While the inclusion of physically based groundwater in the integrated terrestrial systems model is essential to further improve our understanding of the terrestrial water cycle, the increased complexity also introduces uncertainty associated with poor understanding of subsurface soil texture and grid scale dependence of simulated soil moisture. Such grid scale dependence was also found for boundary layer mixing parameterisations. Increased computational resources available at the Jülich Supercomputing Centre (JSC) will partly contribute to mitigate these issues by using hyper-resolutions, along with simultaneous efforts on optimising the convergence of groundwater model codes for larger domains. Besides, the model representation of vegetation with static plant physiological information also contributes to the uncertainty in the pathways of evapotranspiration. Ensemble simulations are thus a prerequisite to quantify the uncertainty in the terrestrial water cycle simulations, which then could also be utilised for data assimilation to improve prediction.

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