HydroBlocks: A Field-scale Resolving Land Surface Model for Application Over Continental Extents

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Key Points:

- Development and implementation of a field-scale resolving land surface model.
- A novel clustering algorithm is used to derive hydrologic response units from high-resolution environmental data.
- The model is run over the Little Washita watershed and validated using available in-situ soil moisture observations.
- 1000 hydrologic response units are sufficient to robustly model field-scale spatial heterogeneity over the Little Washita watershed.

Abstract

Land surface spatial heterogeneity plays a significant role in the water, energy, and carbon cycles over a range of temporal and spatial scales. Until now, the representation of this spatial heterogeneity in land surface models has been limited to over simplistic schemes due to computation and environmental data limitations. This study introduces HydroBlocks—a novel land surface model that represents field-scale spatial heterogeneity of land surface processes through interacting hydrologic response units (HRUs). HydroBlocks is a coupling between the Noah-MP land surface model and the Dynamic TOPMODEL hydrologic model. The HRUs are defined by clustering proxies of the drivers of spatial heterogeneity using high-resolution land data. The clustering mechanism allows for each HRU's results to be mapped out in space, facilitating field-scale application and validation. The Little Washita watershed in the United States is used to assess HydroBlocks' performance and added benefit from traditional land surface models. A comparison between the semi-distributed and fully distributed versions of the model suggests that using 1000 HRUs is sufficient to accurately approximate the fully distributed solution. A preliminary evaluation of model performance using available in-situ soil moisture observations suggests that HydroBlocks is generally able to reproduce the observed spatial and temporal dynamics of soil moisture. Model performance deficiencies can be primarily attributed to parameter uncertainty. HydroBlocks' ability to explicitly resolve field-scale spatial heterogeneity while only requiring an increase in computation of one to two orders of magnitude when compared to existing land surface models is encouraging—ensemble field-scale land surface modeling over continental extents is now possible.

Keywords: Land surface modeling; Spatial heterogeneity; Hydrologic similarity

1. Introduction

The land surface plays a pivotal role in the Earth system over a range of spatial and temporal scales. It absorbs and releases greenhouse gases, emits aerosols, and interacts with the atmosphere and hydrosphere through the exchange of water, energy, and momentum [*Heimann and Reichstein*, 2008]. As a result, the land surface components and processes have a profound impact on the global climate, food and energy production, freshwater resources, and biodiversity [*Rodriguez-Iturbe and Porporato*, 2004; *Seneviratne et al.*, 2006; *Betts*, 2009; *Wood et al.*, 2011; *Sheffield et al.*, 2014]. These are the primary reasons behind the continued development and use of land surface models—to more fully characterize the land surface's inner-dynamics and to understand how it interacts and co-evolves with the Earth system [*Liang et al.*, 1994; *Ek et al.*, 2003b; *Shevliakova et al.*, 2009; *Niu et al.*, 2011; *Oleson et al.*, 2013].

Current land surface models simulate the global terrestrial water, energy, and biogeochemical cycles using grid sizes ranging from 10-100 km—orders of magnitude coarser than the characteristic spatial scales of many critical land surface processes (e.g., runoff generation) [*Beven et al.*, 2015]. To address this discrepancy, land surface models use parameterizations to represent sub-grid spatial heterogeneity in coarse scale models [*Beven and Kirby*, 1979; *Sivapalan et al.*, 1987; *Liang et al.*, 1994; *Avissar*, 1995]. However, existing schemes continue to oversimplify the role of the fine-scale physical environment (topography, soil properties, parent material, and microclimates) and largely ignore sub-grid spatial interactions among the different land surface components and processes [*Cavender-Bares et al.*, 2004; *Katul et al.*, 2007; *Manzoni and Porporato*, 2009; *Mitchell et al.*, 2012; *Porporato and

Rodriguez-Iturbe, 2013; *Chaney et al.*, 2014; *Clark et al.*, 2015b].

Recognizing the role of fine-scale spatial heterogeneity in land surface processes, the land modeling community is revisiting how spatial heterogeneity is represented in land surface models by capitalizing on existing high-resolution global landscape datasets, high performance computing, and decades of research in hydrology, ecology, geomorphology, and soil science [*Wood et al.*, 2011; *Bierkens et al.*, 2014]. A promising path forward is to use process-based models that aim to fully resolve the subsurface and surface processes [*Kollet and Maxwell*, 2006; *Camporese et al.*, 2010; *Brunner and Simmons*, 2012; *Maxwell et al.*, 2014]. In theory, if these models are run at sufficiently high spatial resolutions, there is a reduced need to parameterize sub-grid spatial heterogeneity. However, compared to classic land surface models, these models require multiple orders of magnitude increase in computation. This is especially relevant given that for operational use, models need to be able to efficiently handle ensemble frameworks to account for the unavoidable input, parameter, and structural uncertainties.

A more immediate solution appears to be between the existing oversimplified parameterizations of spatial heterogeneity in land surface models and the fully distributed process-based models. One emerging approach is to use hydrologic response units—derived from available field-scale landscape information—to formalize and expand existing sub-grid tiling schemes in land models [*Subin et al.*, 2014; *Clark et al.*, 2015a]. A hydrologic response unit (HRU) is defined as the points in a watershed (or macroscale grid cell) with similar characteristics (e.g., topography, soil, and land cover); the points that define the HRU do not need to be spatially contiguous. HRUs are analogous to the tiles in the mosaic schemes in existing land surface models (e.g., [*Oleson et al.*, 2013]). Assuming the subsurface and surface connections between HRUs are defined appropriately, this modeling approach can encompass lumped models (one HRU), semi-distributed models (multiple HRUs), and fully distributed models (one HRU per grid cell). The fully distributed model can be used to define a reduced number of HRUs to accurately represent the fine-scale spatial patterns and interactions of the land surface components and processes in the semi-distributed model. This allows for a robust representation of fine-scale spatial heterogeneity in land surface models while ensuring computational efficiency for use in operational numerical weather prediction and climate modeling and to allow for ensemble frameworks to account for parameter, input, and structural uncertainty.

This study introduces HydroBlocks[1], a land surface model that capitalizes on hydrologic response units to explicitly represent field-scale land surface spatial heterogeneity. HydroBlocks couples Noah-MP, a vertical 1-dimensional (1-d) land surface model that acts independently on each response unit, to Dynamic TOPMODEL, a hydrologic model designed to link the hydrologic response units via a subsurface kinematic wave. The model is developed, implemented, and validated over the Little Washita watershed in Oklahoma, USA. The K-means clustering algorithm is used to cluster available land data to define the HRUs. The number of HRUs required to approximate the spatial heterogeneity of the fully distributed solution is assessed. Finally, HydroBlocks' two main advantages (computational efficiency and its ability to

[1] In earlier versions, the model was known as "HydroBloks". The model name has been changed to "HydroBlocks" to avoid confusion in spelling.

approximate the fully distributed solution) are used to run a Latin Hypercube Sample ensemble to assess the role of model parameter uncertainty and determine the model's ability to reproduce available in-situ soil moisture observations.

2. Land Surface Model: HydroBlocks

This section presents the HydroBlocks land surface model. It is divided into 1) an overview of NoahMP, the 1-d vertical land surface model that acts independently on each hydrologic response unit (HRU); 2) an overview of Dynamic TOPMODEL, the hydrologic model that connects the HRUs via a kinematic subsurface wave; 3) the coupling between Noah-MP and Dynamic TOPMODEL. Figure 1 illustrates how HydroBlocks represents spatial heterogeneity and how each hydrologic response unit interacts.

2.1 Noah-MP

Noah-MP is a process-rich 1-d vertical land surface model that improves on the widely used Noah model [*Ek et al.*, 2003a]. The primary reasons it was chosen for HydroBlocks are: the model represents the primary vertical processes that control the water, energy, and carbon cycles at the land surface, its multi-physics options makes it amenable to tailoring to local needs and data availability, the simplicity of the code makes it readily available for coupling to a hydrologic model, and its use in operational weather forecasting research [*Dudhia*, 2014] ensures it will continue to undergo development and improvements in the future. This section offers a brief overview of the model. For a comprehensive overview see [*Niu et al.*, 2011].

Noah-MP is a complex, physically based model that captures the primary vertical subsurface and surface land processes. It includes an explicit representation of the vegetation canopy layer to separately compute the canopy and surface temperatures; this allows for the representation of the differences in energy fluxes over vegetation and bare ground. A modified two-stream radiation transfer scheme considers vegetation canopy gaps to compute fractions of sunlit and shaded leaves and their absorbed solar radiation [*Yang and Friedl*, 2003]. The controls of atmospheric and soil moisture conditions on transpiration rates can be modeled by choosing from a Jarvis-type or Ball-Berry type scheme to relate stomatal resistance to photosynthesis of sunlit and shaded leaves [*Ball et al.*, 1987; *Jacquemin and Noilhan*, 1990; *Collatz et al.*, 1991]. There is also a dynamic vegetation module for short-term prediction of vegetation condition (e.g., LAI) [*Dickinson et al.*, 1998]. A three-layer snow model is implemented that enables percolation, retention, and refreezing of melt water within the snowpack [*Niu and Yang*, 2004].

2.2 Dynamic TOPMODEL

Dynamic TOPMODEL is a semi-distributed hydrologic model that extends the well-established TOPMODEL [*Beven and Freer*, 2001; *Metcalfe et al.*, 2015]. It aims to maintain its predecessor's computational efficiency achieved through grouping of landscape areas of hydrologic similarity into hydrologic response units (HRUs), while relaxing key assumptions that limit TOPMODEL's application to frequently wetted catchments displaying moderate topography. The primary difference is the replacement of the assumption of a succession of quasi-steady-state water table configurations with a kinematic wave routing algorithm to route subsurface flow between HRUs. This allows a more flexible grouping, or discretization, strategy that can take into account any number of landscape layers considered to provide relevant information on the hydrological characteristics of areas within the catchment. In addition, the introduction of a maximum soil moisture deficit parameter S_{max} allows the simulation of variable contributing areas apparent when hillslope connectivity is broken as upslope areas start to dry out [*Barling et al.*, 1994; *McGuire and McDonnell*, 2010]. When the deficit in any unit reaches S_{max}, flow from that unit ceases.

As in the original TOPMODEL, inter-cell slopes determined from gridded topographic data are assumed to be a reasonable approximation for the local hydraulic gradient [*Beven*, 2012]. Once the HRUs have been defined, the proportions of flow between the cells comprising each HRU are determined. The flow fractions are then aggregated into a flow matrix of weights **W** (*n* by *n*) that encapsulates the proportions of flow between HRUs. The i^{th} row in **W** defines how the HRU i's total output, $Q_{out}{}^{i}$, is distributed to surrounding response units, including itself. The total input, $Q_{in}{}^{i}$ is the weighted sum, using the corresponding entries in **W**, of all the upstream outputs, $Q_{out}{}^{j}$. This can be readily generalized to an arbitrary number *n* of response units and formulated as a simple vector-matrix multiplication. The vector of size *n* of all response units' input, $\mathbf{Q_{in}}$, can be calculated by the product of the vector of size *n* of all response units' output, $\mathbf{Q_{out}}$, and the *n* by *n* matrix of weights, **W**.

$$\mathbf{Q_{in}} = [Q_{in}^{1} \quad Q_{in}^{2} \quad \dots \quad Q_{in}^{n}];\ \mathbf{Q_{out}} = [Q_{out}^{1} \quad Q_{out}^{2} \quad \dots \quad Q_{out}^{n}];\ \mathbf{W} = \begin{bmatrix} w_{11} & \cdots & w_{1n} \\ \vdots & \ddots & \vdots \\ w_{n1} & \cdots & w_{nn} \end{bmatrix}$$

$$\mathbf{Q_{in}} = \mathbf{Q_{out}}\mathbf{W}$$

The HRUs are assumed to be spatially homogenous. This allows us to define the specific input into each unit as $q_{in}^{i} = Q_{in}^{i}/b_i$ and the specific output as $q_{out}^{i} = Q_{out}^{i}/b_i$. Where b_i is the sum of the width of all grid cells that belong to HRU *i*.

Following [*Beven and Freer*, 2001]), the subsurface flow $q_{out,t}^{i}$ is solved at each time step via a four-point implicit finite volume solution to the subsurface kinematic wave equation:

$$\frac{\partial q}{\partial t} = c\frac{\partial q}{\partial x} - cr$$

$$q_{out,t}^{i} = q_{out,t-1}^{i} + \Delta t \omega c_t^i\left(\frac{q_{out,t}^{i} - q_{in,t}^{i}}{\Delta x} - r_t^i\right) + \Delta t(1-\omega)c_{t-1}^{i}\left(\frac{q_{out,t-1}^{i} - q_{in,t-1}^{i}}{\Delta x} - r_{t-1}^{i}\right)$$

where c is the kinematic wave speed, r is the recharge rate, Δt is the time step, Δx is the effective length of each response unit (i.e., grid size), and ω is a time-weighting parameter (explicit to implicit). Assuming the topographic gradient defines the hydraulic gradient and the transmissivity decays exponentially as a function of soil moisture deficit, the kinematic wave speed c is defined as:

$$c = \frac{1}{m}\frac{dq}{ds} = -\frac{1}{m}T_0 \tan(\beta)\, e^{-\frac{s}{m}}$$

The four-point finite volume solution is used each time step to solve for q_{out} at each response unit via a system of equations – there is one equation per HRU. For a complete overview of the solution see [*Metcalfe et al.*, 2015]. The main difference in this study's implementation is that *c* is fixed at the beginning of each time step making the system of equations linear. Although this study uses this solution to the kinematic wave for subsurface flows only, it can also be used for surface flows.

2.3 Coupling between Noah-MP and Dynamic TOPMODEL

The coupling between the land surface and hydrologic model is sequential. At the beginning of each time step, Noah-MP computes the surface and subsurface vertical fluxes and updates the soil moisture content and water table depth at each HRU. The change in subsurface storage deficit per unit time before and after updating Noah-MP is interpreted as the recharge rate. Dynamic TOPMODEL uses this recharge rate in the four-point implicit scheme to compute each response unit's subsurface input and output flow. At the end of each time step, HydroBlocks uses Dynamic TOPMODEL's change in subsurface storage deficit at each HRU to update the water table depth and soil moisture profile in Noah-MP. The current implementation updates both Noah-MP and Dynamic TOPMODEL using a 15-minute time step.

3. Data

3.1 Study area – Little Washita, Oklahoma

The Little Washita watershed is a 610 km^2 tributary of the Washita River in southwest Oklahoma. It has gently to moderately rolling topography with hills and outcrops. Its soils cover a large range from sands and silts to clays, deep to shallow, and are generally well drained. Its land cover includes rangelands, pastures, forests, croplands, quarries, water bodies, urban development, and highways. The catchment's climate is moist and sub-humid (~750 mm annual rainfall) with much of the annual rainfall occurring during the spring and fall. Summers are long, hot, and dry while winters are short and generally temperate (16^{o} Celsius annual mean temperature) [*Allen and Naney*, 1991; *Cosh et al.*, 2006]. The United States Department of Agriculture's Agricultural Research Service (USDA-ARS) began collecting rainfall data in the Little Washita in 1961. In 1994, the catchment's instrumentation was expanded and upgraded to also include measurements of air and soil temperature, relative humidity, and solar radiation. This study uses the 18 sites that were in operation between 2004 and 2007. Each site has high-quality, hourly soil moisture measurements of the top 5 cm making it suitable to assess HydroBlocks' ability to simulate observed field-scale soil moisture values. Figure 2 shows a map of the Little Washita watershed and its channel network. The locations of the 18 soil moisture probes are also shown.

3.2 Land and meteorological data

To define the hydrologic response units and to run the HydroBlocks model, this study relies on available datasets that cover the entire contiguous United States (CONUS) at varying spatial and temporal resolutions.

Land Cover - The land cover data come from the 2006 National Land Cover Database (NLCD), a 16-class land cover classification at a spatial resolution of 30 meters (~1 arcsec) that spans CONUS [*Fry et al.*, 2011]. The parameters associated with each land cover type come from the North American Land Data Assimilation System (NLDAS-2;[*Xia et al.*, 2012]). The annual NDVI product from the Web-enabled Landsat Data (WELD) is also used. This dataset is a 30-meter composite of Landsat Enhanced Thematic Mapper Plus (ETM+) mosaics from 2002 to 2012 over CONUS [*Roy et al.*, 2010].

Topography - The 1-arcsec USGS National Elevation Data set (NED) provides the elevation information. The NED data set covers CONUS and is created primarily from the USGS 10 and 30 meter digital elevation models, and from higher resolution data sources such as light detection and ranging (lidar), interferometric synthetic aperture radar (ifsar), and high resolution imagery [*Gesch et al.*, 2009]. This study uses the DEM and a series of derived products including flow accumulation area, slope, topographic index, eight directional (d8) flow direction, and the number of immediately upslope grid cells that contribute to a given grid cell (NIU).

Soil Properties - The soil properties come from the recently developed POLARIS dataset [*Chaney et al.*, 2016], a new continental soil dataset that uses random forests to spatially disaggregate and harmonize gridded SSURGO (Soil Survey Geographic) [*Staff*, 2013] to provide a consistent 30-meter soil product over the entire contiguous United States. When possible, for each soil series, the hydraulic properties come directly from the SSURGO database. The remaining soil hydraulic properties (e.g. Brooks-Corey parameters) are derived using a series of pedotransfer functions [*Maidment*, 1993]. The flow direction map calculated from the NED dataset is used with the saturated hydraulic conductivity to calculate each grid cell's mean upslope saturated hydraulic conductivity.

Meteorology - The model's meteorological forcing data is provided by the NLDAS-2 [*Xia et al.*, 2012] data system. This dataset uses observations to bias-correct shortwave radiation and surface meteorology reanalysis at a 1/8 degree spatial resolution and 1 hour temporal resolution. When available the precipitation data come from the NCEP's Stage IV radar product (~4km) [*Lin and Mitchell*, 2005].

4. Methods

4.1 Hydrologic response units: K-means clustering

HydroBlocks relies on hydrologic response units to represent the spatial heterogeneity of the water, energy, and carbon cycles. How these HRUs are defined determines the number of response units necessary to approximate the fully distributed solution. Following [*Newman et al.*, 2014]), the HRUs are constructed by clustering proxies of the drivers of spatial heterogeneity (i.e., topography, land cover, soil properties, and meteorology). This method should suffice to represent the heterogeneity of the system when the chosen proxies are representative of the spatial drivers of the land surface states and fluxes. Table 1 provides a summary of the proxies of the drivers of spatial heterogeneity used in the clustering method.

The k-means clustering algorithm is used to partition the n dimensional proxy space into k clusters (hydrologic response units); n is the number of proxies of spatial heterogeneity. The algorithm defines the clusters by iterating each cluster center's position – the mean of its constituent instances – to minimize the within cluster sum of squares [*MacQueen*, 1967]. Having defined the hydrologic response units, each element on the fully distributed grid is assigned an HRU. The model parameters are then assigned by computing the mean of the parameters of all the grid cells that belong to a given HRU. If the chosen proxies are adequate to represent the spatial heterogeneity of the catchment and the number of HRUs is sufficient, the differences between the HRU mean of the parameters and its corresponding grid cells on the fully distributed grid should be relatively small. An additional advantage to including latitude and longitude in the clustering is that spatial heterogeneity in the meteorology can be directly represented in the model; the mean of all the grid cells that belong to a given HRU on the fully distributed grid is computed at each time step for each meteorological variable. Having assembled the HRUs, Dynamic TOPMODEL's flow matrix **W** is constructed by determining the connections between the HRUs. HydroBlocks can then be run using the defined hydrologic response units and their derived parameters and meteorological inputs.

4.2 Approximating the fully distributed solution

The current implementation of HydroBlocks can be run as a lumped, semi-distributed, or fully distributed model; the number of HRUs and their configuration determines the model type. The lumped model version will use a single HRU for the catchment while the fully distributed model will assign a unique HRU to each grid cell. Since the only difference between the models is the HRU configuration, this can be a useful diagnostic tool for existing tiling schemes in land surface models since it allows for a direct assessment of how well these schemes represent the spatial heterogeneity of the fully distributed solution. It can also provide insight into the drivers of spatial heterogeneity that are not adequately represented in the tiling scheme.

Here a method is presented that formalizes how the number and configuration of tiles or hydrologic response units are defined over the Little Washita. First, the fully distributed version of the HydroBlocks model is run over 2004 at a 30-meter spatial resolution and 15-minute time step to produce a synthetic truth of the spatial heterogeneity of the catchment at each time step. This allows for a straightforward evaluation of the performance of semi-distributed model configurations.

Using the proxies defined in Table 1 and the k-means clustering algorithm, a suite of model configurations are constructed by varying the number of hydrologic response units. The chosen number of HRUs is 2, 5, 10, 20, 50, 100, 200, 500, 1,000, 2,000, 5,000, and 10,000. HydroBlocks is run for each model configuration over 2004 at a 15-minute time step. For each simulation (including the fully distributed model configuration), the spatial mean and spatial standard deviation are computed for a suite of model output variables including top-layer soil moisture, precipitation, sensible heat, latent heat, and runoff. The Kling-Gupta efficiency metric calculated between each variable's semi-distributed model time series (spatial mean and spatial standard deviation) and its corresponding fully distributed model time series is used to assess the performance of each semi-distributed model configuration. The Kling-Gupta Efficiency (KGE) metric [*Gupta et al.*, 2009], as shown below, combines linear correlation ρ, standard deviation bias $\alpha = \frac{\sigma_{model}}{\sigma_{obs}}$, and mean bias terms $\beta = \frac{\mu_{model}}{\mu_{obs}}$.

$$KGE = 1 - \sqrt{(\rho - 1)^2 + (\alpha - 1)^2 + (\beta - 1)^2}$$

4.3 Parameter Uncertainty: Latin Hypercube Sample

To validate HydroBlocks' ability to represent field-scale information, the model is run over the Little Washita watershed between 2004 and 2007 at a 15-minute time step. The number of HRUs is set to be 1000. This number, as will be shown in section 5.2, is found to adequately approximate the fully distributed solution. To obtain both optimal model performance while assessing the role of model parameter equifinality, the latin hypercube sampling technique (LHS; [*McKay et al.*, 1979]) is used to assess model performance across the model parameter space.

The LHS is used to generate 100 parameter sets by sampling (assuming uniform distributions) from the 4 parameters listed in Table 2. These parameters are chosen due to their impact on simulated soil moisture; all response units have the same parameter value. For each parameter set, 2004 and 2005 are used to spin-up HydroBlocks. 2006 through 2007 are then used to assess model performance by constraining the ensemble using available in-situ soil moisture observations. The model's ability to simulate soil moisture is analyzed since it is a state variable that is heavily controlled by the fine-scale physical environment and plays an important role in other land surface processes (e.g., latent heat). The Kling-Gupta Efficiency (KGE) metric is used to assess the model performance between each probe and the simulations of its corresponding grid cell on the fully distributed grid (i.e., corresponding HRU). The median of the KGE of all the probes for each ensemble member is computed and used as the sole metric of model performance.

5. Results

5.1 HydroBlocks example over the Little Washita

To further understand the HRU clustering algorithm and the HydroBlocks model, an example over the Little Washita watershed is explored using 3 hydrologic response units. In this case, only the topographic index map is used as input to the k-means algorithm to define the 3 HRUs. The algorithm assigns an HRU to each 30-meter grid cell in the catchment. As shown in Figure 3, k-means uses the topographic index to partition the catchment into three distinctive regions. The HRUs are ranked from lowest to highest accumulation area. In this example this corresponds to ranking them from lowest to highest topographic index, however, this will not always be the case.

Per the definition of topographic index, in general, HRU_1 represents ridges, moderate to steep slopes, and low flow accumulation areas. HRU_3 represents valleys, flat regions, and high flow accumulation areas.

The connections between the HRUs are calculated using the 30-meter d8 flow direction raster derived from the NED DEM. Figure 3 provides an example of the connections between the hydrologic response units. They flow into each other and also into themselves. The flow matrix **W** is also shown in Figure 3. It summarizes these connections and assigns weights to define how the outflow of an HRU is distributed among its surrounding response units. Note that given that the d8 flow direction map defines the connections, if the d8 accumulation area were used as the proxy of heterogeneity instead of the topographic index, the flow matrix would be an upper triangular matrix. However, since this example uses the topographic index there can be backflow from grid cells with higher accumulation area to grid cells with lower accumulation area. This explains the backflow from grid cells in HRU_3 into grid cells in HRU_2 and grid cells in HRU_2 into grid cells in HRU_1.

After assigning each HRU's model parameters and meteorological data, HydroBlocks is run between January 1st, 2004 and December 31st, 2004 at a 15-minute time step. Each HRU has its own output time series of states and fluxes. Figure 4 shows the daily results for precipitation, soil moisture, latent heat, and sensible heat for the three response units. There is negligible difference in the time series of precipitation. If latitude and longitude were also used as proxies to define the hydrologic response units this would no longer be the case. The most noticeable feature in Figure 4 is the clear differences in the time series of soil moisture. This can be attributed solely to subsurface redistribution. The convergence from HRU_1 and HRU_2 into HRU_3 leads to a shallower water table depth in HRU_3. This results in higher surface soil moisture content and an increase in available water in HRU_3. Not surprisingly, this drives the differences in latent heat and sensible heat between the three response units. This provides an example of how a simple representation of spatial heterogeneity in the catchment can lead to large differences in not only the simulated soil moisture but also in the simulated surface fluxes.

5.2 Approximating the fully distributed solution

As shown in section 5.1, using 3 response units in HydroBlocks already defines distinct spatial patterns in the simulated surface fluxes and soil moisture. However, it will be rare that a catchment the size of Little Washita requires only 3 HRUs to approximate the spatial heterogeneity of the fully distributed solution. To address this concern, the method outlined in section 4.2 is used to assess the required number of HRUs to approximate the fully distributed solution. This is accomplished by running HydroBlocks with an increasing number of hydrologic response units. Note that in this section all the proxies from Table 1 are used to define the HRUs.

Given that each grid cell is assigned an HRU in the clustering algorithm, the model results can be readily mapped out in space. This not only allows for field-scale predictions but also facilitates robust comparison between the semi-distributed and fully distributed solutions. Figure 5 compares the 30-meter mapped model output for the different model configurations on October 22nd, 2004 for daily soil moisture, storage deficit, latent heat, and precipitation. The apparent coarse grid at 10 HRUs is because the latitude and longitude proxies are driving the heterogeneity of the model. From visual inspection, the simulations using 1,000 and 10,000

HRUs most closely approximate the fully distributed solution. The increase in coarseness of the rainfall product as the number of HRUs increase is due to the effective spatial resolution of the input meteorological data set (~ 4 km).

Figure 6 shows the change in the time series of the spatial mean and spatial standard deviation of soil moisture as the number of hydrologic response units increases. At 10 HRUs, the model reproduces the soil moisture mean of the fully distributed model. However, 10 HRUs is not sufficient when the goal is to reproduce the fully distributed model's time series of spatial standard deviation. At 2 HRUs, the spatial heterogeneity is driven mainly by rain events. There is a noticeable improvement when using 10 HRUs; a further increase in the number of HRUs continues to improve the performance. However, it appears that the semi-distributed model only approximates but never completely reproduces the fully distributed simulation. This is not surprising since a fraction of the spatial heterogeneity will be due to field-scale heterogeneity that will be represented only if every grid cell on the fully distributed grid is assigned a unique HRU.

Figure 7 uses the KGE metric and its components (α, β, and ρ) to formalize the comparison of the time series of the spatial mean and standard deviation between the semi-distributed and fully distributed model simulations. It assesses how the performance metrics vary as a function of the number of hydrologic response units. The variables used in this comparison are top-layer soil moisture content, surface runoff, baseflow, sensible heat, precipitation, and latent heat. The results from Figure 7 for both the spatial mean and spatial standard deviation are analyzed below.

Spatial mean - The linear correlation (ρ) between the time series of spatial mean of the semi-distributed and fully distributed simulations is close to 1 for all variables at 10 HRUs except baseflow; the same result applies to the bias in the standard deviation (α). The noticeable weakness when using a low number of response units (n_{hru}) is the bias in the mean (β). In these cases, latent heat is positively biased and sensible heat and runoff are negatively biased. This suggests that at low n_{hru}, HydroBlocks releases too much water as evapotranspiration and not enough as runoff. At around 100 HRUs, these biases in sensible heat and latent heat diminish. Although diminished, the negative bias in baseflow continues at 10,000 HRUs – and most likely beyond.

Spatial standard deviation – As expected from Figure 6, the time series of the spatial standard deviation converges to the fully distributed solution at a slower rate than the spatial mean. The linear correlation of precipitation spatial heterogeneity is high because at many time steps the rainfall is 0 throughout the catchment regardless of the model configuration. This also helps explain the excellent linear correlation of surface runoff at relatively low number of response units. However, the biases in the mean and standard deviation terms suggest that the semi-distributed model never completely represents the spatial heterogeneity of the fully distributed model – regardless of the number of HRUs. This appears to be especially true for baseflow. Closer inspection of the modeled surface runoff and baseflow spatial heterogeneity suggests that the semi-distributed model struggles to adequately represent the spatial properties of baseflow. As will be addressed in the discussion, this further suggests that assuming homogenous HRUs is not adequate; instead sub-HRU parameterizations may be required to ensure convergence with the fully distributed solution when attempting to represent baseflow spatial heterogeneity.

5.3 Computational efficiency

The primary reason to use a semi-distributed model instead of relying exclusively on the fully distributed model is due to computation and storage limitations. For example, on a 32-core machine it takes 60 hours to run the fully distributed version of HydroBlocks over the Little Washita at a 30-meter spatial resolution between January 1st, 2004 and December 31st, 2004 at a 15-minute time step. Furthermore, more than 250 gigabytes is necessary to store the model output. To assess the computational benefits of using a reduced number of hydrologic response units to run HydroBlocks, Figure 8 shows the change in model runtime as a function of the number of hydrologic response units. Up to 100 HRUs, the computation savings with respect to the fully distributed model is above three orders of magnitude. At 1,000 HRUs it is above 2 orders of magnitude.

The growth in runtime per HRU after 500 is explained by the complexity of the flow matrix used in the subsurface redistribution scheme in Dynamic TOPMODEL (see section 2.2). The flow matrix defines the number of terms and their positions in a system of linear equations; this system is used to solve for the subsurface outflow at each HRU. In the fully distributed model, although the number of unknowns is very large, it is straightforward to solve the system of linear equations at each time step since each HRU flows into one and only one HRU. This is not the case for the semi-distributed model where one HRU can flow into multiple HRUs and backflows occur. The storage requirements of HydroBlocks do scale linearly. In this example, for 1,000 HRUs the simulation for 2004 requires less than 0.5 gigabytes of storage – orders of magnitude less than the fully distributed model.

5.4 Model Validation: Latin Hypercube Sample

One of the primary goals behind the development of HydroBlocks is the accurate simulation of field-scale soil moisture. To assess whether HydroBlocks achieves this goal, it is evaluated using the USDA-ARS Micronet network of soil moisture probes in the Little Washita (see Figure 2). The model is run using 1000 HRUs; the results in section 5.2 suggest that this is an acceptable threshold to approximate the soil moisture spatial heterogeneity simulated by the fully distributed model. HydroBlocks is run between 2004 and 2007 using 100 different parameter sets drawn from a Latin Hypercube Sample (see section 4.3 for more details). Point soil moisture observations available between 2006 and 2007 are used to evaluate the model performance of each probe's corresponding grid cell (HRU). The performance of the model at each soil moisture probe collocated HRU is calculated using the KGE metric and its components (α, β, and ρ). The optimal catchment parameter set is chosen as the set that leads to the highest median KGE among all the probes – the same parameter values are used at each response unit in the catchment.

Figure 9 shows the model performance at the 18 soil moisture probes when using the catchment's optimal parameter set. It also shows the spread in model performance from the top performing parameter sets from the LHS ensemble. Figure 10 summarizes these results by using the KGE, linear correlation ρ, bias in the mean β, and bias in the standard deviation α. For most probes, the linear correlation ρ between the probes and their corresponding simulated grid cells is high. This result appears to be driven primarily by the quality and spatial detail of the input precipitation data. Not being able to represent the consistently high soil moisture values towards the beginning of 2006 appears to drive the low correlation at a number of sites. The choice of parameter set does not have a large impact on the correlation. The simulations are generally unbiased at many sites; at these sites α and β approach 1. There are 6 sites at which there are noticeable positive biases. These biases are driven by the modeled soil moisture being too wet; this can most likely be attributed to biases in the prescribed soil properties including soil porosity, field capacity, wilting point, and residual soil water content. Overall, these model validation results over the Little Washita suggest that 1) the accuracy of the precipitation product is the primary driver of the linear correlation between the probes and the simulation and 2) uncertainty in the soil hydraulic properties is the primary driver of bias in the mean and standard deviation in the simulated soil moisture content.

6. Discussion

6.1 Improving sub-grid spatial heterogeneity in land surface models

A primary motivation behind the development of HydroBlocks is to capitalize on decades of research and existing field-scale global datasets to improve the representation of spatial heterogeneity in land surface models. Existing models represent sub-grid heterogeneity through a mosaic approach; each tile represents a fraction of the grid cell. These tiles account for the spatial heterogeneity of land cover, lakes, wetlands, water management, urban areas, soil heterogeneity, topography, and glaciers [*Avissar and Pielke*, 1989; *Koster and Suarez*, 1992; *Nijssen et al.*, 1997; *Essery et al.*, 2003; *Shevliakova et al.*, 2009; *Oleson et al.*, 2013]. A persistent weakness in the mosaic approach is the lack of spatial interactions among tiles. In HydroBlocks, tiles (i.e. HRUs) interact laterally via a subsurface kinematic wave. This approach enables HydroBlocks to explicitly represent subsurface water redistribution while maintaining computational efficiency. As shown in Figures 3, 4, and 5 and discussed in section 5.1, accounting for the lateral interactions among HRUs has an important role in the modeled soil moisture spatial heterogeneity, which, in turn, contributes to the simulated spatial patterns of latent heat and sensible heat, among others.

Although not used in this study, HydroBlocks also uses a surface kinematic wave to model overland and channel flow; in the future, this could be used to account for surface water redistribution, erosion, and reinfiltration. Interactions among tiles could also be used in land surface models to improve the representation of processes that are influenced by lateral movement due to surface wind patterns including fires, blowing snow, and seed dispersal, among others. HydroBlocks presents a straightforward and computationally efficient path towards a more explicit accounting of the impact of lateral interactions among tiles. This will lead to an improved representation of field-scale land surface components and processes and provide a more complete coupling between the modeled water, energy, and carbon cycles.

6.2 Deriving the hydrologic response units

HydroBlocks can be run as a semi-distributed model (multiple HRUs) or fully distributed model (one HRU per grid cell). The goal with the semi-distributed model is to reproduce the fully distributed model while minimizing computational expense; this relies on the number and configuration of the prescribed HRUs. Over the Little Washita watershed, the results in section

5.2 suggest that around 1000 HRUs are necessary to successfully approximate the fully distributed model's catchment mean and standard deviation for latent heat, soil moisture, surface runoff, and sensible heat, among others (except baseflow). This result is dependent on both the clustering mechanism and the chosen proxies of spatial heterogeneity (see Table 1). For example, when using 1000 HRUs—assembled by using NDVI as the single proxy of spatial heterogeneity—the results vary; the semi-distributed model's ability to reproduce the fully distributed fine-scale spatial patterns of soil moisture and surface runoff decreases substantially.

The role that the proxies of spatial heterogeneity play in deriving the appropriate HRUs is further exemplified in baseflow generation. To produce baseflow, HydroBlocks requires an HRU's water table to be above ground. This condition becomes a significant challenge when trying to approximate the fully distributed solution during the dry season. In the fully distributed simulation, during this period, baseflow generation ceases except for a small subset of grid cells within the catchment that have highly specific environmental characteristics (local and upslope). This was the rationale for using as proxies of spatial heterogeneity the number of immediately upslope grid cells that contribute to a given grid cell (NIU) and the mean upslope saturated hydraulic conductivity. Without these two variables, the model performance at 1000 HRUs decreases substantially when trying to reproduce the spatial patterns of baseflow of the fully distributed simulation. Future work should investigate other proxies that improve the semi-distributed model's spatial patterns of baseflow during the dry season. Following [*Newman et al.*, 2014], one promising path forward is to use the fully distributed model output maps (e.g., baseflow) as the proxies of spatial heterogeneity. By identifying the key areas that play a dominant role in the fully distributed spatial patterns, this approach might also lead to a reduction in the number of required HRUs.

Another potential path forward to both minimize the number of necessary HRUs and to improve the modeled spatial patterns of baseflow in the semi-distributed model is to improve the clustering algorithm. Using the K-means clustering algorithm is a brute force approach that does not necessarily account for the physical configuration of the catchment. For example, dividing the catchment into sub-basins is a more realistic spatial division than the latitude and longitude grid used in this study (see Table 1). However, there is no straightforward mechanism to include the sub-basin structure within K-means. A more plausible path forward is to first divide the catchment into a predefined number of sub-basins and then use K-means to find each sub-basins characteristic HRUs. A preliminary evaluation shows that this type of clustering approach also speeds up the simulations when compared to the original clustering algorithm since it leads to a more simplified flow matrix that results in a system of linear equations that is faster to solve for each update of Dynamic TOPMODEL.

6.3 Revisiting the representative elementary area concept

Through a set of model experiments using a modified version of TOPMODEL, [*Wood et al.*, 1988] and [*Famiglietti and Wood*, 1995] introduced the concept of a representative elementary area (REA) for hydrologic and land surface modeling; the REA is defined as the catchment scale above which field-scale spatial heterogeneity can be represented through sub-grid parameterizations instead of needing to rely on fully distributed modeling. In other words, it is the spatial scale (~grid cell size) above which macroscale land surface models are applicable.

The REA has been found to be around 1 km^2, although the REA is known to vary as a function of the catchment's physical environmental characteristics and the model complexity [*Blöschl et al.*, 1995].

Usually, HRU models consider HRUs to be spatially contiguous regions within a catchment (e.g., sub-basin); each HRU's field-scale processes are modeled via sub-HRU parameterizations. In these models, an REA can be established for the minimum HRU spatial scale. However, this is not how HRUs are defined in HydroBlocks. In this study, HRUs are defined as points in a catchment with similar field-scale environmental characteristics that need not be spatially contiguous (see Figure 3). The HRUs are defined such that each one will have a unique hydrologic response. Therefore, the concept of REA is not applicable to the HRUs currently defined in HydroBlocks. However, as discussed in section 6.2, the authors are implementing a hierarchical clustering method to more adequately define the HRUs. First, the catchment is divided into sub-basins and then the HRUs are defined per sub-basin. In this scenario, the REA would be the area of the sub-basin. Future work will use this hierarchical clustering method in HydroBlocks to further explore the REA concept in hydrologic and land surface modeling. The available field-scale environmental datasets and computational resources makes it feasible to perform this study over the entire contiguous United States. This will provide further understanding on how environmental characteristics impact the REA spatial scale and lead to a more informed configuration of sub-grid spatial heterogeneity in macroscale land surface models.

6.4 Quantifying and constraining model uncertainty

Although an explicit representation of field-scale land surface processes has the potential to more accurately depict the observed spatial and temporal dynamics over the land surface, it will also lead to an increase in model uncertainty due to the need for higher resolution model parameters and meteorological input data [*Beven and Cloke*, 2012]. To ensure the increase in process detail in the next generation of land surface models results in improved modeling of the land surface, these models must be able to handle robust ensemble frameworks to quantify and constrain model uncertainty [*Chaney et al.*, 2015]. The possibility to run thousands of simulations in a short time period was one of the primary benefits of the original TOPMODEL and an important driver in the development of Dynamic TOPMODEL [*Beven and Freer*, 2001]. Although using around 100 to 1000 HRUs in HydroBlocks increases computational demand when compared to current land surface models, the model is still highly computationally efficient. The results in section 5.3 show how the model can be run around 500 times using 1000 HRUs in the time it takes to run the fully distributed mode once. This makes it possible to resolve the physical processes at field-scales enabling the model results to be directly compared to in-situ observations while accounting for model uncertainty through robust ensemble frameworks (e.g., Latin Hypercube Sample). Although this study focused exclusively on assessing the performance of the simulated surface soil moisture (see section 5.4), future validation efforts should extend the analysis to include other states and fluxes of the water, energy, and carbon cycles including streamflow, latent heat, and sensible heat, among others.

6. Conclusions

This study introduces HydroBlocks, a novel land surface model that couples the NOAH-MP land surface model and the Dynamic TOPMODEL hydrologic model. HydroBlocks represents a catchment's spatial heterogeneity via dynamically interacting hydrologic response units (HRUs). The model defines the response units by using the K-means algorithm to cluster high-resolution drivers of spatial heterogeneity (soil, topography, land cover, and position). The model's structure provides a seamless link between lumped, semi-distributed, and fully distributed modeling. A set of simulations with an increasing number of HRUs show that over the Little Washita watershed, the semi-distributed version of the model can adequately approximate the spatial mean and spatial standard deviation of the fully distributed version of the model with around 1000 HRUs. In other words, the spatial patterns of the fully distributed model can be reproduced with a fraction of the computational expense. A 100 Latin Hypercube Sample is then used to evaluate model performance over each catchment's network of soil moisture observations and to assess the role of model parameter uncertainty. The results confirm that HydroBlocks' ability to handle large ensembles is crucial to provide reliable fine scale detail. HydroBlocks' reliance on interacting hydrologic response units provides a promising path forward for macroscale land surface modeling. It will enable land surface models to improve the representation of the role of the fine-scale physical environment in land surface processes and to explicitly model the sub-grid spatial interactions of the water, energy, and carbon cycles.

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Table 1. Drivers of the spatial heterogeneity of land surface processes and their corresponding proxies used for defining the hydrologic response units.

Driver of Spatial Heterogeneity	Proxy	Dataset*	Spatial Resolution
Land Cover	NDVI	WELD	30 meters
Soil Properties	K_{sat}	POLARIS	30 meters
	Mean upslope K_{sat}		
Topography	Accumulation area	NED	30 meters
	NIU		
Meteorology	Latitude	N/A	30 meters
	Longitude		

* See section 3.2 for a description of these datasets and the proxies.

Table 2. Parameter definition and ranges used in the 100 set Latin Hypercube Sample.

Parameter	Description	Lower Limit	Upper Limit
m (meters)	Form of the exponential decline in conductivity	0.001	10.0
S_{max} (meters)	Maximum effective soil moisture deficit	0.1	1.0
p_{soil}	Scaling factor of the residual point, wilting point, field capacity, and porosity.	0.5	1.0
p_{ksat}	Scaling factor of the saturated hydraulic conductivity	0.25	4.0

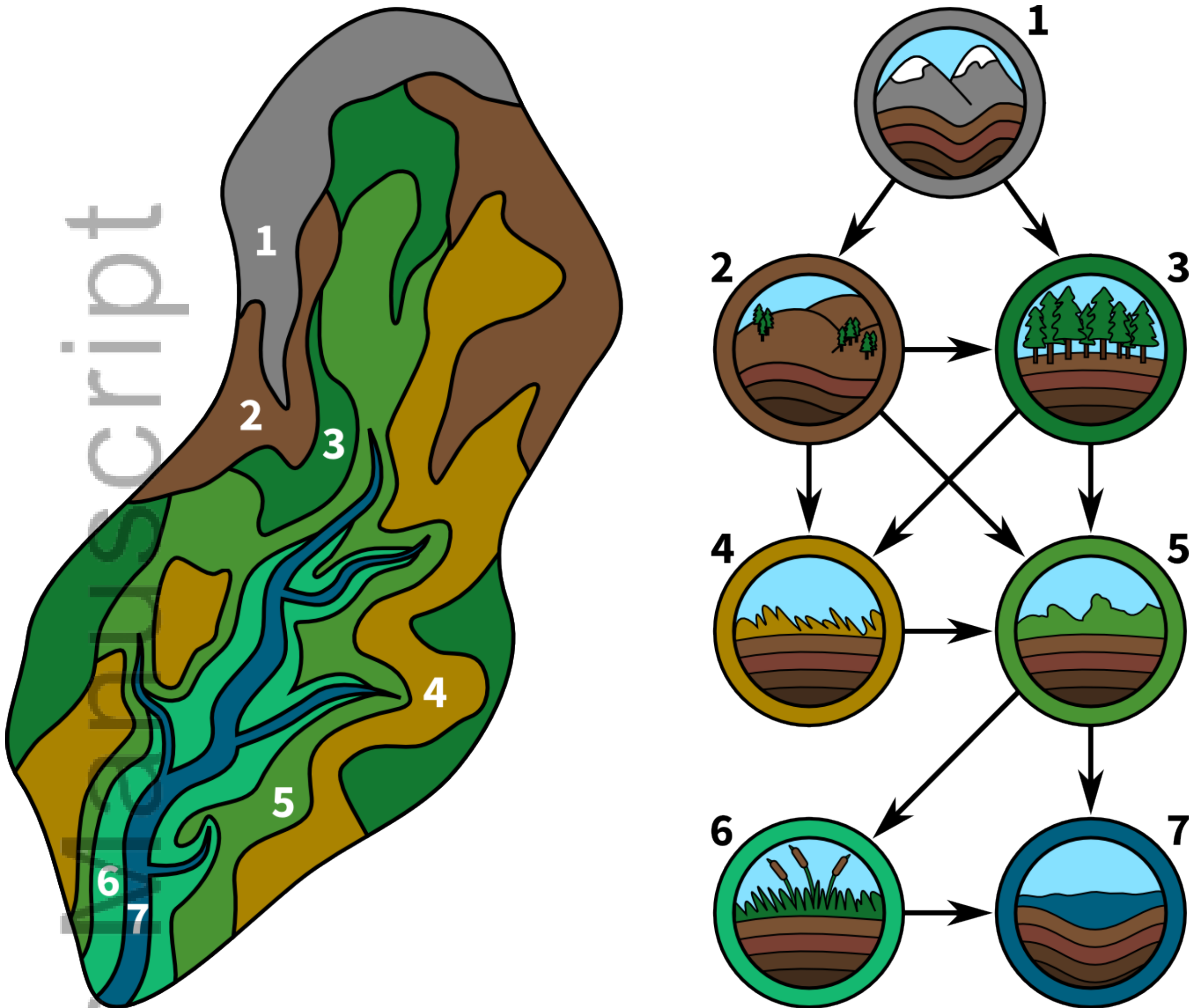

Figure 1. HydroBlocks represents spatial heterogeneity through hydrologic response units (HRUs). These response units are defined according to a catchment's land cover, topography, soil, and position maps. At each time step, the Noah-MP land surface model updates the vertical profile of each response unit and Dynamic TOPMODEL connects the response units via a subsurface kinematic wave.

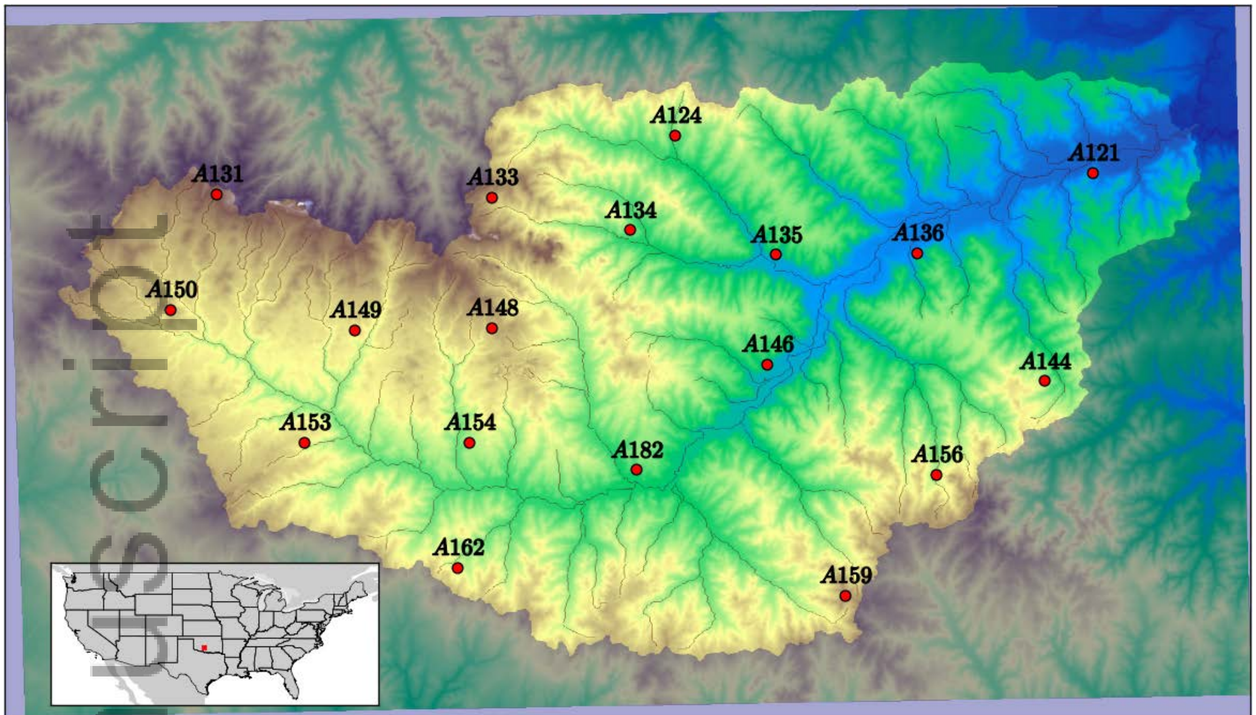

Figure 2. The Little Washita watershed is a 610 km^2 tributary of the Washita River in southwest Oklahoma, United States. The catchment is shown via the NED elevation data and the derived channel network. The ids and locations of the soil moisture probes in the USDA-ARS Micronet network are also shown.

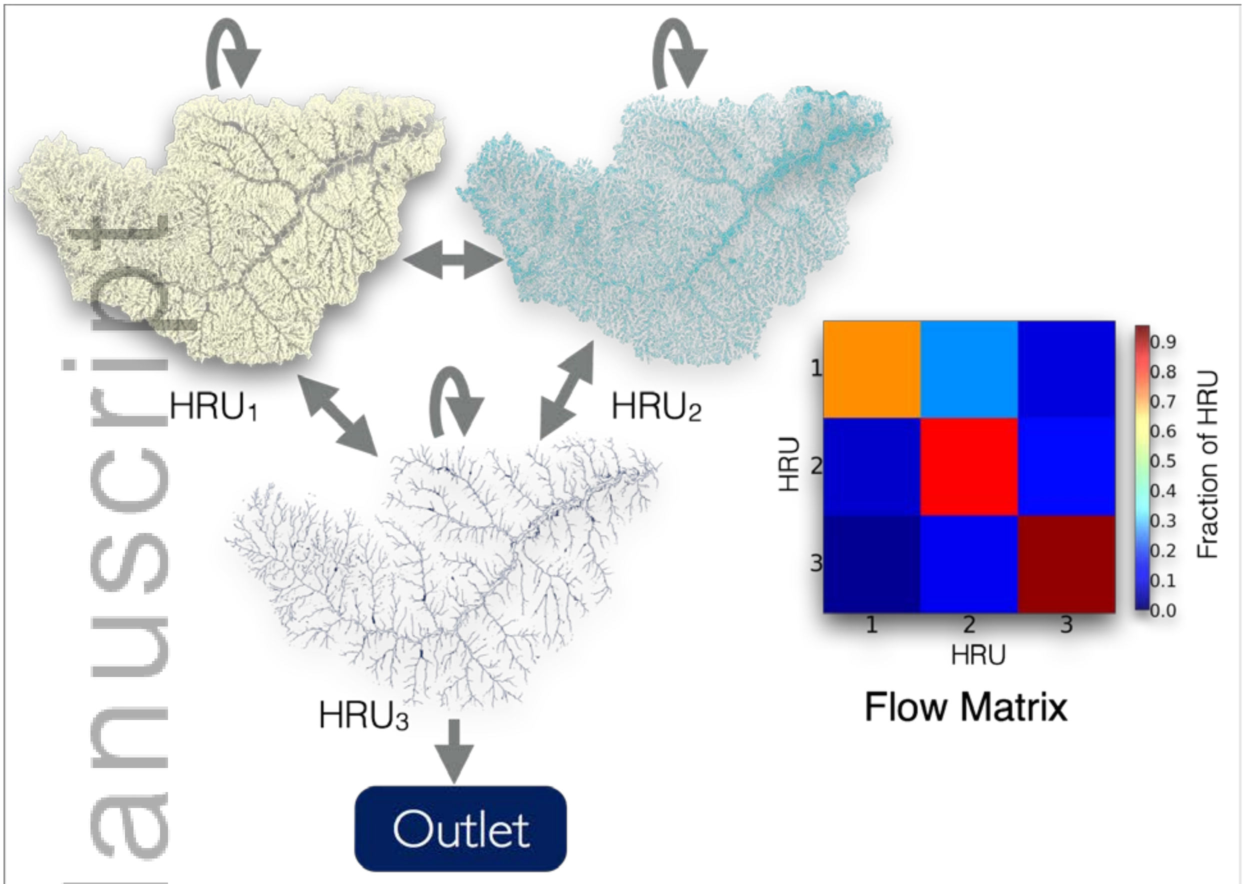

Figure 3. As an example, the K-means clustering algorithm is applied to the topographic index map to define 3 hydrologic response units over the Little Washita. The flow direction map derived from the 30-meter NED DEM is then used to compute the connections between the HRUs. As shown in the flow matrix, the HRUs either flow into themselves or into another HRU.

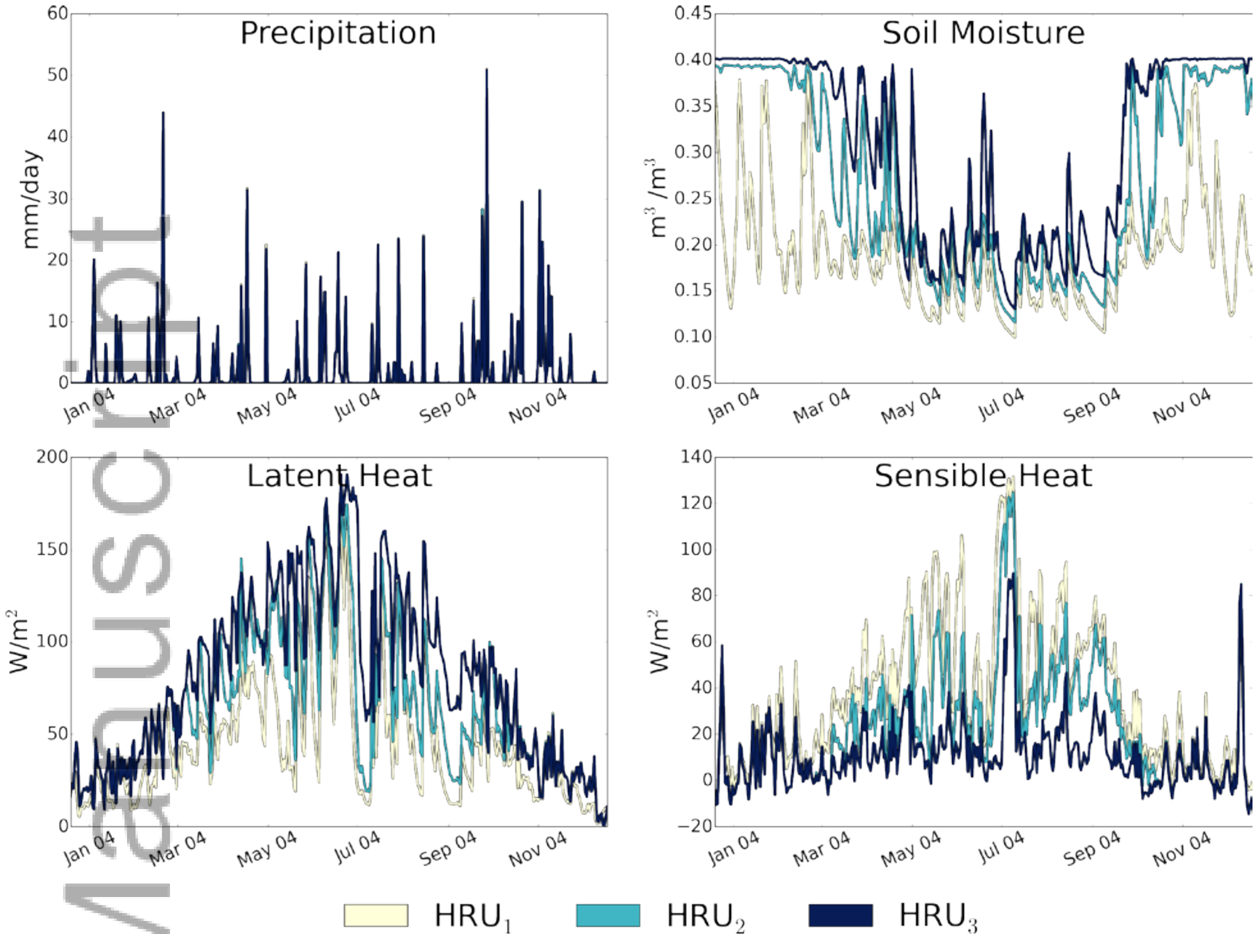

Figure 4. HydroBlocks is run over the Little Washita watershed using the 3 hydrologic response units defined in Figure 3. This simple example illustrates the semi-distributed model's ability to represent spatial heterogeneity of soil moisture, latent heat, and sensible heat.

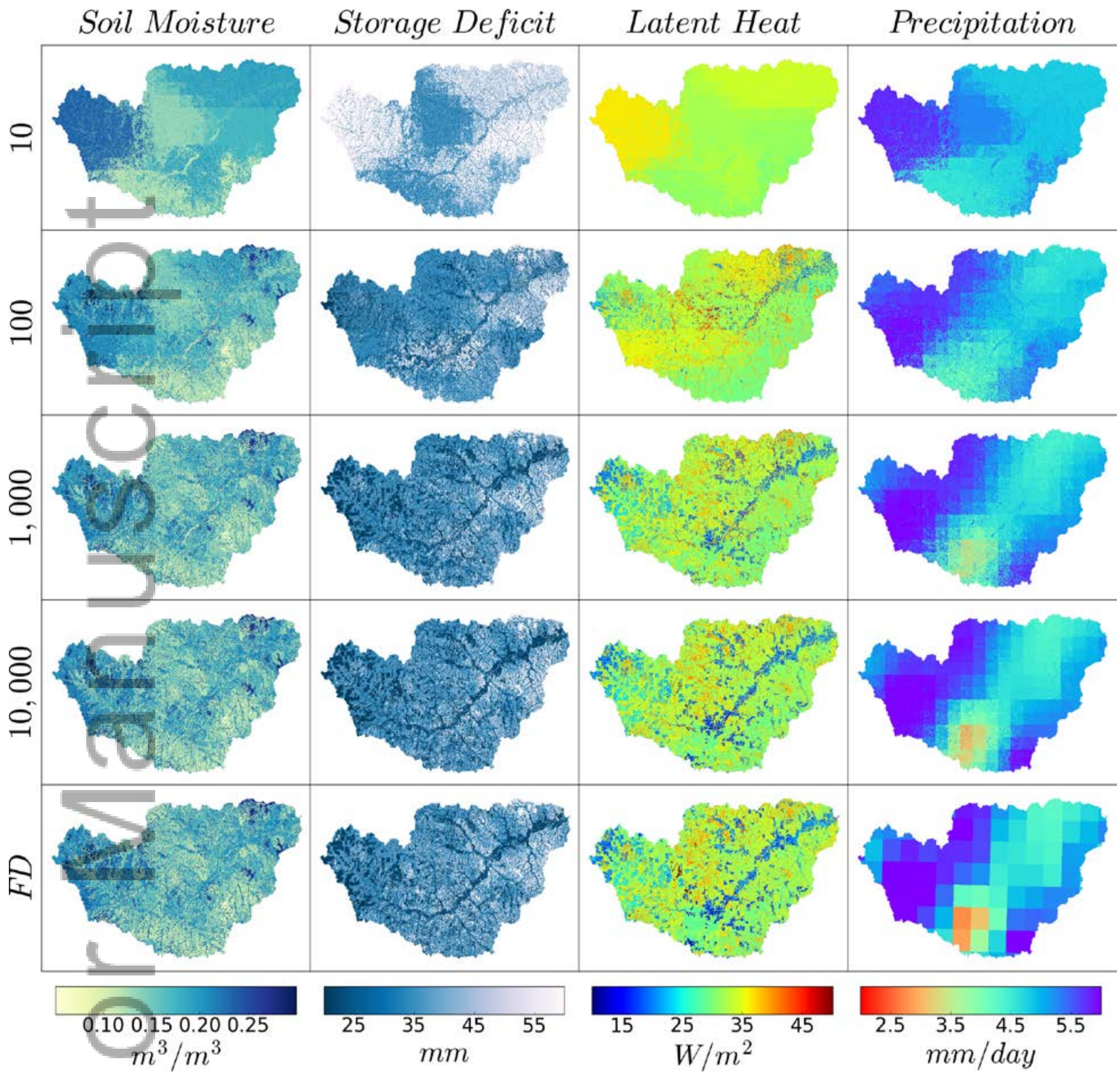

Figure 5. Comparison between the semi-distributed and fully distributed HydroBlocks model output over the Little Washita on October, 22nd 2004. The panels offer a visual comparison between the mapped daily top-layer soil moisture content, soil water storage deficit, latent heat, and precipitation for the different model configurations (10, 100, 1,000, 10,000 HRUs, and fully distributed).

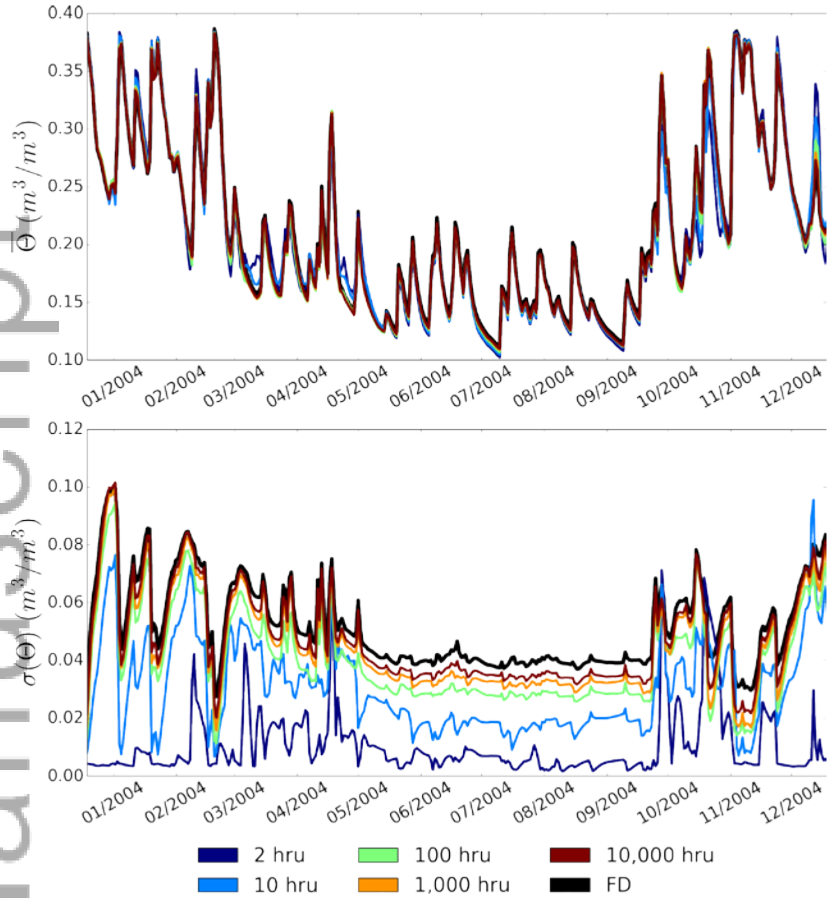

Figure 6. Modeled catchment soil moisture mean and standard deviation using HydroBlocks with 2, 10, 100, 1,000, and 10,000 HRUs and the fully distributed model over the Little Washita watershed.

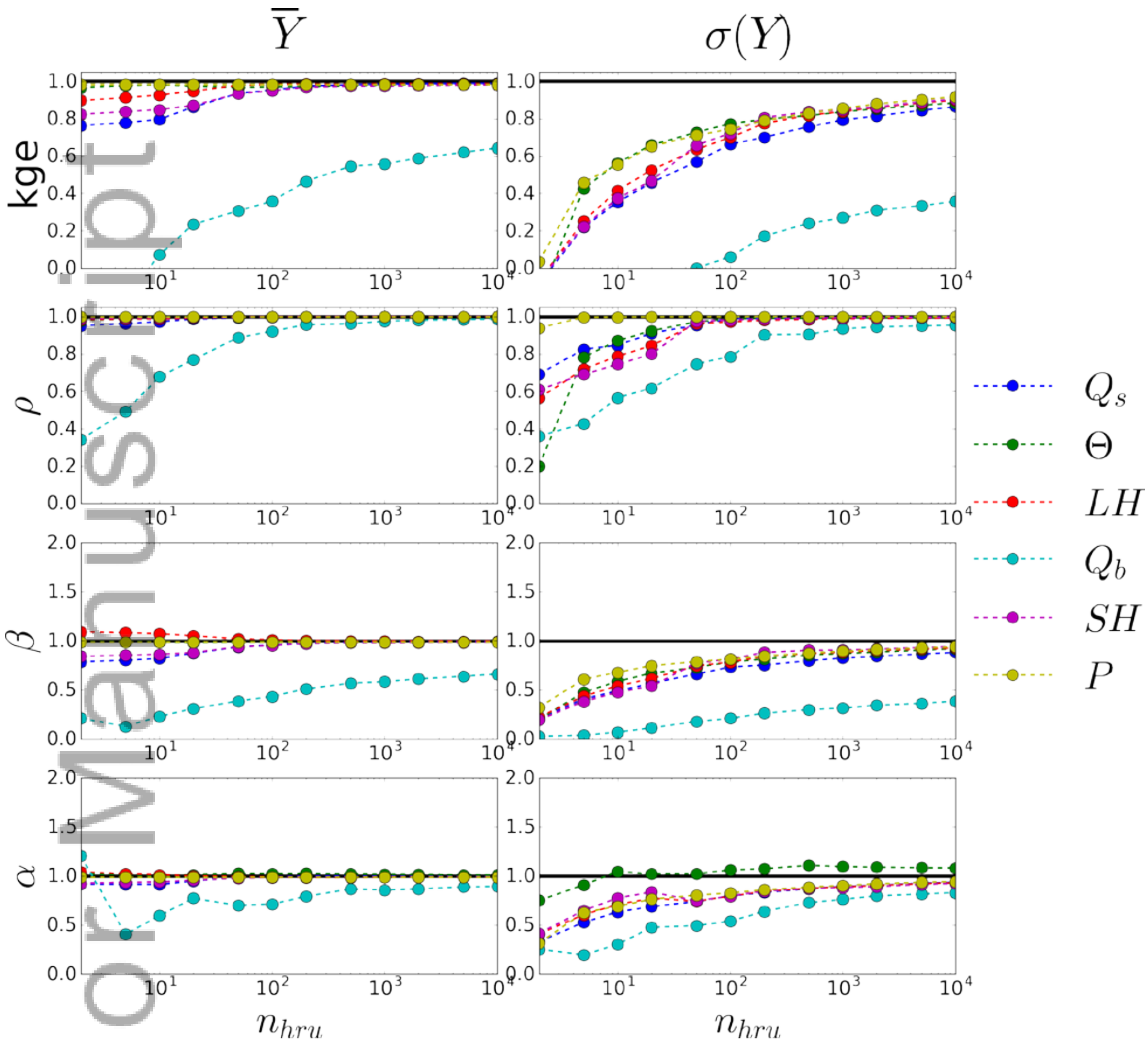

Figure 7. Convergence of the Kling-Gupta efficiency metric KGE, linear correlation ρ, bias in the mean β, and the bias in the standard deviation α with increasing number of HRUs. Metrics are based on comparisons of daily time series of simulated spatial mean (left) and the spatial standard deviation (right) of the semi-distributed and fully distributed versions of the HydroBlocks model, and are provided for soil moisture (θ), baseflow (Q_b), surface runoff (Q_s), precipitation (P), sensible heat (SH) and latent heat (LH).

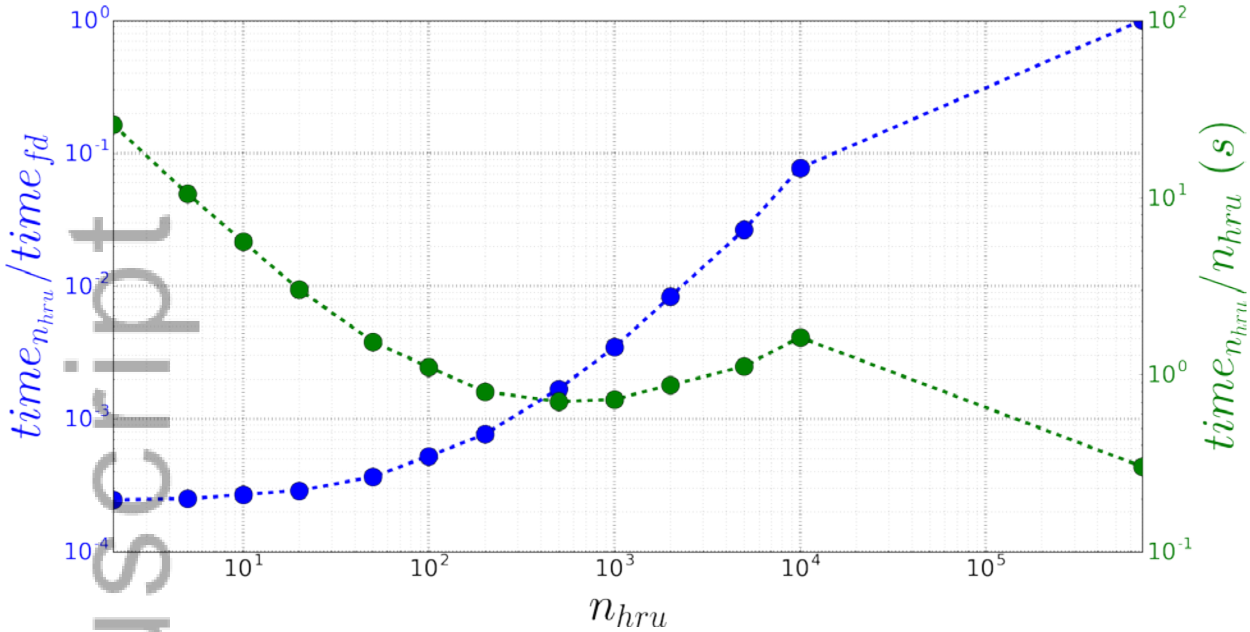

Figure 8. Analysis of the time it takes to run the HydroBlocks model for one year over the Little Washita as a function of the number of hydrologic response units. The blue line is the semi-distributed runtime divided by the fully distributed run-time. The green line is the semi-distributed runtime divided by the number of hydrologic response units.

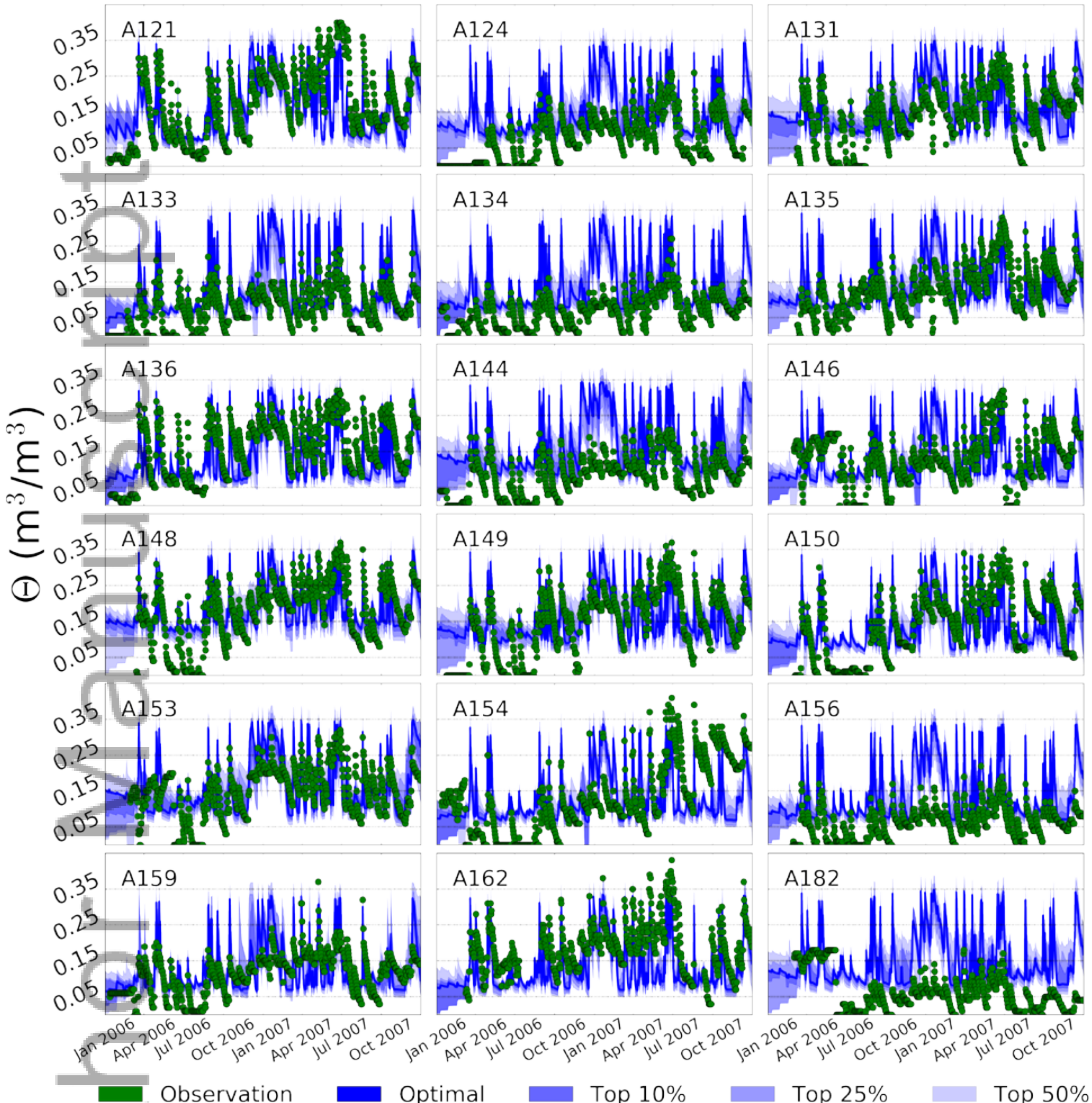

Figure 9. The observations of 18 soil moisture probes (green dots) in the ARS Micronet network in the Little Washita watershed are used to validate the HydroBlocks model output from the Latin Hypercube Sample. The optimal parameter set simulations (blue line) are bounded by the simulations of the best performing 10%, 25%, and 50% parameter sets.

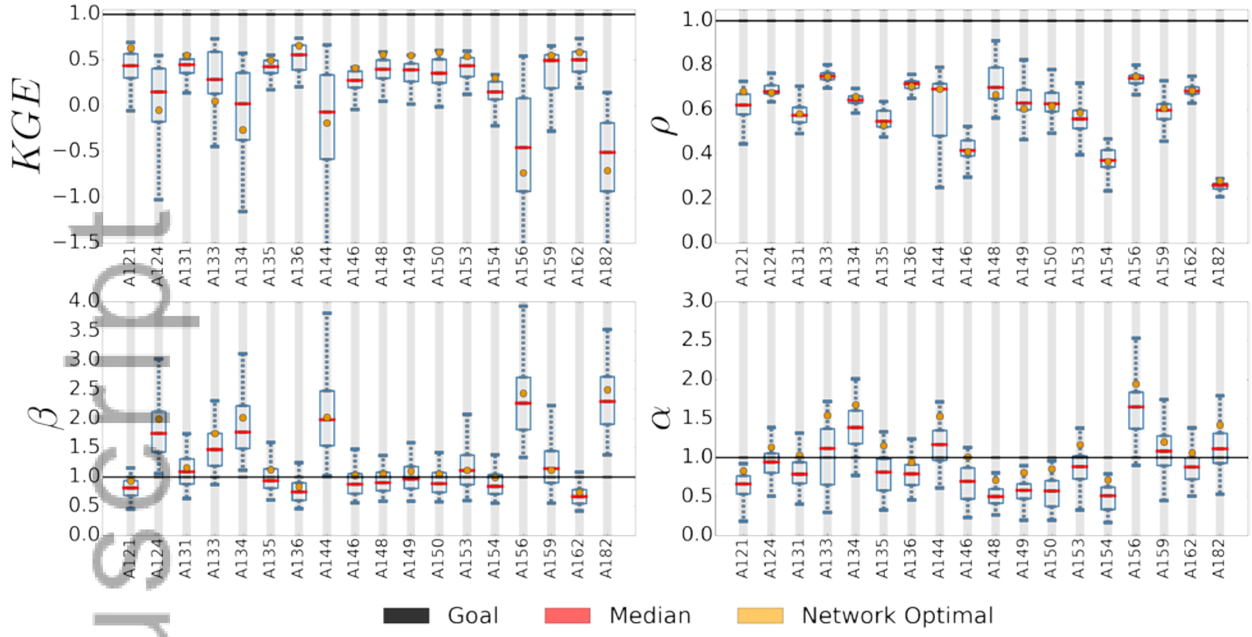

Figure 10. The spread in model performance from the 100 set Latin Hypercube Sample is visualized at each of the 18 soil moisture probes in the Little Washita watershed via boxplots of a suite of performance metrics including Kling-Gupta Efficiency (upper left panel), linear correlation (upper right panel), bias in the mean (lower left panel), and bias in the standard deviation (lower right panel). The performance at each site when the catchment optimal parameter set is used is shown via the light orange dots.

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