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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 the application of coupled or 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 reducing uncertainty in model initialization is to run the model recursively using either a single year 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 the spin-up procedure by using a combination of model simulations and an empirical DTWT function. The methodology is examined across two distinct catchments located in a temperate region of Denmark and a semi-arid region of Australia. Our results illustrate that the hybrid approach reduced the spin-up period required for an integrated groundwater–surface water–land surface model (ParFlow.CLM) by up to 50 %. To generalize results to different climate and catchment conditions, we outline a methodology that is applicable to other coupled or integrated modeling frameworks when initialization from an equilibrium state is required.

1 Introduction

The issue of model initialization is important for hydrologic simulation and prediction, as the initial state has a major impact on a catchment's modeled response (Berthet et al., 2009). In coupled or integrated surface–subsurface models, uncertainty in a catchment antecedent condition is of particular importance, as both the 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 information on the spatial pattern of water table and soil moisture distributions is generally unavailable, various approaches have been developed to determine the 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 or integrated distributed hydrologic models are the following: (1) an initial depth-to-water table is specified at a certain uniform depth below the land surface (Kollet

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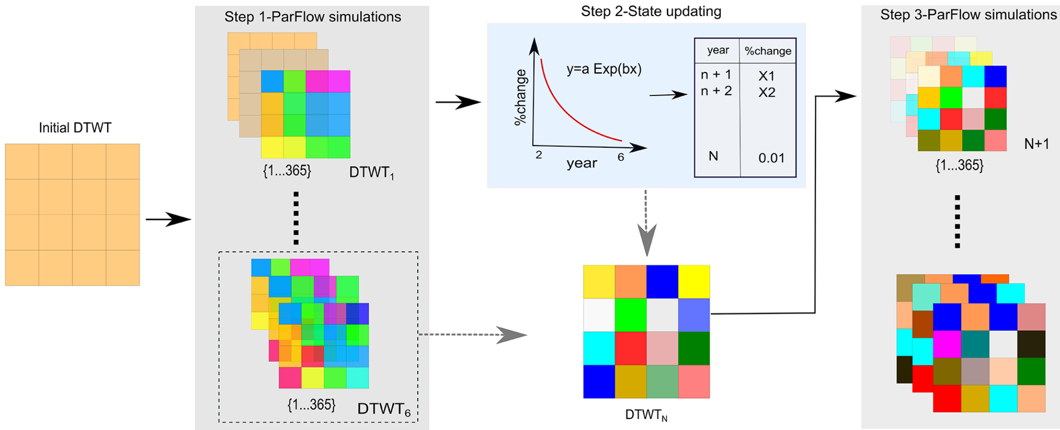

Figure 1. The hybrid spin-up approach consists of three main steps: (1) initial ParFlow.CLM spin-up simulations based on an arbitrary DTWT distribution, (2) a state-updating step by developing a DTWT function based on percentage changes in mean annual DTWT in initial spin-up simulations, and (3) stage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

and Maxwell, 2008), and the impact of initialization is reduced through recursive simulations over either a single year or multiple years of forcing data, until equilibrium conditions are reached, which are 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 the modeled baseflow matches the observations (Jones et al., 2008). Equilibrium-based initializations have been utilized previously for exploring land surface–groundwater coupling (Kollet and Maxwell, 2008) and assessing the impact of climate change on groundwater–land surface interactions using an integrated hydrologic model (Ferguson and Maxwell, 2010).

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 occurring when percentage 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 (a service unit is equivalent to 1 h of time used by one processor) 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 the spin-up period in computationally intensive integrated hydrologic 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. In integrated hydrologic models like ParFlow, numerical solution of the Richards equation in 3-D increases computational time (Kim et al., 1997; Maxwell et al., 2014), in comparison to approaches that use a 1-D Richards equation for the vadose zone and a 2-D groundwater flow formulation for simulating subsurface flow.

The objective of the current study is to develop a hybrid spin-up approach that significantly reduces the number of years of spin-up required for model state equilibrium. The equilibrium-based initialization represents a correct initial state for catchments in which the land use does not change over time and the interannual variability of atmospheric forcing is very small, assumptions that are common to most simulation frameworks. This technical note provides a method for improving the efficiency of this commonly used initialization technique. The performance of the proposed approach in reducing the spin-up period for a catchment-scale application of the ParFlow.CLM model is evaluated against the standard continuous recursive simulation approach that is commonly applied for land surface model spin-up, and is referred to here as the baseline spin-up approach.

2 Data and methodology

The hybrid approach consists of three main stages: 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 utility of the proposed scheme is compared against the equilibrated initial condition for a sub-catchment of the Skjern River basin in Denmark, using the ParFlow.CLM model as developed by Ajami et al. (2014) that employed a traditional baseline spin-up approach. An additional assessment of the hybrid approach in reducing the spin-up period is undertaken by developing ParFlow.CLM for a semi-arid catchment in Australia.

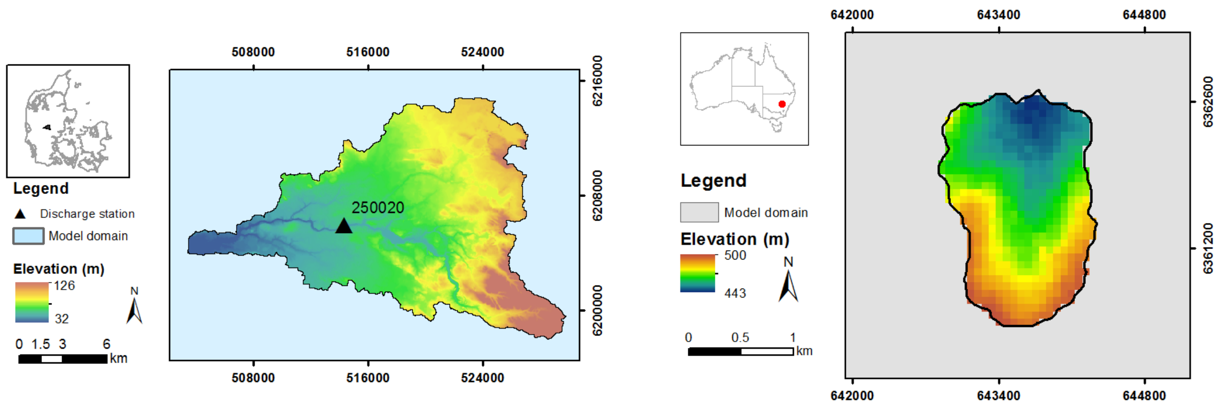

Figure 2. Sub-catchment of the Skjern River basin located in western Denmark (reproduced from Ajami et al., 2014) (left), and the Baldry sub-catchment in Australia (right). Modeling domains are extended beyond the catchment boundary to remove the impact of boundary conditions on catchment fluxes.

2.1 Overview of the ParFlow.CLM model

ParFlow is a 3-D variably saturated groundwater flow model that solves the mixed form of the 3-D Richards equation for the subsurface (Ashby and Falgout, 1996; Jones and Woodward, 2001; Maxwell et al., 2014). ParFlow has a fully integrated overland flow simulator (Kollet and Maxwell, 2006) and performs routing of the ponded water on the land surface via the kinematic wave equation. The Common Land Model (CLM 3.0) (Dai et al., 2003) is integrated into ParFlow to simulate water and energy fluxes at the land surface (Maxwell and Miller, 2005; Kollet and Maxwell, 2008). ParFlow.CLM versions 605 and 653 were used for the Skjern River and Baldry simulations, respectively, which are described below. The terrain-following grid of Maxwell (2013) is not implemented in these modeling setups.

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) and 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.

To reduce the impact of boundary conditions on catchment-scale fluxes, the computational domain is extended beyond the delineated catchment boundary. As such, the ParFlow.CLM model domain covered a 28 km by 20 km area that encompasses the Skjern River sub-catchment (Fig. 2). The modeling 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, resulting in a 56 × 40 × 406 dimension grid.

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 the bottom boundary. Spatially uniform hourly atmospheric forcing (air temperature, wind speed, specific humidity, air pressure, precipitation, and incoming shortwave and downward longwave radiation) for the year 2003 was used for spin-up. In 2003, annual precipitation was 801.6 mm, and the minimum and maximum daily air temperatures were 261.2 K and 295.2 K, respectively. Initial DTWT was assigned uniformly at 3 m below the land surface. 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 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 western New South Wales of Australia, has an area of 1.9 km^2, with an elevation range from 443 m to 500 m inside the catchment boundary (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 sub-catchment (Fig. 2) in order to reduce the impact of boundary conditions on catchment-scale fluxes. Catchment topography was represented using a 60 m pre-processed DEM. The bottom elevation of the modeling grid was a uniform 400 m, resulting in a subsurface thickness of 43 to 101 m across the computational domain. The modeling grid had a 60 m resolution in the x and y directions and a vertical discretization of 0.5 m, resulting in a 48 × 48 × 203 dimension grid.

As for the Skjern River implementation, the ParFlow free-surface overland flow boundary condition was assigned at the land surface. A no-flow boundary condition was specified for the lateral and bottom boundaries of the computational domain (gray domain in Fig. 2). 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) reanalysis data interpolated to $0.25° \times 0.25°$ resolution were used (Decker et al., 2012). In 2004, annual precipitation was 674.8 mm, and the minimum and maximum daily air temperatures were 277 K and 305.5 K, respectively. 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 the mean annual air temperature of 288.1 (K).

2.2 Development of empirical DTWT functions for model re-initialization

Analysis of ParFlow.CLM spin-up behavior using the baseline spin-up approach for the sub-catchment of the Skjern River identified the fact that percentage changes in subsurface storages and DTWT had the form of an exponential decay for a model initialized from a uniform 3 m DTWT (Ajami et al., 2014). Due to spatial adjustment of the water table during the spin-up, groundwater levels declined near the catchment divide and reached the land surface along the channel network, causing an overall decline in mean annual DTWT relative to the initial condition. Using the functional relationships between the number of simulation years and the percentage change of a variable, Ajami et al. (2014) produced 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., a 0.1 % or 0.01 % change for a given variable. Sensitivity of spin-up functions across multiple criteria and variables showed that the estimated spin-up period based on mean annual DTWT was more stable when compared to other spin-up criteria, such as changes in the mean DTWT for the last day of recursive simulations (Ajami et al., 2014).

The inverse of a spin-up function for DTWT predicts percentage 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 of 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 was performed based on an arbitrary initial state (DTWT of 3 m below the land surface for the Skjern River sub-catchment 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 years of the spin-up simulation, the first year of data is removed from the analysis. As a minimum of four data points (i.e., six cycles of ParFlow.CLM simulations) is required to fit a double exponential function, 6 years of spin-up simulations are performed using a single year of forcing data. To assess the sensitivity of DTWT functions to the number of ParFlow.CLM cycles, various exponential functions with single (Eq. 1) or double exponential (Eq. 2) terms are fit to ParFlow.CLM cycles 2 to 6:

$$y = a\exp(bx) \tag{1}$$

$$y = a\exp(bx) + c\exp(\mathrm{d}x), \tag{2}$$

where y is the percentage change in DTWT, x is the number of simulation years, and a, b, c, and d are the fitting parameters. Coefficient of determination and root mean square error are used as goodness-of-fit measures. Furthermore, the performances of global- versus local-scale DTWT functions are evaluated. In this analysis, a domain-based global DTWT function is based on percentage changes in mean annual DTWT values from all the grid cells inside the computational domain, while a catchment-based DTWT function is based on the grid cells inside the catchment boundary. Local DTWT functions are developed for every grid cell based on percentage changes in mean annual DTWT values in that grid cell.

The empirical DTWT functions calculated above estimate percentage changes in mean annual DTWT as a function of simulation year. To predict spatially distributed mean annual DTWT from a global DTWT function, the mean annual DTWT from the final cycle of the ParFlow.CLM spin-up simulation for every grid cell is used as the initial value to estimate successively DTWT distributions as a function of simulation year. These DTWT distributions are based on the predicted percentage change values from the global DTWT function. The sensitivity of DTWT functions to the number of ParFlow.CLM cycles was also examined by developing a number of DTWT functions using data from two to six cycles of ParFlow.CLM. To assess the performance of these DTWT functions, estimated mean annual DTWT values from the DTWT functions were compared against mean annual DTWT from the ParFlow.CLM model of Ajami et al. (2014) that had been spun up for 20 years. Root mean square difference (RMSD), mean absolute error (MAE) and bias were computed to find the best-performing DTWT function. These objective functions are calculated as follows:

$$\mathrm{RMSD} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(B_i - M_i)^2}, \tag{3}$$

$$\mathrm{MAE} = \frac{1}{N}\sum_{i=1}^{N}|B_i - M_i|, \quad (4)$$

$$\%\mathrm{bias} = \frac{\sum_{i=1}^{N}(B_i - M_i)}{\sum_{i=1}^{N}(B_i)} \times 100, \quad (5)$$

where N is the number of grid cells in the domain, B is the mean annual DTWT from the baseline simulation of Ajami et al. (2014) for every grid cell, and M is the estimated mean annual DTWT in a grid cell obtained from a DTWT function.

In the state-updating stage, the best performing empirical DTWT function (a double exponential DTWT function as discussed in Sect. 3.1) was used to estimate percentage changes in DTWT as a function of simulation years, until percentage changes reached the 0.01 % threshold. Using the percentage change values and the mean annual DTWT distribution from the sixth cycle of the ParFlow.CLM spin-up simulation, spatially distributed DTWT was predicted for the entire computational domain.

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 defining pressure head distribution above the water table: (1) implementing the commonly used hydrostatic equilibrium assumption, where the 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 from the DTWT function. In the adjusted pressure head 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 (Fig. 3). This adjustment may represent a lack of consistency in the proposed approach, as the DTWT function estimates mean annual DTWT, while pressure head adjustments in the unsaturated zone are taken from the last day of the sixth cycle of ParFlow.CLM. While it is possible to use DTWT values

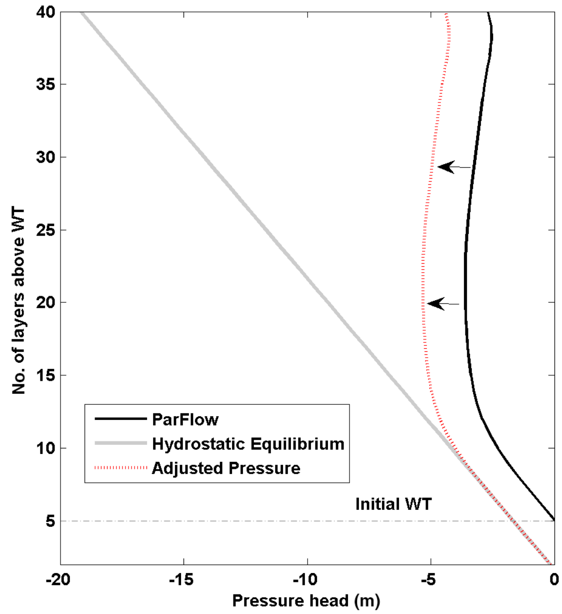

Figure 3. Adjusted pressure head distribution above the estimated DTWT from the DTWT function. Pressure head distribution of the last day of ParFlow. CLM spin-up simulation 6 was adjusted in every grid cell based on the position of DTWT estimated from the DTWT function. In this approach, the hydrostatic 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 head distribution is shown as a reference for the new DTWT, which is lower than the WT in simulation 6.

from the last day of simulations to develop a DTWT function, estimated DTWT values from such a function exhibit larger variability and result in a larger bias. For the Skjern River sub-catchment, the percentage bias values between the estimated DTWT values from the DTWT functions and the baseline simulation of Ajami et al. (2014) for the equilibrium year (simulation 20) were −4 % and −1.6 % for the DTWT functions based on the last day and mean annual DTWT values, respectively.

2.3 Evaluating the hybrid spin-up approach

The performance of the hybrid spin-up approach in reducing the spin-up period 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 and an arbitrary initial state (DTWT of 2 m below the land surface). The equilibrium condition was achieved when percentage changes in catchment-averaged monthly groundwater storages were below the 0.1 % threshold level. Similar to the Skjern River sub-catchment, the sensitivity of empirical DTWT functions to the number of ParFlow.CLM cy-

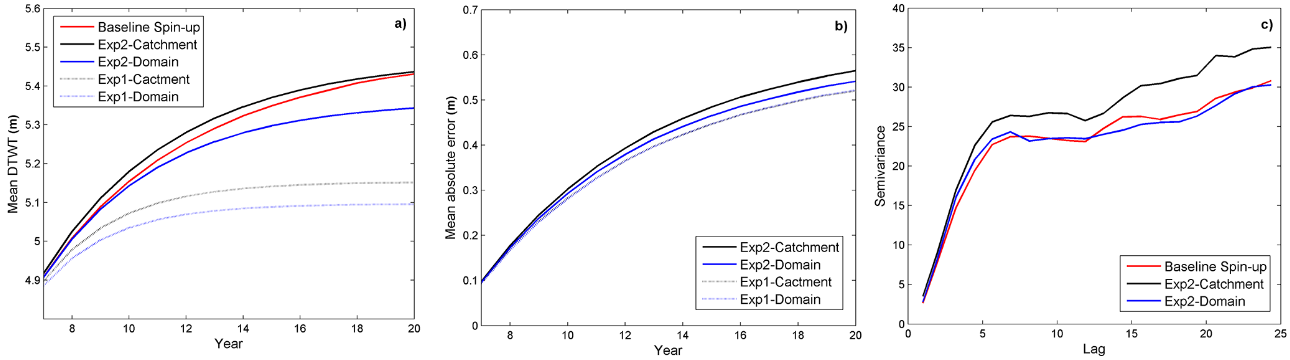

Figure 4. (a) Comparison between the simulated mean annual DTWT obtained from the baseline spin-up approach of ParFlow.CLM of the Skjern River sub-catchment and empirical DTWT functions. The single exponential model was formulated using the domain- and catchment-averaged data from spin-up simulations 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 the 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.

cles (i.e., cycles 2 to 6) is explored and assessed against the baseline spin-up simulations of the Baldry sub-catchment. In the next step, the hybrid spin-up approach outlined in Sect. 2.2 was implemented to re-initialize ParFlow.CLM using a domain-based double exponential DTWT function to estimate spatially distributed DTWT and 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–Skjern River sub-catchment

Optimum parameter values for single and double exponential DTWT functions were obtained using the nonlinear least squares method. Performance of the single and double exponential DTWT functions in predicting 14 years of DTWT were compared against the 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 percentage changes in DTWT oscillate between positive and negative values through initial spin-up simulations. Spatial distributions of these grid cells are shown in Supplement Fig. S1.

Calculated RMSD and percentage 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 (2 to 4, 2 to 5, etc.). Because the first six cycles of ParFlow.CLM simulations were the same between the baseline spin-up simulations and DTWT distributions from the DTWT functions presented in Fig. 4, 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. 4a, the mean annual DTWT over the domain derived from the single exponential functions (fitted to the percentage change data from simulations 2 to 6) underpredicts the baseline spin-up simulations, due to their consistently small underestimates in comparison to double exponential functions fitted to the same data points. Only for the mean absolute error (MAE) calculated at each pixel do single exponential functions based on simulations 2 to 6 perform slightly better and produce smaller errors on average than the double exponential functions (Fig. 4b). It should be noted that the percentage bias in mean annual DTWT for simulation cycle 20 is $-1.6\,\%$ for the domain-based double exponential function and $-6.2\,\%$ for the single exponential function, with both functions derived from simulation cycles 2 to 6. Therefore, single exponential functions are not examined further in re-initializations of the DTWT. In terms of mean DTWT across the domain (Fig. 4a), the catchment-based double exponential DTWT function provides a better prediction and the smallest mean bias when compared to the function based on the entire model domain. However, Fig. 4b indicates that the mean absolute error values are slightly smaller for the domain-based double exponential function. The higher MAE of the catchment-based double exponential function is a result of slightly more regions with overestimated and underestimated DTWT values that contribute to a good overall mean DTWT (Fig. 4a), but which contain more errors spatially compared to the domain-based double exponential function.

To investigate this result further, three empirical semi-variograms were generated. As the impact of an east–west spatial trend on the mean annual DTWT values was evident in the semi-variograms, the trend should first be removed from the mean annual DTWT values. To remove the trend, a plane was fitted to the observed mean annual DTWT values, with an equation of the form

$$z = ax + by + c, \tag{6}$$

where a, b and c are fitted coefficients, x and y are the coordinates of every grid cell, and z is the mean annual DTWT. Residuals are computed by subtracting the estimated mean annual DTWT from Eq. (6) from the observed mean annual DTWT values. Finally, the semi-variogram of the residuals as a function of distance is calculated. The semi-variance is a measure of spatial variance, and presents the average (dis-)similarity between data pairs at a given distance. Investigating the empirical semi-variograms of mean annual DTWT values (Fig. 4c) indicates that the domain-based double DTWT function is a better predictor of mean annual DTWT, because the spatial structure of DTWT is sufficiently reproduced by the domain-based function, and the catchment-based function has 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 topographically driven flow, and equilibrates more slowly than in other regions (Ajami et al., 2014). In summary, double exponential functions are chosen as they have less bias compared to single exponential functions, and there is very little difference in terms of MAE amongst predictions. The choice is further supported by the RMSD and semi-variograms.

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

Impacts of re-initializing the unsaturated zone using the hydrostatic equilibrium versus adjusted vertical pressure distribution on the spin-up period were also explored using the ParFlow.CLM simulations of the Skjern River sub-catchment. As can be seen from Fig. 3, the difference between the two initialization methods is more pronounced in areas of the 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 sub-

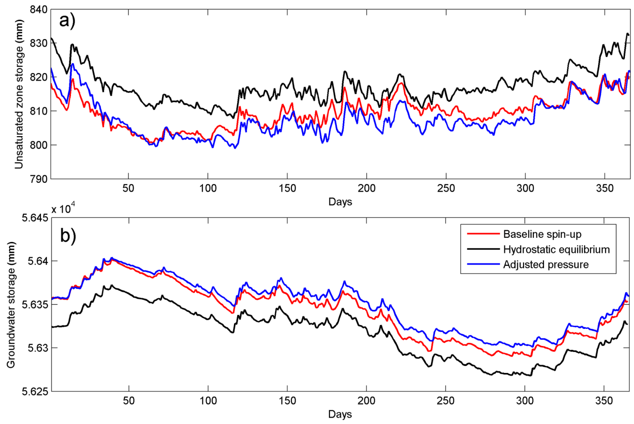

Figure 5. Comparison of **(a)** unsaturated and **(b)** groundwater storages of the ParFlow.CLM equilibrium year using the hybrid and baseline spin-up approaches (Ajami et al., 2014). The equilibrium year corresponds to simulation cycles of 10, 12 and 20 for the adjusted pressure head, hydrostatic equilibrium, and baseline simulations, respectively. 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.

surface storage equilibrium, reducing the spin-up time by 40 or 50 %, compared to the baseline spin-up approach.

The 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). While in both re-initializations, DTWT and subsequently groundwater storage volume were the same at the start of the simulations, unsaturated zone storage of the hydrostatic equilibrium option was drier than the adjusted pressure head option. Additional ParFlow.CLM simulations after re-initialization ensured equilibrium of groundwater storage. As can be seen from Fig. 6a, hydrostatic re-initialization results in a deeper WT at equilibrium (simulation 12) relative to the baseline equilibrium year (simulation 20). Higher DTWT values of the hydrostatic option at equilibrium correspond to smaller groundwater storage and subsequently larger unsaturated zone storage compared to the baseline spin-up (Fig. 5). It should be noted that in ParFlow.CLM, groundwater and unsaturated zone storages are not explicitly determined by fixed size compartments, and the extent of an unsaturated zone is determined by the location of the water table. Percentage changes in mean annual unsaturated zone storage between the last 2 years of recursive simulations were 0.1 % for the hydrostatic equilibrium and 0.3 % for the ad-

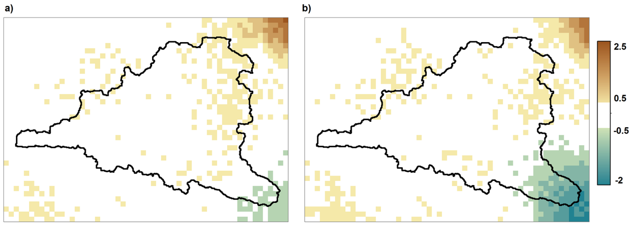

Figure 6. Differences in equilibrium DTWT between ParFlow.CLM simulations after re-initializations and ParFlow.CLM after 20 years of baseline spin-up simulations in meters, where **(a)** is based on hydrostatic pressure head distribution above the water table for the initial condition, while **(b)** is based on adjusted pressure head distribution above the water table for the Skjern River sub-catchment. White regions correspond to grid cells where the differences in equilibrium DTWT are less than 0.5.

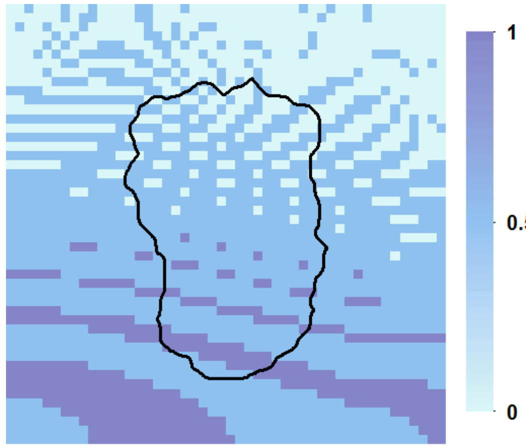

Figure 7. Differences in equilibrium DTWT of Baldry ParFlow.CLM simulations after re-initialization with the adjusted pressure head distribution above the water table and ParFlow.CLM after 28 years of baseline spin-up simulations, in meters. The contours of DTWT overestimation are along the direction of flow lines from high-elevation areas towards the catchment outlet.

justed pressure head re-initializations, indicating unsaturated zone equilibrium at different threshold levels.

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), the percentage 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-initialization, DTWT decreased as simulations proceeded and the system reached equilibrium (Fig. 5). At equilibrium, differences in simulated DTWT from the last day of the ParFlow.CLM simulations after re-initializations (hydrostatic equilibrium and adjusted pressure head distribution) 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 overestimation of the DTWT, while the adjusted vertical pressure distribution produces a distribution of pressure head errors centered on the expected value.

3.3 Evaluation of the hybrid spin-up approach over the Baldry sub-catchment

Similar to the Skjern River sub-catchment, percentage changes in monthly groundwater storages were used to assess the 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, which is equivalent to 24 days of computation using 64 processors of a high-performance computing cluster.

To obtain optimum parameter values for single and double exponential DTWT functions, the nonlinear least squares method is used. 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 percentage bias, relative to the baseline spin-up simulations. For Baldry, a domain-based double exponential function had the closest mean over the domain (Fig. S2a) and the smallest mean absolute error relative to the baseline simulation (Fig. S2b). However, DTWT semi-variograms showed higher variances in the domain-based double exponential function relative to the catchment-based function (Fig. S2c). 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. After re-initialization with the adjusted pressure head distribution, only 8 additional simulation years were required until percentage changes in monthly groundwater storages reached below the 0.1 % level. This result indicates a 50 % reduction in the spin-up period 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 less than 0.5 m. Similar to the Skjern River sub-catchment, the largest differences in WT distribution were

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

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.

observed in higher-elevation areas in the southern part of the catchment. Lower WT levels in the hybrid spin-up approach resulted in larger unsaturated zone storage compared to the baseline spin-up (Fig. S3). In this semi-arid catchment, no stream flow was generated at the catchment 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 period of spin-up required to reach equilibrium with the ParFlow.CLM integrated hydrological model. In the case of the Skjern River and Baldry sub-catchments, the simulation period 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 or integrated hydrologic models.

A general approach to spin-up should include the following steps: (1) perform 6 years of hydrologic model simulations with DTWT initialized via expert knowledge or 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 the desired equilibration level is reached. Previous efforts in calibrating coupled or integrated hydrologic models required a spin-up process after every parameter update (Stisen et al., 2011; Weill et al., 2013). Development of a computationally efficient spin-up approach will enable this type of systematic calibration of integrated or coupled hydrologic models.

Additional experiments across multiple catchments with different climate and subsurface heterogeneity and DTWT initializations are required to assess the efficiency of the proposed approach in reducing the simulation period to equilibration in a variety of settings. In addition, the role of topography and spatially distributed forcing should be examined further. Reducing the required spin-up years of coupled or integrated hydrologic models will expand their application for hydrological investigations and facilitate the use of these models in investigating both real-world and theoretical system behavior.

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