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Technical Note: Reducing the spin-up time of integrated surface water–groundwater models

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Abstract

One of the main challenges in catchment scale application of coupled/integrated hydrologic models is specifying a catchment's initial conditions in terms of soil moisture and depth to water table (DTWT) distributions. One approach to reduce uncertainty in model initialization is to run the model recursively using a single or multiple years of forcing data until the system equilibrates with respect to state and diagnostic variables. However, such "spin-up" approaches often require many years of simulations, making them computationally intensive. In this study, a new hybrid approach was developed to reduce the computational burden of spin-up time for an integrated groundwater-surface water-land surface model (ParFlow.CLM) by using a combination of ParFlow.CLM simulations and an empirical DTWT function. The methodology is examined in two catchments located in the temperate and semi-arid regions of Denmark and Australia respectively. Our results illustrate that the hybrid approach reduced the spin-up time required by ParFlow.CLM by up to 50 %, and we outline a methodology that is applicable to other coupled/integrated modelling frameworks when initialization from equilibrium state is required.

1 Introduction

The issue of model initialization is important for hydrologic predictions as the model state has a major impact on catchment's response (Berthet et al., 2009). In coupled/integrated surface–subsurface models uncertainty in a catchment antecedent condition is of particluar importance because both soil moisture distribution and depth to water table (DTWT) need to be specified at the start of a simulation (Ivanov et al., 2004; Noto et al., 2008).

Since there is often no a priori information on the spatial pattern of water table and soil moisture distributions, various approaches have been developed to determine initial DTWT variation. Sivapalan et al. (1987) used a topography-soil index to map the spatial distribution of initial DTWT. In another approach, Troch et al. (1993) used recession flow analysis to estimate the effective water table height of a catchment. Regardless of the choice of initial DTWT, the uncertainty involved is such that a period of spin-up is always required (Cloke et al., 2003) as the applied atmospheric forcing is often inconsistent with the hydrodynamic initialization of the catchment inferred from limited observations (Ajami et al., 2014).

The two most common initialization approaches in coupled/integrated distributed hydrologic models are as follows: (1) initial depth to water table is specified at a certain uniform depth below the land surface (Kollet and Maxwell, 2008), with the impact of initialization reduced through recursive simulations over a single or multiple years of forcing data, until equilibrium conditions are reached: usually related to spin-up criteria based on changes in groundwater heads (Refsgaard, 1997) or changes in water and energy balances (Kollet and Maxwell, 2008); or (2) the model is initialized from a fully saturated condition and simulations are continued until modelled baseflow matches the observations (Jones et al., 2008).

Results of a ParFlow.CLM spin-up study for a catchment in Denmark showed that at least 20 years of recursive simulations were required to reach equilibrium in subsurface storages, defined as when percent changes in monthly unsaturated and saturated zone storages were less than 0.1 and 0.01 % respectively (Ajami et al., 2014). For reference, 20 years of spin-up simulations required 20 000 service units on a high performance parallel computing cluster: equivalent to over 26 days of computation using 32 processors. The challenge lies in designing methodologies to reduce spin-up time in computationally intensive integrated models such as ParFlow.CLM (Ashby and Falgout, 1996; Jones and Woodward, 2001; Kollet and Maxwell, 2006) when initialization from equilibrium states is required for transient simulations.

The objective of the current study is to develop a *hybrid* spin-up approach that significantly reduces the time required for model state equilibrium. The performance of the proposed approach in reducing the spin-up time for a catchment scale application of the ParFlow.CLM model is evaluated against a standard continuous recursive

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simulation approach commonly applied for land surface model spin-up and referred to here as a baseline spin-up approach.

2 Data and methodology

The hybrid approach consists of a two-stage model simulation step and an intermediate state updating step using the DTWT function. Figure 1 illustrates this hybrid spin-up approach. The applicability of the proposed scheme is examined against the equilibrated ParFlow.CLM model of the sub-catchment of the Skjern River basin in Denmark, developed by Ajami et al. (2014) using a traditional baseline spin-up approach. Further, performance of the hybrid approach in reducing spin-up time is evaluated by developing a ParFlow.CLM model for a semi-arid catchment in Australia.

2.1 Overview of the ParFlow.CLM models

2.1.1 Sub-catchment of the Skjern River Basin, Denmark

The sub-catchment of the Skjern River basin in western Denmark has an area of 208 km^2 (Fig. 2) that is characterized by mild topography and a temperate climate (Jensen and Illangasekare, 2011). Agricultural land is the dominant cover type (78 %), with the remainder of the catchment area covered by evergreen needle leaf forest.

The catchment's ParFlow.CLM model covered a 28 km by 20 km area. The modelling grid had a horizontal resolution of 500 m and a vertical discretization of 0.5 m. Catchment topography was determined via a 500 m digital elevation model (DEM) and the bottom elevation of the domain was a uniform −75 m. At the land surface, the ParFlow free-surface overland flow boundary condition was assigned. A no-flow boundary condition was specified for the sides and bottom boundary. Spatially uniform hourly atmospheric forcing (air temperature, wind speed, specific humidity, air pressure, precipitation, incoming shortwave and downward longwave radiation) for the year 2003 were used for spin-up. Initial DTWT was assigned uniformly at 3 m below the land surface.

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Ground surface temperature was set to the mean annual air temperature (281 K) at the start of a simulation. Prescribed subsurface hydraulic parameters include the saturated hydraulic conductivity ($0.3\,\mathrm{m\,h^{-1}}$), porosity (0.39), van Genuchten parameters ($\alpha = 1.5\,\mathrm{m^{-1}}$ and $n = 2$), and relative residual saturation (0.1).

2.1.2 Baldry sub-catchment, Australia

The Baldry sub-catchment, located in central west New South Wales of Australia, has an area of $1.9\,\mathrm{km^2}$ with an elevation range from 443 m to 500 m (Fig. 2). For the spin-up experiment, the catchment land cover was assumed to be evergreen broadleaf forest representing eucalyptus plantation.

The ParFlow.CLM model of the site was set up over a 2.9 km by 2.9 km area encompassing the Baldry catchment. Catchment topography was represented using a 60 m pre-processed DEM. The bottom elevation of the modelling grid was a uniform 400 m. The modelling grid had a 60 m resolution in the x and y directions and its vertical discretization was 0.5 m resulting in a $48 \times 48 \times 203$ grid. At the land surface, the ParFlow free-surface overland flow boundary condition was assigned. A no-flow boundary condition was specified for the lateral and bottom boundaries. Hourly forcing data for the year 2004 were obtained from a weather station at the site. For the hourly downward longwave radiation, the Modern Era Retrospective Analysis for Research and Applications (MERRA) reanalyses data interpolated to $0.25^\circ \times 0.25^\circ$ resolution was used (Decker et al., 2012). Prescribed subsurface hydraulic parameters include the saturated hydraulic conductivity ($0.18\,\mathrm{m\,h^{-1}}$), porosity (0.25), van Genuchten parameters ($\alpha = 1.5\,\mathrm{m^{-1}}$ and $n = 2$), and relative residual saturation (0.1). The model was initialized with a uniform DTWT of 2 m below the land surface. Ground surface temperature was set to mean annual air temperature 288.1 [K].

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2.2 Development of empirical DTWT functions for model re-initialization

Analysis of ParFlow.CLM spin-up behavior via the baseline spin-up approach for the sub-catchment of the Skjern River identified that percentage changes in subsurface storages and DTWT had the form of an exponential decay (Ajami et al., 2014). Using the functional relationships between number of simulation years and percentage change of a variable, Ajami et al. (2014) developed a series of spin-up functions based on 16 years of initial ParFlow.CLM simulations. These spin-up functions were used to predict the number of years required until the model equilibrated, based on a predefined threshold i.e. 0.1 or 0.01 % change for a given variable.

Conversely, the inverse of a spin-up function for DTWT predicts percent changes in DTWT as a function of simulation years, which hereinafter is referred to as the empirical DTWT function. In this study, we examined the capabilities of empirical DTWT functions as a means for updating DTWT and hence groundwater storage after just a few initial ParFlow.CLM spin-up simulations. The expectation is that this state updating should reduce the total number of spin-up years of simulation, substantially reducing the computational burden. To do this, a series of spin-up simulations were performed based on an arbitrary initial state (DTWT was 3 m below the land surface as in Ajami et al., 2014), in order to identify the minimum number of data points required to develop an empirical DTWT function (stage 1 of model simulation).

Due to the anticipated large changes in mean annual DTWT values between the first and second year of the spin-up simulation, the first year of data is removed from the analysis. This means that a minimum of four data points (i.e. 6 cycles of ParFlow.CLM simulations) are required to fit a double exponential function to percentage change values. Therefore, six years of spin-up simulations were performed using forcing data for the year 2003. Percent changes in catchment and domain averaged annual DTWT values, as well as changes in DTWT at every grid cell, were used to fit exponential functions at the global and local scales respectively, using single (Eq. 1) or double

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exponential (Eq. 2) terms:

$$y = a\exp(bx) \quad (1)$$

$$y = a\exp(bx) + c\exp(dx) \quad (2)$$

where y is the percentage change in DTWT, x is the number of simulation years, and a, b, c, d are the fitting parameters.

These empirical DTWT functions estimate percentage changes in DTWT as a function of simulation years. Depending on the number of ParFlow.CLM cycles used to fit the DTWT functions (i.e. 2 to 6, cycles), the mean annual DTWT from the last cycle of the ParFlow.CLM spin-up simulation for every grid cell was used as the initial value to estimate DTWT distributions based on the predicted percent change values. To assess the performance of these DTWT functions, estimated mean annual DTWT from the DTWT functions were compared against mean annual DTWT from the ParFlow.CLM model of Ajami et al. (2014) spun-up for 20 years.

In the state updating stage, the best performing empirical DTWT function (a double exponential DTWT function) was used to estimate percentage changes in DTWT as a function of simulation years, until percentage changes reached the 0.01 % threshold. Using the percent change values and mean annual DTWT distribution from the sixth cycle of the ParFlow.CLM spin-up simulation, spatially distributed DTWT was predicted.

In the second stage of model simulations, the ParFlow.CLM was re-initialized using newly estimated DTWT values from a double exponential DTWT function, and spin-up simulations were continued until equilibration based on subsurface storage spin-up criteria. The second stage of spin-up simulations was necessary to ensure equilibrium after re-initialization, especially for the unsaturated zone storage.

One issue with the re-initialization of DTWT using the DTWT function is that the distribution of soil moisture above the water table cannot be estimated. Here, we considered two approaches to define pressure head distribution above the water table: (1) implementing the commonly used hydrostatic equilibrium assumption, where pressure head at the water table was linearly decreased as a function of elevation head towards the land surface; and (2) adjusting the pressure head distribution of the unsaturated zone from the last day of the sixth cycle of ParFlow.CLM spin-up simulations based on new DTWT values.

2.3 Evaluation of the hybrid spin-up approach

Performance of the hybrid spin-up approach in reducing the spin-up time is evaluated by developing a ParFlow.CLM model for the Baldry sub-catchment. The baseline spin-up simulations were performed using spatially uniform, hourly forcing data for the year 2004. The equilibrium condition was achieved when percent changes in catchment averaged monthly groundwater storages were below 0.1 % threshold level. In the next step, the hybrid spin-up approach outlined in Sect. 2.2 was implemented to re-initialize the ParFlow.CLM using the adjusted pressure head distribution approach above the water table. Recursive simulations after re-initialization continued until equilibrium condition was achieved.

3 Results

3.1 Performance of empirical DTWT functions in predicting DTWT

Performance of the single and double exponential DTWT functions in predicting 14 years of DTWT were compared against ParFlow.CLM baseline spin-up simulations (years 7 through 20) of Ajami et al. (2014) to find the optimum empirical DTWT function for the Skjern River sub-catchment. Post-simulation analysis indicates that global DTWT functions based on domain or catchment averaged percentage change values are better predictors of DTWT response compared to local DTWT functions developed for every grid cell. Instability of local DTWT functions occurs in grid cells where percent changes in DTWT oscillate between positive and negative values through initial spin-up simulations.

Calculated root mean square difference (RMSD) and percent bias relative to the baseline spin-up simulations indicate that global double exponential functions using ParFlow.CLM spin-up simulations 2 to 6 provide a better fit compared to various single exponential functions obtained from different spin-up simulation years (e.g. 2 to 3, 2 to 4, etc.). Only for the mean absolute error (MAE) do single exponential functions based on simulations 2 to 6 perform better than the double exponential functions (Fig. 3b). Because the first six cycles of ParFlow.CLM simulations were the same between the baseline spin-up simulations and DTWT distributions presented in Fig. 3, comparisons were made with simulations 7 to 20 of the baseline spin-up approach of Ajami et al. (2014). As can be seen from Fig. 3, the mean annual DTWT from single exponential functions (fitted to percentage change data from simulations 2 to 6) underpredict the baseline spin-up simulations in comparison to double exponential functions fitted to the same data points. In terms of mean DTWT (Fig. 3a), the catchment delineated double exponential DTWT function provides a better prediction when compared to the function based on the entire model domain. However, Fig. 3b indicates that the mean absolute error values are slightly smaller for the domain based double exponential function.

To investigate this further, three empirical semi-variograms were generated by removing the trend from DTWT values using a polynomial function and calculating the semi-variance of the residuals as a function of distance. The semi-variance is a measure for spatial variance of a variable and presents average dissimilarity between data pairs at a given distance. Investigating the empirical semi-variograms of DTWT values (Fig. 3c) indicates that the domain based double DTWT function is a better predictor of DTWT, because the spatial structure of DTWT is sufficiently reproduced by the domain based function, and the catchment based function had a higher variance compared to the baseline simulations. Therefore, it is recommended to use the domain based DTWT function as it contains data from high elevation regions on the eastern side of the domain that contribute to topography driven flow and equilibrate slower than other regions (Ajami et al., 2014).

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3.2 Impact of unsaturated zone re-initialization on ParFlow.CLM spin-up

Impacts of re-initializing the unsaturated zone using the hydrostatic equilibrium vs. adjusted vertical pressure distribution on the spin-up time were also explored using the ParFlow.CLM simulations of the Skjern River sub-catchment. As can be seen from Fig. 4, the difference between the two initialization methods is more pronounced in areas of deep water table, where hydrostatic pressure head distribution results in a drier unsaturated zone compared to adjusted pressure head distribution. Results indicate that after re-initialization, the system equilibrated after 6 additional years of spin-up simulation when using the hydrostatic equilibrium option. With the adjusted pressure head distribution option, only 4 additional years of spin-up simulation were required. Therefore, depending on the pressure head distribution above the water table, either 10 or 12 years of ParFlow.CLM simulations were sufficient to ensure subsurface storage equilibrium, reducing the spin-up time by 40 or 50 %, compared to the baseline spin-up approach. Improved performance of the adjusted pressure distribution is related to the fact that information about soil moisture distribution from stage 1 of spin-up simulations is preserved in this approach. In both initialization approaches, the groundwater storage was equilibrated at the 0.01 % threshold level, based on changes in mean monthly values. In comparison to the baseline spin-up approach, both groundwater and unsaturated zone storages of the equilibrium year are closely reproduced by the adjusted pressure head distribution option (Fig. 5). For the hydrostatic equilibrium, increases in unsaturated zone storage compared to the baseline spin-up resulted in unsaturated zone equilibrium at different threshold level.

Changes in annual water balance after re-initialization were also compared against the baseline spin-up approach of Ajami et al. (2014). While changes in annual evapotranspiration were approximately 1 mm between the two spin-up approaches (annual baseline evapotranspiration of 447.3 mm), percent bias in annual discharge against observations decreased by about 2 % compared to the baseline approach (Table 1). In the hybrid approach, changes in groundwater storage were positive, because after re-

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initialization, DTWT decreased as simulations proceed and the system reached equilibrium (Fig. 5). Differences in simulated DTWT from the last day of the ParFlow.CLM simulations after re-initialization and the baseline spin-up approach varied by up to 2 m inside the catchment boundary (Fig. 6), although most areas were within 0.5 m. Differences were more pronounced in areas of higher elevation in the catchment. Figure 6 shows that the hydrostatic equilibrium pressure head adjustment leads to a clear bias with consistent over estimation of the DTWT, while the adjusted vertical pressure distribution produces a distribution of pressure head errors centred on the expected value.

3.3 Evaluation of the hybrid spin-up approach

Similar to the Skjern River sub-catchment, percent changes in monthly groundwater storages were used to assess equilibrium condition. However, for the Baldry sub-catchment a threshold level of 0.1 % was chosen as the convergence criterion. Results indicated that 28 years of recursive simulations were required until the model equilibrated based on monthly groundwater storage changes. For reference, 28 years of baseline spin-up simulations for Baldry required 37 000 service units equivalent to 24 days of computation using 64 processors of a high performance computing cluster.

Similar to the Skjern River sub-catchment, a double exponential DTWT function using simulations 2 to 6 resulted in WT distributions with the smallest RMSD and percent bias relative to the baseline spin-up simulations. For Baldry, a domain based double exponential function had the closest mean (Fig. S1a in the Supplement) and the smallest mean absolute error relative to the baseline simulation (Fig. S1b in the Supplement). However, DTWT semi-variograms showed higher variances in the domain based double exponential function relative to the catchment based function. Despite the slight differences in the predictive power of DTWT functions between the two catchments, a double exponential function seems to perform best based on most of the criteria.

To re-initialize the ParFlow.CLM model of the Baldry sub-catchment, the new DTWT distribution obtained from the domain based double exponential function was used.

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After re-initialization with the adjusted pressure head distribution, only 8 additional simulations were required until percent changes in monthly groundwater storages reached below the 0.1 % level. This result indicates a 50 % reduction in the spin-up time of a semi-arid catchment when the hybrid spin-up approach is used.

Comparison of WT distributions from the last day of equilibrium simulations (baseline simulation and the hybrid approach) illustrated differences of up to 1 m (Fig. 7). However, for the majority of cells inside the catchment, differences were up to 0.5 m. Similar to the Skjern River sub-catchment, the largest differences in WT distribution were observed in higher elevation areas. Lower WT levels in the hybrid spin-up approach resulted in larger unsaturated zone storage compared to the baseline spin-up (Fig. S2 in the Supplement). In this semi-arid catchment, no stream flow was generated at the catchment's outlet for the equilibrium year. The difference in annual evapotranspiration was only 0.2 mm between the two equilibrium simulations (Table 2).

4 Summary

We present a hybrid approach for reducing the number of spin-up simulations of the integrated hydrological model ParFlow.CLM. In the case of the Skjern River and the Baldry sub-catchments, simulation time decreased by 50 % compared to the baseline spin-up approach when an adjusted pressure head distribution was specified above the water table. Although, ParFlow.CLM was used as a modeling platform, the developed methodology is applicable to other coupled/integrated hydrologic models. Therefore, a general approach to spin-up should include the following steps: (1) perform six years of hydrologic model simulations with DTWT initialized via an informed guess (here 2 m and 3 m below the land surface for the Baldry and Skjern River sub-catchments respectively), (2) calculate a global double exponential DTWT function using domain wide data and estimate the new DTWT for the desired equilibration level, (3) implement the adjusted pressure head approach for the unsaturated zone initialization; and (4) continue spin-up simulations until desired equilibration level is reached. Beyond

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being used to define initial states of the model, this process has the potential to assist in parameter calibration. Previous efforts in calibrating coupled/integrated hydrologic models required a spin-up process after every parameter update (Stisen et al., 2011; Weill et al., 2013). Development of the hybrid spin-up approach could be one step towards enabling systematic calibration of integrated/coupled hydrologic models. However, further refinement is required to facilitate automatic calibration approaches. Additional experiments across multiple catchments with different climate and subsurface heterogeneity and DTWT initializations are also required to assess the efficiency of the proposed approach in reducing time to equilibration in a variety of settings. Reducing the required spin-up time of integrated/coupled hydrologic models will expand their application for hydrological investigations and facilitate the use of these models to investigate both real world and theoretical system behavior.

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Table 1. Skjern River sub-catchment annual water balance for the equilibrium year after the baseline spin-up approach and the hybrid approach using the hydrostatic equilibrium and adjusted pressure head distribution options above the water table. Annual precipitation is 801.6 mm.

Simulation Name	Number of simulations	%bias[1] Q	ET [mm yr^{-1}]	dS[2] GW[3] [mm]	dS UZ[4] [mm]
ParFlow baseline simulation	20	20.3	447.3	−3.3	−0.2
ParFlow + DTWT function (Hydrostatic equilibrium)	12	18.1	446.8	3.3	−0.7
ParFlow + DTWT function (Adjusted Pressure)	10	18.5	446.3	3	−1.6

[1] Percent bias is based on observed discharge at the gauge shown in Fig. 2.
[2] Changes in storage.
[3] Groundwater storage.
[4] Unsaturated zone storage.

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Table 2. Baldry sub-catchment annual water balance for the equilibrium year after the baseline spin-up approach and the hybrid approach with the adjusted pressure head distribution option above the water table. Annual precipitation is 674.8 mm.

Simulation Name	Number of simulations	ET [mm yr^{-1}]	dS[1] GW[2] [mm]	dS UZ[3] [mm]
ParFlow baseline simulation	28	519.2	−12	4.4
ParFlow + DTWT function (Adjusted Pressure)	14	519	−0.2	1.0

[1] Changes in storage.
[2] Groundwater storage.
[3] Unsaturated zone storage.

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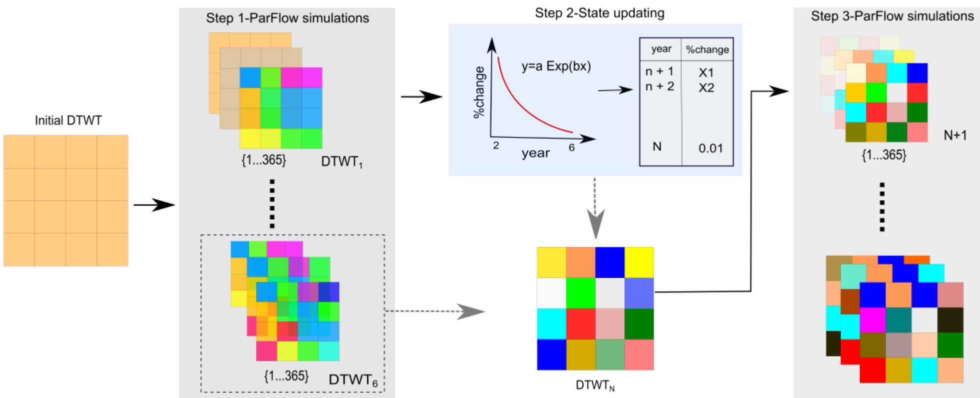

Figure 1. The hybrid spin-up approach consists of three main steps: (1) initial ParFlow.CLM spin-up simulations based an arbitrary DTWT distribution, (2) state updating step by developing a DTWT function based on percent changes in mean annual DTWT in initial spin-up simulations, and (3) stage 2 of ParFlow.CLM spin-up simulations until desired equilibration level is reached.

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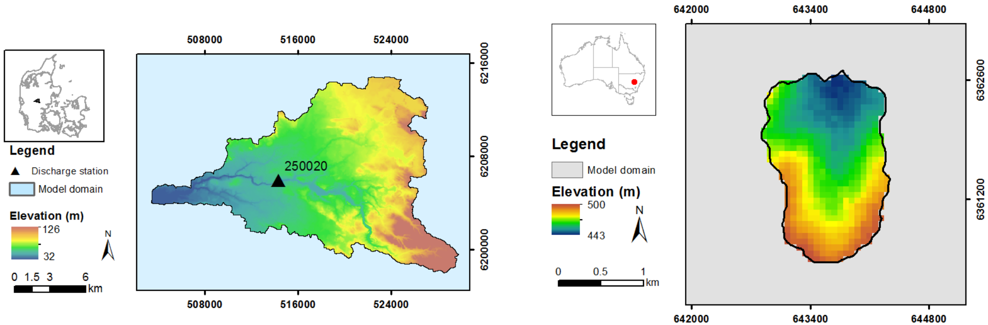

Figure 2. Sub-catchment of the Skjern river basin located in western Denmark (reproduced from Ajami et al., 2014) (left), and Baldry sub-catchment in Australia (right). Modelling domains are extended beyond the catchment boundary to remove the impact of boundary conditions on catchment fluxes.

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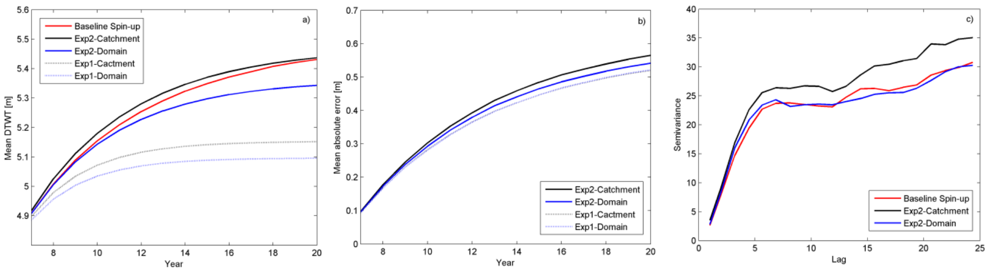

Figure 3. (a) Comparison between the simulated mean annual DTWT obtained from the baseline spin-up approach of ParFlow.CLM of the Skjern River sub-catchment and empirical DTWT functions. The single exponential model was formulated using the domain and catchment averaged data from spin-up simulations 2 to 6; **(b)** estimated mean absolute error based on simulated DTWT from the baseline spin-up together with both catchment and domain averaged single and double exponential functions; and **(c)** experimental semi-variograms of mean annual DTWT from ParFlow.CLM equilibrium year (after 20 years of simulations) and DTWT from catchment and domain averaged double exponential functions, showing that catchment based semi-variances are higher than the baseline simulation. Exp1 and Exp2 refer to single and double exponential functions respectively.

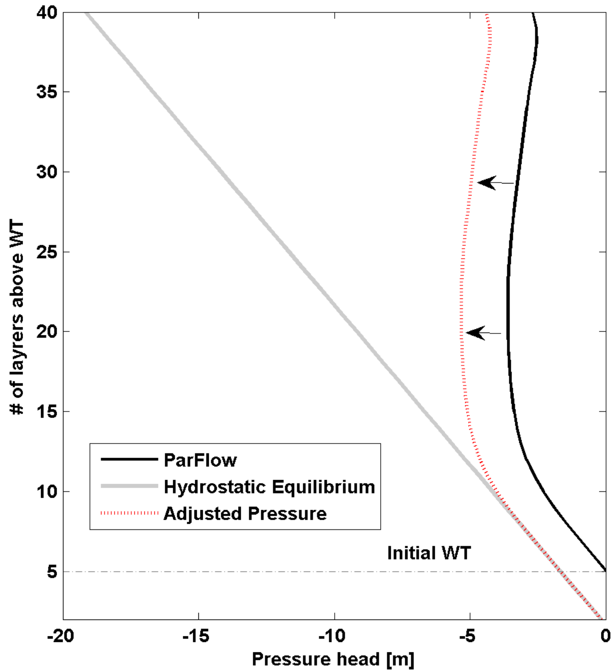

Figure 4. Adjusted pressure head distribution above the estimated DTWT from the DTWT function. Pressure head distribution of the last day of ParFlow.CLM spin-up simulation 6 was adjusted at every grid cell based on the position of DTWT estimated from the DTWT function. In this approach, the hydrostatic equilibrium assumption is used in regions between the new DTWT and the initial DTWT. The ParFlow.CLM pressure head distribution is adjusted to begin at the new pressure head from the initial WT such that the vertical profile is maintained. Hydrostatic pressure distribution is shown as a reference for the new DTWT which is lower than the WT in simulation 6.

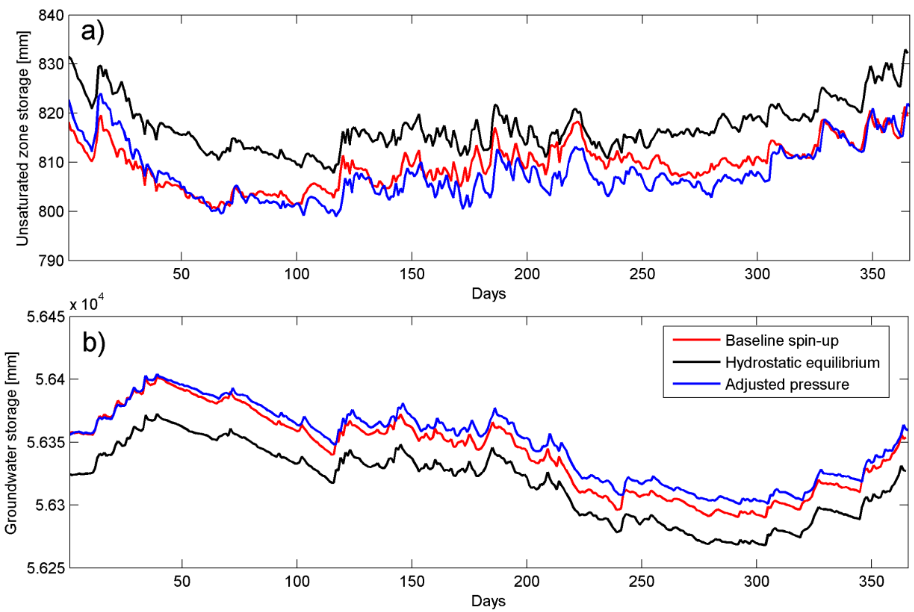

Figure 5. Comparison of **(a)** unsaturated and **(b)** groundwater storages of ParFlow.CLM equilibrium year using the hybrid and baseline spin-up approaches (Ajami et al., 2014). The dynamics of groundwater and unsaturated zone storages are closely reproduced by the adjusted pressure head distribution approach relative to the baseline spin-up approach for the Skjern River sub-catchment.

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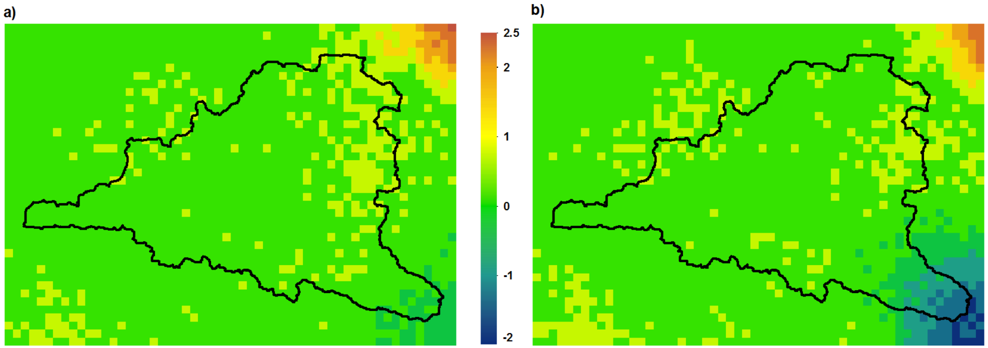

Figure 6. Differences in equilibrium DTWT between ParFlow.CLM simulations after re-initializations and ParFlow.CLM after 20 years of baseline spin-up simulations in (m), where **(a)** is based on hydrostatic pressure distribution above the water table for the initial condition, while **(b)** is based on adjusted pressure head distribution above the water table for the Skjern River sub-catchment.

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Technical Note: Reducing the spin-up time of

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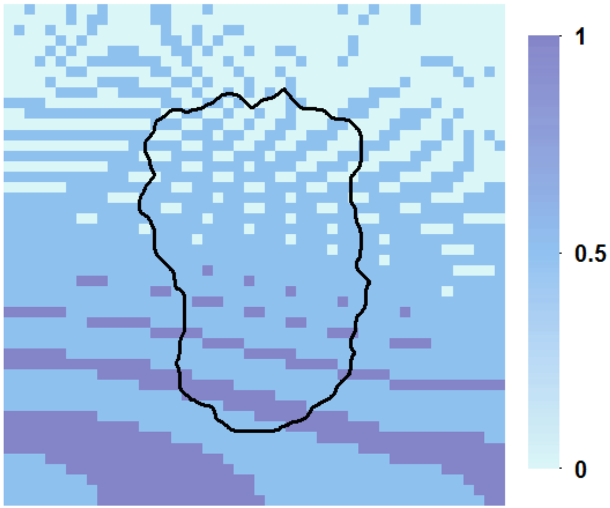

Figure 7. Differences in equilibrium DTWT of Baldry ParFlow.CLM simulations after re-initialization with the adjusted pressure head distribution above the water table and ParFlow.CLM after 28 years of baseline spin-up simulations in (m).

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