Development of a Coupled Groundwater–Atmosphere Model

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ABSTRACT

Complete models of the hydrologic cycle have gained recent attention as research has shown interdependence between the coupled land and energy balance of the subsurface, land surface, and lower atmosphere. PF.WRF is a new model that is a combination of the Weather Research and Forecasting (WRF) atmospheric model and a parallel hydrology model (ParFlow) that fully integrates three-dimensional, variably saturated subsurface flow with overland flow. These models are coupled in an explicit, operator-splitting manner via the Noah land surface model (LSM). Here, the coupled model formulation and equations are presented and a balance of water between the subsurface, land surface, and atmosphere is verified. The improvement in important physical processes afforded by the coupled model using a number of semi-idealized simulations over the Little Washita watershed in the southern Great Plains is demonstrated. These simulations are initialized with a set of offline spinups to achieve a balanced state of initial conditions. To quantify the significance of subsurface physics, compared with other physical processes calculated in WRF, these simulations are carried out with two different surface spinups and three different microphysics parameterizations in WRF. These simulations illustrate enhancements to coupled model physics for two applications: water resources and wind-energy forecasting. For the water resources example, it is demonstrated how PF.WRF simulates explicit rainfall and water storage within the basin and runoff. Then the hydrographs predicted by different microphysics schemes within WRF are compared. Because soil moisture is expected to impact boundary layer winds, the applicability of the model to wind-energy applications is demonstrated by using PF.WRF and WRF simulations to provide estimates of wind and wind shear that are useful indicators of wind-power output.

1. Introduction

Surface–atmospheric interactions modulate the energy available to the atmosphere. As such, these processes (e.g., feedback between soil moisture and precipitation) may play a key role in improving the predictability of weather and climate (Betts et al. 1996; Chen and Avisar 1994; Chen and Dudhia 2001b; Hong and Kalnay 2000; Koster et al. 2004; Trier et al. 2004). Patton et al. (2005) and Chow et al. (2006b) found soil moisture initialization to be a strong influence on boundary layer flows, while Holt et al. (2006) found that soil moisture influences the prediction of cloud patterns in frontal systems. Zhong

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et al. (1996) found that soil moisture is a primary driver of the nocturnal low-level jet, a significant resource for the generation of renewable power from the wind. These results highlight the critical importance of representing land–atmospheric interactions in atmospheric models used in water resources and wind-energy applications and boundary layer simulation research in general. However, two important components of the hydrologic cycle related to the land surface—groundwater and overland flow—have only recently been considered in atmospheric models. The full effects of these components on atmospheric processes, for example, the development of the atmospheric boundary layer, remain unknown (NRC 2004). More research is needed to fully understand the relationship between land surface heterogeneity and atmospheric heterogeneity, and the spatial and temporal scales over which the impacts of soil moisture variations persist in the atmosphere. A complete understanding of these processes will involve further theoretical and observational studies. This present study advances how best to represent these processes in numerical simulations of atmospheric flow through enhancements to a widely used community modeling platform.

Several recent studies have shown that groundwater storage and redistribution play an important role in the land energy and water balances (Kollet and Maxwell 2008a), in short-term atmospheric feedbacks (Maxwell et al. 2007), and in local response to global climate change (Maxwell and Kollet 2008a). There is also evidence that, while the timing of extreme events such as drought is strongly influenced by ocean–atmosphere forcing, the duration and severity of these events, for example in regions such as the southern Great Plains, likewise depend upon soil moisture and land–atmosphere feedbacks (Hong and Kalnay 2000, 2002; Koster et al. 2004; Schubert et al. 2004, 2008). This evidence indicates that not only will climate change impact the hydrologic cycle (Allen et al. 2004; Cayan et al. 2008; Dettinger et al. 2004; Scibek and Allen 2006; Scibek et al. 2007; Seager et al. 2007; Tague et al. 2008; Vanrheenen et al. 2004), but that changes in the hydrologic cycle, particularly the terrestrial system, will feed back to alter the climate at local and possibly larger scales. These feedbacks are a function of water table depth (Kollet and Maxwell 2008a; Maxwell and Kollet 2008a; Maxwell et al. 2007) and seasonal atmospheric conditions (Kollet and Maxwell 2008a), and are expected to vary across different geographic and climatic regions.

A small, but growing body of work has addressed the inclusion of groundwater and detailed representations of surface hydrology into atmospheric models. York et al. (2002) coupled a single-column atmospheric model to a single-layer groundwater model via a land surface model. Seuffert et al. (2002) and Molders and Ruhaak (2002) both coupled watershed models with more sophisticated representations of lateral, overland flow to regional-scale atmospheric models and found improvements in energy fluxes and rainfall. Maxwell et al. (2007) used a coupled watershed and atmospheric model to demonstrate feedbacks as well as the connection between water table depth and the atmospheric boundary layer at regional watershed scales. More recently, Anyah et al. (2008) and Jiang et al. (2009) coupled a simple groundwater scheme into atmospheric models and showed differences in atmospheric fluxes and improvements to predicted precipitation over seasonal time periods at continental scales.

Here we present the development and application of a coupled hydrologic–atmospheric model. This model is the result of coupling the parallel hydrology model (ParFlow) to the community numerical weather prediction Weather Research and Forecasting model (WRF). By including ParFlow, the coupled model extends the WRF platform and previous approaches to include the following additional surface and subsurface hydrologic processes:

1) Highly resolved groundwater flow in complex, three-dimensional, heterogeneous aquifers, ranging from deep storage to a free or confined water table;
2) Variably saturated flow in three dimensions, with the potential for a shallow or deep vadose zone, ranging from the water table to the land surface;
3) Fully integrated lateral flow over the land surface, with explicit routing, in full communication with subsurface flow (groundwater and vadose zone) at every surface grid cell.

These processes extend the capabilities of the Noah land surface model (LSM) within WRF, which does not provide for any lateral flows (surface or subsurface) or any deep-groundwater processes. Although a similar coupling between a mesoscale atmospheric model and ParFlow has been achieved (PF.ARPS, as in Maxwell et al. 2007), this research extends that effort by integrating ParFlow with the WRF model. In addition to having a broad user base, the WRF model will continue to benefit from a broad research and developer base for improved physics, dynamics, and data assimilation options in the future. WRF presently offers an already extensive suite of options for physics parameterizations, the benefits of which are demonstrated in this work, as a means for uncertainty quantification in the evaluation of the significance of coupling an atmospheric model with a groundwater and watershed model. We present the development of this model and demonstrate its performance using a semi-idealized set of simulations to delineate the critical role of spinup in coupled simulations.
These simulations vary the microphysics parameterizations within WRF and compare the uncoupled and coupled models. The impact of the coupled model on boundary layer winds is also explored, with a focus on those altitudes relevant for the generation of power from the wind, to explore the relevance of subsurface moisture transport for forecasting parameters of interest to wind-power production. We show that the coupled model very accurately balances water between terrestrial and atmospheric systems and that it may be employed in water resources and wind-energy applications.

2. Model description

Here we briefly describe the two models used in this study; ParFlow and the WRF model, version 3.0, in uncoupled form, then discuss the coupling process in more detail.

a. WRF

The Advanced Research (ARW) core of the WRF model used in this study is described in Skamarock and Klemp (2008; more information is available online at http://www.wrf-model.org). The ARW contains both a dynamical core that advances the governing equations (using an explicit time integration scheme), and an extensive package of parameterization options for the various atmospheric and land surface processes that force the evolution of the flow. Jointly developed by the National Center for Atmospheric Research (NCAR), a number of government agencies, and the university research community, the WRF model is continually benefitting from new physical process parameterizations developed within the broad user community and integrated into future releases of the model. The ARW version 3.0 contains nine microphysics parameterizations, three longwave radiation schemes, four shortwave radiation schemes, three surface layer physics schemes, four land surface schemes, four planetary boundary layer schemes, and five cumulus parameterization schemes. With a wide range of users and developers, and an established pathway for integration of new options into the model, subsequent WRF releases will continue to offer expanded options.

In addition to its extensive suite of mesoscale physics options, WRF also contains physics and dynamics options appropriate for both global-scale and large-eddy simulations, as well as various data assimilation schemes. As such, the WRF model is applicable to a wide range of operational and research activities. Many such applications could benefit from improved representation of subsurface, land surface, atmosphere exchanges provided by coupling to a subsurface hydrologic model as described below.

b. ParFlow

ParFlow is a parallel, variably saturated, groundwater flow model, and is described in detail by Ashby and Falgout (1996), Jones and Woodward (2001), and Kollet and Maxwell (2008a). (Additional information is available online at https://computation.llnl.gov/casc/parflow/parflow_home.html.) It is an open-source, community code and freely available for download (available online at http://inside.mines.edu/~rmaxwell/maxwell_software.shtml). In the mode employed here, it solves the Richards equation, which describes the movement of water in saturated and unsaturated soil [see Eq. (A1)] in three dimensions. Additionally, this platform has an integrated overland flow boundary condition (Kollet and Maxwell 2006), which solves the kinematic wave equation [see Eq. (A5)]. Thus ParFlow has the capability to resolve streamflow and two-way flows between surface and groundwater explicitly without the use of parameterized river routing or runoff schemes.

ParFlow requires specification of subsurface hydraulic properties, such as the saturated hydraulic conductivity, porosity, and the parameters [see Eqs. (A3)–(A4)] for the pressure–saturation and pressure–relative permeability relationships. These parameters may be specified using commonly available databases (Schaap and Leij 1998) and are specific to the soil and geology present at a particular study site. ParFlow has been modified to optionally include the Common Land Model (CLM; Dai et al. 2003), as described in Maxwell and Miller (2005) and Kollet and Maxwell (2008b) allowing for full-coupling between land–energy processes and hydrology. This option is used during the spinup process for the numerical experiments presented in this work.

c. Coupled model PF.WRF

The coupled model used in this study was created by combining the ParFlow variably saturated groundwater flow model with the WRF mesoscale numerical weather prediction system. The surface water and soil moisture components of ParFlow provide WRF with soil moisture information that includes the effects of ponding, runoff, and subsurface flow, including an explicitly resolved water table. In turn, WRF provides ParFlow with spatially variable precipitation and evapotranspiration rates. In this effort, the CLM component of stand-alone ParFlow was replaced by the Noah LSM that is used in WRF (Chen et al. 2001, 1996; Ek et al. 2003; Pan and Mahrt 1987). Modifications to Noah involved in the coupling process are described more fully below and in the appendix.

The coupling of these two models provides each model with boundary condition information at a level of detail that is usually not available from common data
sources used as forcing. This coupled system (PF.WRF) can represent spatial variations in land surface processes, as well as groundwater–land surface and land surface–atmosphere feedbacks, driven by physical processes in the atmosphere and the subsurface. This coupled modeling approach is general, allowing for physically accurate representation of subsurface, land surface, and atmospheric processes. Coupling ParFlow with WRF both enables the use of the broad range of physics applications in WRF, as well as extending the potential user base of the model given WRF’s popularity and wide range of applications.

The coupled simulations detailed herein utilized the full suite of atmospheric physics parameterizations (e.g., radiation, cloud and precipitation microphysics, and planetary boundary layer turbulence). These simulations require the simultaneous solution of the three-dimensional (3D) groundwater and two-dimensional (2D) overland flow equations (provided by ParFlow) and the 3D atmospheric flow equations (provided by WRF). The Noah LSM constitutes the interface between the subsurface hydrology (ParFlow) and the atmosphere (WRF), and passes surface energy and moisture fluxes between the two models. In PF.WRF, ParFlow is incorporated as a subroutine within WRF’s Noah LSM, with communication over the top four soil layers (for complete details, please see the appendix). Subsurface hydrology in the WRF Noah LSM is entirely replaced by ParFlow in the coupled model.

The general solution procedure begins with the explicit advancement of the atmospheric solver. An operator-splitting approach is employed, allowing the ParFlow model to use the internal time step of WRF (1 s in these simulations). As with other physical process modules, larger time steps can be taken in ParFlow as part of a subcycling option (e.g., 1 h). Such an approach can potentially take advantage of the slower dynamics in the terrestrial flow regime to improve computational efficiency at an acceptable loss of solution accuracy. For all the simulations in this work other than the subcycling-specific tests, ParFlow is advanced using the same time step as WRF. The subsurface moisture field calculated by ParFlow is passed directly to the Noah LSM within WRF and is used by Noah LSM in the next time step. The Noah LSM is advanced for each internal WRF time step to provide all the surface fluxes, but the soil moisture values are now specified by ParFlow. A schematic of the coupling process is shown in Fig. 1.

3. Numerical simulations, results, and discussion

Two numerical experiments are used to demonstrate the capabilities of the coupled model and to explore details of the coupled-model physics. The first is an idealized simulation that strongly forces the model with heavy precipitation to test the error in the water balance and to test temporal subcycling between ParFlow and WRF. This idealized simulation also demonstrates the impact of ParFlow processes on atmospheric parameters. The second is a semi-idealized set of coupled and uncoupled simulations based upon data from a real watershed.

a. Idealized simulation

The atmospheric portion of the idealized simulations, shown in Fig. 2, uses a flat $15 \times 15 \times 14.462$ km domain discretized using $16 \times 16 \times 25$ computational nodes, with horizontal grid spacing of 1 km in each direction, and vertical resolution of approximately 40 m near the surface and stretched toward the top of the atmosphere. The WRF model domain had periodic boundary conditions on the lateral sides. No mean winds were specified, but small random perturbations were added to the initial horizontal flow components, and the temperature was initialized to be slightly stable, given by $T = 300.0 - 0.005 z$, where $T$ is in kelvin, $z$ is height above the surface in meters, and 0.005 represents the vertical temperature gradient in kelvin per meter. Atmospheric pressure was initialized to be hydrostatic; based on a temperature of 300 K, and relative humidity was initialized to 50% everywhere. Rain was imposed by adding a source term to the tendency (time derivative) of the water vapor mixing ratio $q_v$ (kilogram H$_2$O per kilogram dry air). For this simulation the average column mass was 85 037.4 Pa. Hence, the unit vapor tendency prescribed was $1.0/85 037.4 = 1.175 95 \times 10^{-5} \text{s}^{-1}$, or 0.042 kg H$_2$O h$^{-1}$. This tendency was applied over a horizontal array of nine grid points, three in each direction, at the middle of the domain. These points included grid points 6, 7, 8 in both $x$ and $y$ and 9 grid points in the vertical spanning a height of roughly 1.3–8.1 km.

The ParFlow domain used the same lateral dimensions with the same horizontal grid spacing as WRF (1 km) over a depth of 5 m, with a constant vertical grid spacing of 0.25 m. The subsurface pressure head was initialized as hydrostatic with the water table 3 m below the ground surface (i.e., 3 m below the top of the ParFlow domain). Subsurface parameters were set as follows: saturated hydraulic conductivity $K_{sat} = 0.1$ (m h$^{-1}$), and porosity $\phi = 0.3$. No-flow boundary conditions were imposed on the subsurface sides and bottom. A slope, $S_x = 0.001$, was used to route ponded water to the $x = 0$ face, where it was allowed to exit the domain. The land cover was specified as bare soil everywhere. The entire simulation was run for 48 h with $\Delta t = 5$ s and the positive moisture tendency as...
specified above for the first 24 h then a tendency of 0 for 24–48 h.

1) IMPACT OF PF.WRF

The spatial distribution of cumulative rainfall over the entire 48-h simulation appears in Fig. 3. This figure clearly shows the large rainfall (2498 mm) accumulations in the middle of the domain. This maximum rainfall value lies directly below the area of injected moisture. Rainfall totals in areas around the rainfall maximum decrease rapidly with zero rainfall 4 km away from the center point and zero accumulated rainfall over much of the domain.

Figure 4 plots the spatial distribution of soil saturation at two times during the simulation at the ground surface. After 1.5 h of simulation time (left) the spatial distribution of soil saturation very closely matches the distribution of rainfall. However, after 16 h of simulation time, the distribution of soil saturation is much different than the distribution of rainfall. This difference is due to the coupled physical processes present in PF.WRF. Because the maximum rainfall rate is less than the saturated hydraulic conductivity of the subsurface, the rainfall quickly infiltrates into the subsurface. When the infiltrated water reaches the water table, it causes a saturation mound (increased saturation above the water table) in the subsurface, which eventually reaches the land surface. This surface saturation creates ponded conditions, which results in surface water storage and nonzero values for $h$ in the rhs of Eq. (A5). This ponded water is automatically routed downslope, to the left in this case, to adjacent cells that are not fully saturated. Over time, as a result of the continuing precipitation and runoff from cells upslope, those cells also become saturated. This process repeats, until all the cells from the point of initial rainfall to the edge of the domain are fully saturated. At the end of the 24-h rainfall period, the subsurface and surface from the area of maximum rainfall to the $x = 0$ face of the domain are fully ponded and routing water out of the domain. These conditions create the saturation distribution shown in Fig. 4.

Figure 5 shows conditions at 30 h, after the rainfall has ceased and the surface has begun to dry. The distribution of soil saturation at hour 30 is similar to that shown at earlier times, for example hour 16 (Fig. 4). Examination of the contours of latent heat flux ($LH, W m^{-2}$) at 30 h of simulation time shown in Fig. 5 reveals that the contours of LH follow saturation very closely. The
maximum instantaneous LH is located in a region not coincident with the peak rainfall, but in a region where rainfall was zero. This displacement occurs because of the new physical processes in PF.WRF, listed earlier. Though rain may fall at the ground surface in one location, it infiltrates into an unsaturated zone that is in full contact with the saturated zone (or groundwater), and the water table may eventually rise to reach the land surface. At the land surface, water is transported laterally due to overland flow, whereupon it may then re-infiltrate or continue to flow laterally, resulting in the very different soil saturation seen in Fig. 5.

Figure 6 summarizes the partitioning of water into subsurface water, surface water, and runoff, accumulated over the entire ParFlow domain. This figure plots the cumulative change of water, in cubic meters, for each of these components along with the total flux provided to ParFlow from WRF. Initially, the heavy rainfall in the idealized test case mainly infiltrates into the subsurface resulting in the change in subsurface storage as shown. After about 6 h of rainfall, surface storage increases, indicating ponded water on the ground surface that is routed laterally from cell to cell within the domain. At 16 h the surface water storage reaches a maximum value (note this is the time for Fig. 4, right panel). At this point, ponded water reaches the edge of the domain and runs off through the \( x = 0 \) face.

Figure 6 may also be used to assess the total water balance and water balance error in the coupled simulation. At all times, the cumulative surface, subsurface and runoff amounts must total the input from WRF to balance the water in the domain. The difference between the cumulative WRF flux and the two storage and runoff components is the water balance error. The water balance error can be defined as the difference between the water storage terms, on the lhs of Eq. (A1) and the corresponding flux terms, on the rhs of this equation, accumulated over a given time period, in this case a single model time step. At any time in the simulation the instantaneous normalized water balance error is less than \( 6.8 \times 10^{-12} \) and the total normalized water balance error is \( 2 \times 10^{-13} \), which corresponds to an absolute error of \( 2 \times 10^{-6} \) m\(^3\) or 2 mL of water.

2) SUBCYCLING

To explore the potential gains in computational efficiency afforded by subcycling ParFlow relative to WRF, we employed a similar test case to the idealized one described above. However, in order to strongly force the coupled model, the subcycling simulations used a prescribed vapor tendency 5 times greater than the previous simulations (0.21 kilograms H\(_2\)O per hour) applied over a shorter simulation time (3 h) to create a very intense

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rainfall episode. The subcycling interval between WRF and ParFlow was varied from 1 (a case with no subcycling of ParFlow) to 72 (e.g., ParFlow takes one step for every 72 WRF time steps).

In Fig. 7a, the water balance error (as defined above) between WRF and PF appears as a function of time, for subcycling intervals of 1 (no subcycling and $\Delta t_{PF} = \Delta t_{WRF} = 5$ s), 2 (2 WRF time steps for every PF time step and $\Delta t_{PF} = 10$ s), 12 (12 WRF time steps for every PF time step, and $\Delta t_{PF} = 60$ s), and 72 (72 WRF time steps for every PF time step, and $\Delta t_{PF} = 360$ s). The water balance error is always less than $1 \times 10^{-12}$ % for all cases and does not vary significantly with the subcycling interval. Figure 7b depicts the total water storage, surface and subsurface, in ParFlow over time as a function of all subcycling intervals; this quantity should be the same for all intervals. While differences in water balance indicate errors due to the subcycling, differences in the total amount of water indicate divergence of the solutions due to differing land feedbacks. The water storage is consistent among simulations up to a subcycling interval of 12, while the simulation with a subcycling interval of 72 appears to diverge from the other solutions. These results suggest that accurate solutions that are not divergent are achieved for up to an order of magnitude difference in time step between atmospheric and surface–subsurface systems (provided that the time steps are adequate to resolve relevant physical and dynamic processes).

The results of a timing test for the different subcycling cases appear in Fig. 8. In this test, the time spent in WRF and ParFlow are calculated and plotted separately. Note that ParFlow solves for the pressures everywhere at the land and subsurface using an implicit time integration method with an iterative solution technique. As a result, ParFlow time steps may be chosen by accuracy constraints of dynamics of interest. The results of Fig. 8 demonstrate that the overall simulation time decreases with increases in temporal subcycling. For the temporal subcycling of one (equal WRF and ParFlow time steps) the time spent in ParFlow is almost equal to that of WRF. At the greatest subcycling interval (i.e., 72) the total time in ParFlow is less than 7% of the total simulation time (which exceeds 1/72). These results indicate that, of the choices tested here, the subcycling interval of 12 is an acceptable number where simulation accuracy, fidelity, and efficiency may be balanced. Here, the solution is very similar to the case with no subcycling.

Fig. 4. Plot of soil saturation at the ground surface at simulation times of (left) 1.5 and (right) 16 h. Note that the early saturations follow the rainfall pattern closely, while later saturations show the effects of lateral flow.
ParFlow takes approximately 12% of the total simulation time, and disagreement in water balance between ParFlow and WRF is less than $1 \times 10^{-12}$%.

In general, whether one can subcycle ParFlow within a given simulation will be dependent on the dominant physics within the simulation. Specifically, when parameterizations within Noah that rely on soil moisture from ParFlow are highly nonlinear and rapid changes are occurring, subcycling will lead to very different results. We leave a thorough analysis of the couplings involved in a determination of best subcycling interval for a future study. However, a general strategy for determining a subcycling interval would be the following:

1) Determine the quantities of interest (QOI) of the specific study to be run (i.e., precipitation) and the amount of variance that can be tolerated for the purpose of the study.
2) Run the coupled model without subcycling ParFlow and using a fairly large time step.
3) Subcycle ParFlow relative to WRF with intervals of 2, 4, 6, etc., until results from a given interval produce a variation in the QOI larger than its prescribed tolerance. The last interval that produced acceptable variation is a likely candidate for a good subcycling interval.
4) Run the coupled model with the small time step of choice and subcycling interval found in step 3.
5) Run the coupled model with small time step and subcycling with an interval of 1 or 2 greater than in step 4) to determine if the variation is small relative to the tolerated variation. If so, then use the interval found in step 3). If not, decrease the subcycling interval and try again.

This strategy gives very general guidance. However, it should help in determining when and at what interval subcycling will give a faster solution with similar (to within the prescribed tolerance) behavior for the specific study.

b. Semi-idealized simulations

A series of semi-idealized simulations were performed on a $45 \times 32$ km$^2$ domain in Oklahoma. This domain encompasses the Little Washita watershed, which has been studied previously using both modeling (e.g., Famiglietti and Wood 1994; Peters-Lidard et al. 1997) and
field campaigns (e.g., Jackson et al. 1999). This domain has been used previously in atmospherically coupled (Maxwell et al. 2007) and uncoupled (Kollet and Maxwell 2008b,a; Maxwell and Kollet 2008a) model simulations. The goals of these tests are to quantify the impact of model spinup and coupled execution in short-term (36 h) atmospheric simulations. For comparison to other physical processes represented in WRF, microphysics options are also varied. Three microphysics options and two initialization options were used for the coupled (PF.WRF) and uncoupled (WRF) simulations for a total of 12 cases all of which are listed in Table 1.

1) OFFLINE SPINUP PROCESS

A challenge in coupled simulations lies in initializing the land surface conditions, namely, pressure (or soil moisture) and temperature. If observations of soil moisture, subsurface pressure-head, and soil temperature are available, they may be interpolated to fill the domain. Because of data scarcity, often a spinup process is used instead. During a spinup, a single (water) year of atmospheric forcing (e.g., solar radiation, wind, precipitation, humidity, and pressure) is used to repeatedly provide near-surface conditions for a land surface model over multiple years. This process is repeated until the yearly difference in the water and energy balances drop below a threshold of less than $10^{-6}$.

The soil moutes and soil temperatures of WRF and PF.WRF were initialized using the offline spinup approach described above. As discussed previously, the recent literature has shown that initialization of soil moisture fields (i.e., the memory of the soil moisture to previous atmospheric events) has an important effect on prediction. Because of this, we desired a spinup process that was different, yet consistent, for the uncoupled WRF and the coupled PF.WRF models: a spinup without groundwater or lateral flow for WRF and with these processes for PF.WRF. To achieve this goal, two models were spun up: the CLM (Dai et al. 2001), to initialize the WRF model, and ParFlow with CLM integrated (PF.CLM; Kollet and Maxwell 2008b), to initialize the PF.WRF model. The land surface physics, energy balances, and vegetation specifications are completely equivalent in the two models. The key difference between them is in the surface and subsurface hydrology, with PF.CLM having a more advanced description of these physical processes. One water year (1998) of atmospheric forcing data derived from the North American Regional Reanalysis (NARR; Mesinger et al. 2006) was used to repeatedly force the land surface model. This water year was chosen because an existing spinup and validation (by comparing to observations from that watershed) of the offline PF.CLM model (Kollet and Maxwell 2008a) and complete details may be found in that study. Both models were set up over the same domain (45 km × 32 km at 1 km × 1 km horizontal resolution), with the same land and soil cover as described in Kollet and Maxwell (2008a). The land cover and soil characteristics used for these simulations were adjusted to match those in Maxwell et al. (2007) and therefore do not match those characteristics provided by the standard WRF datasets.

The results of the spinup process may be seen in Fig. 9, which plots the instantaneous soil moisture and temperature fields at the beginning of the simulation. This figure clearly shows the differences in soil moisture and temperature between CLM and PF.CLM and highlights the effects of lateral flow during the spinup process. The river valley in the PF.CLM simulation is fully saturated, leading to generally cooler temperatures. Additionally, the hilltop in the PF.CLM spinup is considerably dryer. Both of these shifts are due to the explicit representation of lateral, subsurface flow that converges in the river valleys providing water that alters land surface processes. The CLM simulation shows variability due only to differences in land-cover type and generally shows much less spatial variability than the PF.CLM simulations. These results are quite similar to previous studies (Kollet and Maxwell 2008a; Maxwell and Kollet 2008a; Maxwell et al. 2007).
2) HYDROLOGIC IMPACTS

As discussed in section 3a, the PF.WRF model calculates infiltration and runoff using the integrated solution of Eqs. (A1), (A2), and (A5). Figure 10 plots total domain outflow, or runoff that leaves the domain boundaries, and the total precipitation $P$ minus evaporation combined with transpiration—so-called evapotranspiration (ET, i.e., $P - ET$) at the land surface for the PF.WRF simulations. Note that $P - ET$ may be formally defined as $q_s - q_r$ in Eqs. (A7)–(A8). This figure shows that PF.WRF routes rainfall to runoff for three different microphysics parameterizations and the two temperature initializations. The total domain runoff for the NARR temperature initialization cases and three microphysics options appears in Fig. 10a. In this figure we see the influence of the microphysics parameterizations on runoff: each of the three cases produces different spatial rainfall patterns that then generate different amounts of runoff and infiltration, resulting in different hydrographs.

Recall that ParFlow routes water across the ground surface and through the subsurface as a function of calculated pressure head distributions and that the results shown in Fig. 10 are unique to PF.WRF. In Fig. 10a we see that the total outflow is quite different between cases (i.e., microphysics options). These differences are due to variability in the total amount of precipitation as well as its spatial distribution and timing. Each of the

![Figure 7](image_url)
three microphysics cases (the gray, blue, and black curves) produces similar values for evapotranspiration during the first 5 h of simulation time (shown as the negative portion of the $P - ET$ curve in Fig. 10a) when $P$ is zero and total outflow is small. Each of the three microphysics cases also produces similar times for the onset of rainfall, around noon of day one as seen by the large, positive trends in $P - ET$ when $P$ is much larger than ET. The large differences in outflow between microphysics options are created by large differences in the predicted precipitation rates.

In Fig. 10b we see the runoff generated from three microphysics parameterizations when initialized using the temperature from the spinup. We also see large differences in both predicted rainfall and subsequent outflow between Figs. 10a,b, corresponding to the differences in temperature initialization. For example, of the three microphysics options, case clmQ_mp1 has the greatest rainfall amount at 40.2 mm over the column with a corresponding 7.4 mm of outflow, while case clmTQ_mp1 has the least with almost half the rainfall total with 24.8 mm and 1.4 mm of outflow. This indicates that, for these semi-idealized simulations, the temperature initialization is as important as the microphysics parameterization in determining rainfall amount. The temperature at the bottom level in the Noah model is held constant at the initialized value during the simulation. This boundary condition will change the energy fluxes at the land surface, as has been recently explored (Kollet et al. 2009).

Figure 10 also shows a strong nonlinearity between rainfall and outflow totals. This is due in part to the spatial distribution of rainfall. For example, rain that falls on the

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hilltop areas would produce less runoff than rain that falls farther down the hillslopes or in the valleys since the water table is closer to the ground surface in the valleys. Rainfall infiltration in these regions results in greater increases in subsurface pressures—and thus streamflow—than on the drier hilltops. These nonlinearities are also due to land surface feedbacks. These feedbacks are illustrated in the idealized simulation results described in section 3a and are shown in Figs. 4 and 5. In the same way that lateral flow in the coupled model creates land fluxes in locations other than directly under clouds that produce precipitation in the idealized case, similar feedbacks will also occur in the Little Washita simulations. These feedbacks can further enhance differences in microphysics parameterization, as seen by the strong divergence in the $P - ET$ curves in Fig. 10, resulting in an additional nonlinearity in rainfall–runoff response.

3) ATMOSPHERIC BOUNDARY LAYER IMPACTS

The second set of results demonstrates the relevance of this coupled model for boundary layer applications such as wind-energy forecasting or transport and dispersion modeling. It is expected that changes in surface soil moisture afforded by the coupled PF.WRF model would impact hydrological parameters as discussed above. It is somewhat surprising to see the impact on low-level winds over short-time-scale (36 h) simulations. Both $a$, a measure of wind shear, and the wind speed at 40 m above the surface are investigated to compare coupled and uncoupled simulations.
A power-law relationship is often assumed for winds in the lower boundary layer (Elliott et al. 1987):

\[ U(z) = U_R \left( \frac{z}{z_R} \right)^\alpha, \]  

where \( U \) is the mean horizontal wind speed (m s\(^{-1}\)) at height \( z \) (m), and \( U_R \) is the mean horizontal wind speed (m s\(^{-1}\)) at reference height \( z_R \) (m). In Eq. (1) the reference height \( z_R \) is by convention closer to the ground than height \( z \). An \( \alpha \)-value of 0 indicates a perfectly well-mixed wind profile; \( \alpha > 0 \) indicates that winds aloft are stronger than winds near the surface, which is the usual case, while \( \alpha < 0 \) indicates that winds aloft are weaker than winds near the surface, which can happen in the case of shallow downslope drainage flows that frequently happen overnight in regions of complex terrain, for instance. An \( \alpha \) value of 1/7 (0.144) is commonly used to extrapolate the wind speed taken at a reference height on the meteorological tower to greater heights within a turbine-blade-swept area, assuming a neutral boundary layer. Although this extrapolation is common, it is also widely recognized that boundary layer winds are more complex than predicted by the power law. For the data:

**Fig. 10.** Plot of \( P - ET \) (solid lines, left vertical axis) and outflow (dotted lines, right vertical axis) fluxes (m\(^3\) h\(^{-1}\)) between WRF and ParFlow for each of the simulated PF.WRF cases and the corresponding runoff that exits the ParFlow simulation domain. Note cases are grouped by temperature initialization as (a) NARR and (b) PF.CLM spinup, with each microphysics option plotted as well as indicated in the figure for both \( P - ET \) and outflow.
presented here, height $z$ is defined as $\sim 120$ m above the surface, near the top of the rotor disk on a modern turbine, while the reference height $z_R$ is $\sim 20$ m above the surface, consistent with the height of wind speed sensors used for extrapolation to the hub height. These levels correspond to the first and third levels above the surface in the simulations.

Comparison of six WRF-alone and six PF.WRF simulations for the same time period (with three different choices of cloud microphysics schemes and two different surface spinup choices) appear in Fig. 11. In this figure we see that both the WRF-alone (left, Fig. 11a) and PF.WRF (right, Fig. 11b) simulations exhibit behavior consistent with expectations for a diurnal cycle. The first 6 h of the simulation, during the initial growth of a convective boundary layer, show variability that is consistent expectations for model spinup, but also likely includes some effect of turbulent mixing forced by surface heating. By hour 12, when the surface heat flux has changed sign and the surface starts to cool, $\alpha$ increases as winds above the surface decouple from the surface, consistent with expectations for a nocturnal boundary layer. During the nighttime hours, hours 14–22, $\alpha$ values continue to increase, indicating that winds at $\sim 120$-m elevation continue to decouple from those nearer to the surface. As low-level jets are frequently observed in this region (Lundquist and Mirocha 2008; Whiteman et al. 1997; Zhong et al. 1996), the acceleration of flow aloft could be interpreted as evidence of low-level jet formation; however, as the idealization of the test problem removed synoptic-scale forcing, such a conclusion cannot be verified. The following morning, surface heating generates convective plumes that reestablish the coupling between the lower-level winds and the surface during the daytime (hours 26–36), which exhibit little variability amongst the simulations, as would be expected during a convective well-mixed boundary layer.

Some notable differences exist between the sets of WRF-alone (left, Fig. 11a) and PF.WRF (right, Fig. 11b) simulations. Differences between the domain averaged WRF-alone averages of the ensemble of all spinups and microphysics and PF.WRF, all spinups and all microphysics, appear in Fig. 11c. The horizontal line represents $\alpha = 0.144$ or $\frac{1}{7}$, the most commonly used value. This value rarely appeared during any of our simulations, coupled or otherwise.

During the night (hours 14–22), the PF.WRF simulations, on average, exhibit both higher and more variable $\alpha$ values than the WRF simulations. The maximum difference between WRF and PF.WRF occurs between 16 and 18 h into the simulation, halfway through the night. The higher alpha values predicted by the PF.WRF simulations indicate either an acceleration of the PF.WRF winds aloft, or a deceleration of the PF.WRF winds very close to the surface, relative to the WRF alone simulations. The wind speeds at approximately 40 m, shown in Fig. 12, indicate generally lower wind speeds near the surface on the PF.WRF simulations relative to the WRF simulations. The lower wind speeds near the surface suggest that the increased spatial heterogeneity in soil moisture and temperature introduced by the PF.WRF model promotes stronger coupling of the near-surface flow with the surface.

The wind speeds shown in Fig. 12 afford additional insights into differences between the WRF-alone and PF.WRF simulations. A first daytime wind speed maximum can be seen in the early evening (around hour 10). At night (hours 14–22) winds near the surface tend to decrease, with a subsequent increase in the morning (by hour 26). Different physical processes are at work at different points in the diurnal cycle. During the daytime periods, convective heating from the surface dominates the flow; the convective heating is strongly coupled to the surface characteristics. The surface soil temperatures for WRF-alone simulations are significantly higher ($\sim 5$ K) on the first morning (see Fig. 9), which generates stronger convective plumes and therefore inducing stronger horizontal advection or winds in the WRF-alone open-boundary-condition simulations. At night, the domain and ensemble-averaged differences in 40-m winds (Fig. 12c) between the WRF and PF.WRF lessen or approach zero. At all times of day, the PF.WRF winds encounter a more heterogeneous surface, and therefore tend to exhibit lower spatial and temporal correlations.

4. Conclusions and future directions

Here we present improvements to the model physics for the community-based WRF simulation platform. These enhancements include fully integrated, lateral overland and subsurface flow, in addition to complete treatment of flow in the subsurface via solution of the three-dimensional Richards equation. We demonstrate, using an idealized simulation designed to strongly force the integration, 1) that this model balances water extremely well between terrestrial and atmospheric systems, and 2) that this model’s ability to include more precise runoff mechanisms and lateral water flow will change the spatial pattern of land surface fluxes. Additionally, we use a number of semi-idealized simulations using a real watershed to demonstrate how the coupled model may be used in rainfall–runoff predictions for water resources applications and in wind-energy forecasting. We see several significant differences between coupled and uncoupled model simulations, across a range of microphysics parameterization choices, in the magnitude, timing, and
spatial distributions of rainfall and runoff, and in atmospheric parameters of interest to wind-power production, including low-level wind speeds and vertical shear.

We reach the following specific conclusions in this work:

1) As shown by the idealized simulation, the coupled model balances water very accurately across the

![Fig. 11. Plots of $\alpha$ for (top) valley, (middle) hilltop, and (bottom) domain averaged for (a) WRF and (b) PF.WRF simulations. (c) Plots of differences in $\alpha$ between WRF and PF.WRF averaged across case.](image)
combined terrestrial and atmospheric system and the overall spatial pattern of land surface moisture and energy fluxes was shown to change as a result of including more accurate runoff mechanisms and deeper, lateral subsurface flows;

2) The time step of ParFlow may be subcycled relative to WRF; for the test problem studied, subcycling ParFlow relative to WRF at an interval of 12 increased the overall computational efficiency of PF.WRF with little change in overall system behavior; more
importantly, we outline a general strategy for how the subcycling could be applied to coupled problems;

3) As shown by the more substantive, semi-idealized problem, the coupled model may be used to develop rainfall–runoff predictions for water resource applications as well as to interrogate atmospheric boundary layer dynamics for wind-energy forecast applications. Differences between coupled (PF.WRF) and uncoupled (WRF) model simulations, across a range of microphysics parameterization choices, were evident, especially as they affected wind shear and lower atmosphere wind velocities.

Future work will include additional investigation of the numerical methods, validation of the coupled model, and further exploration of feedbacks between the subsurface and atmosphere for synoptic cases. We plan a thorough analysis of the parameterizations expressing the dependences of the subsurface, surface, and atmosphere on each other with the goals of providing definitive guidance on frequency of subcycling and determining whether tightening the coupling between the regimes may lead to more accurate simulations. Additionally, we plan to explore synoptic simulations to understand the regimes in which the PF.WRF coupled model does and does not produce differences relative to the WRF model and to further validate the coupled model. Given recent work that successfully scaled the ParFlow model out to almost $10^{10}$ unknowns using greater than 16-K processors (Kollet et al. 2010) the application of this coupled model to very large scales (e.g., continental) with very high resolution (e.g., $\sim$1 km) is within current capability. Though some data gaps still exist, particularly in the subsurface, these recent developments represent a very exciting opportunity to extend the boundaries of current coupled hydrologic simulation.

The coupled PF.WRF model extends the applicability of the WRF model platform to many new and important arenas. In addition to the shorter-term hydrological and wind-power prediction applications demonstrated herein, coupled simulations forced with climate simulation data could assist longer-term water resources planning as well as prediction of future wind-energy resources. Overall, the coupled PF.WRF model will provide many new avenues for more robust application of the WRF platform. Such applications can include more complete validation studies of the coupled model with the appropriate observations and might include more substantive, integrated simulations of climate downscaling for water resources management, flood prediction, and wind-energy forecasting.

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APPENDIX

Governing Equations for Surface and Subsurface Water Flow and Evapotranspiration

The PF.WRF model couples lateral surface and subsurface flow to the WRF platform through the Noah LSM within WRF. This coupling creates differences within both the energy and water balance formulations of the LSM (Kollet and Maxwell 2008a; Maxwell et al. 2007)—discussed in detail in (Kollet et al. 2009). Here we present only the primary hydrologic processes to better formalize the coupled relationships and to mathematically illustrate the interdependence between shallow soil moisture and evapotranspiration.

Figure A1 demonstrates the coupling of the two systems. ParFlow and WRF each use structured grids and the land surface representations used by each model must be mapped onto these grids. As shown in Fig. A1, the four Noah grid cells beneath the surface ($k_{Noah}$) must coincide with the first four nodes of the ParFlow grid $k$. This grid matching provides the interface between the two codes. Details on the coupled terms in the balance equations are provided below.

While complete details of the solution approach that ParFlow uses to solve for coupled surface–subsurface flow are given in (Kollet and Maxwell 2006) a brief summary of the equations is presented here. Fundamentally, ParFlow solves the Richards equation for variably saturated flow (Richards 1931) in three spatial dimensions given as

$$ S_s S_w \frac{\partial h}{\partial t} + \phi \frac{\partial S_w(h)}{\partial t} = \nabla \cdot q + q_s(x, z), \quad (A1) $$

where

$$ q = \phi S_w v = -K_s(x)k_r(h) \cdot \nabla (h - z). \quad (A2) $$

In these expressions, $h$ is the pressure head [unit is defined as length (L)], $z$ is the vertical coordinate (L), $K_s(x)$ is the
saturated hydraulic conductivity tensor (length per unit time), \( k_r \) is the relative permeability (-), \( S_p \) is the specific storage coefficient (L\(^{-2}\)), \( \phi \) is the porosity (-), \( S_w \) is the relative saturation (-), and \( q_r \) is a general source–sink term that represents transpiration, wells, and other fluxes (length per unit time). The subsurface flow velocity is denoted by \( y \) (length per unit time) and the specific volumetric (Darcy) flux is denoted by \( q \) (length per unit time).

The van Genuchten (1980) relationships are used to describe the relative saturation and permeability functions:

\[
S_w(h) = \frac{s_{\text{sat}} - s_{\text{res}}}{[1 + (\alpha h)^n]^{1/(1-n)}} + s_{\text{res}} \quad \text{and} \quad (A3)
\]

\[
k_r(h) = \left\{ 1 - \frac{(\alpha h)^{n-1}}{[1 + (\alpha h)^n]^{1-1/(1-n)}} \right\}^{1/(1-n)} \quad \text{and} \quad (A4)
\]

where \( \alpha \) (L\(^{-1}\)) and \( n \) (-) are soil parameters, the values \( s_{\text{sat}} \) (-) is the relative saturated water content and the value \( s_{\text{res}} \) (-) is the relative residual saturation.

Overland flow is represented in ParFlow by the two-dimensional kinematic wave equation included as the overland flow boundary condition resulting from application of continuity conditions for pressure and flux:

\[
k \cdot [ - K_s(x) k_r \cdot V(h - z) ] = \frac{\partial [h,0]}{\partial t} - V \cdot \partial [h,0] \mathbf{v}^{\text{sw}} = q_r(x).
\]

where \( \mathbf{v}^{\text{sw}} \) is the two-dimensional, depth-averaged surface water velocity (length per unit time); \( h \) is the surface ponding depth (L), if \( h > 0 \); \( q_r(x) \) is a general source–sink (e.g., rainfall, ET) rate (length per unit time); and \( k \) is the unit vector in the vertical. Note that \( ||h, 0|| \) indicates the greater value of the two quantities, that the lhs of Eq. (A5) represents vertical fluxes (e.g., in–exfiltration) across the land surface boundary and that the overland flow condition assumes that pressure \( h \) represents both surface pressure and the ponding depth at the ground surface under saturated conditions (Kollet and Maxwell 2006). Equation (A5) represents the connection between surface and subsurface flow processes. At any time in which the pressure head at the land surface (as shown in Fig. A1) is greater than zero, corresponding to a saturation of one as shown in Eq. (A3), the two terms representing the storage and continuity of water become active. This can be due to either excess saturation or excess infiltration and allows fully coupled routing of water and subsurface flow. Complete details on the formulation and verification of this approach are provided in Kollet and Maxwell (2006), application at the watershed scale as well as comparison to observations are provided in Kollet and Maxwell (2008a), and detailed exploration of this approach’s ability to represent very tightly coupled overland flow and heterogeneity are given in Maxwell and Kollet (2008b).

Manning’s equation is used to establish a flow depth–discharge relationship, the \( \mathbf{v}^{\text{sw}} \) in Eq. (A5), as follows:

\[
\mathbf{v}_x^{\text{sw}} = \frac{\sqrt{S_{f,x}}}{n} h^{2/3} \quad \text{and} \quad \mathbf{v}_y^{\text{sw}} = \frac{\sqrt{S_{f,y}}}{n} h^{2/3}, \quad (A6)
\]

where \( S_{f,x} \) (L) is the friction slope, \( i \) stands for the \( x \) and \( y \) direction, and \( n \) (time per cube root of length) is Manning’s coefficient.
For the groundwater flow solution, ParFlow employs an implicit backward Euler scheme in time, and a cell-centered finite-difference scheme in space. At the cell interfaces, the harmonic averages of the saturated hydraulic conductivities and a one-point upstream weighting of the relative permeabilities are used. For the overland flow component, ParFlow uses an upwind finite-volume scheme in space and an implicit backward Euler scheme in time.

As shown in Fig. A1, the Noah LSM is in communication with ParFlow over the top four soil layers below the ground surface. Note that these four layers are not constant (i.e., flat) in the vertical index $k$, as the ground surface elevation varies within the ParFlow model domain. The Noah model passes three water fluxes to ParFlow at every time step: precipitation throughfall and canopy drip, $P(x)$ (length per unit time); direct evaporation from the soil, $E(x)$ (length per unit time); and plant transpiration, $T(x, z)$ (length per unit time). The first two fluxes are applied to the top soil layer ($k_{Noah} = 1$) at the ground surface through the boundary source–sink term, $q_r(x)$, in Eq. (A5). The boundary condition source is then formulated as

$$q_r(x) = P(x) - E(x). \quad \text{(A7)}$$

The transpiration flux is applied over the root zone, which may encompass cells $k_{Noah} = 2$–4 below the ground surface, depending on land-cover type. This flux is applied to the general source–sink term, $q_r(x)$, in Eq. (A1) as follows:

$$q_r(x, z) = T(x, z). \quad \text{(A8)}$$

In both the evaporation and transpiration, the potential evaporation, $E_{pot}$ (length per unit time), is calculated based on atmospheric conditions as provided by the WRF boundary layer scheme (see, e.g., Chen and Dudhia 2001a; Ek et al. 2003). The actual evaporation and transpiration based upon the potential evaporation is modified according to local soil moisture and plant resistances. The evaporation is calculated as follows (Chen et al. 1996; Ek et al. 2003):

$$E(x) = F_{\text{fx}}(1 - f_{\text{veg}})E_{\text{pot}}, \quad \text{(A9)}$$

where $f_{\text{veg}}$ is the fraction of vegetation covering that particular tile; $f_{\text{fx}}$ is an empirical coefficient and the resistance of vapor flux to local soil moisture, $F$, is parameterized as (Ek et al. 2003):

$$F = \left( \frac{\phi S_w - \phi S_{\text{res}}}{\phi - \phi S_{\text{res}}} \right). \quad \text{(A10)}$$

Note that the functional form of $F$ is linear for $f_{\text{fx}} = 1$ and nonlinear for other values ($f_{\text{fx}} = 2$ is used in the simulations presented in this work). Here $F$ is the parameterization of the interdependence between evaporation and shallow soil moisture and provides one of the connections between ParFlow and Noah, and thus WRF.

The plant transpiration is calculated as follows (Chen et al. 1996):

$$T(x, z) = G(z)C_{\text{plant}}f_{\text{veg}}E_{\text{pot}}, \quad \text{(A11)}$$

where $C_{\text{plant}}$ is a constant coefficient between 0 and 1, and is dependent on vegetation species (Chen et al. 1996; Pan and Marht 1987). The $G(z)$ function represents soil moisture stress and takes the form (Chen and Dudhia 2001b; Chen et al. 1996; Pan and Marht 1987):

$$G(z) = \frac{(\phi S_{\text{ref}} - \phi S_{\text{wilt}})\Delta z_{k_{Noah}}}{(\phi S_{\text{ref}} - \phi S_{\text{wilt}})z_{\text{root}}} \left| \frac{n_{\text{root}}}{k_{Noah} = 2} \right|, \quad \text{(A12)}$$

where $n_{\text{root}}$ is the number of soil layers over which the root zone extends and is dependent upon plant type, $S_{\text{wilt}}$ is the saturation at which plants wilt, $S_{\text{ref}}$ is a reference saturation (often taken to be the field capacity), $\Delta z_{k_{Noah}}(L)$ is the thickness of each soil layer, and $z_{\text{root}}(L)$ is the depth of the bottom of the root zone. The $G(z)$ provides the other primary link between ParFlow, Noah, and WRF. As mentioned previously, the evapotranspiration fluxes also appear in the land–energy balance as the latent heat flux. The soil moisture values provided by ParFlow to Noah also influence the diffusion of heat in the subsurface. This influence provides a connection between surface and subsurface hydrology and the land–energy budget.

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