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A priori discretization error metrics for distributed hydrologic modeling applications

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Abstract:

Watershed spatial discretization is an important step in developing a distributed hydrologic model. A key difficulty in the spatial discretization process is maintaining a balance between the aggregation-induced information loss and the increase in computational burden caused by the inclusion of additional computational units. Objective identification of an appropriate discretization scheme still remains a challenge, in part because of the lack of quantitative measures for assessing discretization quality, particularly prior to simulation. This study proposes *a priori* discretization error metrics to quantify the information loss of any candidate discretization scheme without having to run and calibrate a hydrologic model. These error metrics are applicable to multi-variable and multi-site discretization evaluation and provide directly interpretable information to the hydrologic modeler about discretization quality. The first metric, a subbasin error metric, quantifies the routing information loss from discretization, and the second, a hydrological response unit (HRU) error metric, improves upon existing *a priori* metrics by quantifying the information loss due to changes in land cover or soil type property aggregation. The metrics are straightforward to understand and easy to recode. Informed by the error metrics, a two-step discretization decision-making approach is proposed with the advantage of reducing extreme errors and meeting the user-specified discretization error targets. The metrics and decision-making approach are applied to the discretization of the Grand River watershed in Ontario, Canada. Results show that information loss increases as discretization gets coarser. Moreover, results help to explain the modeling difficulties associated with smaller upstream subbasins since the worst discretization errors and highest error variability appear in smaller upstream areas instead of larger downstream drainage areas. Hydrologic modeling experiments under candidate discretization schemes validate the strong correlation between the

proposed discretization error metrics and hydrologic simulation responses. Discretization decision-making results show that the common and convenient approach of making uniform discretization decisions across the watershed performs worse than the proposed non-uniform discretization approach in terms of preserving spatial heterogeneity under the same computational cost.

KEY WORDS: *a priori* spatial discretization error metrics; distributed hydrologic modeling; spatial heterogeneity; information loss; routing errors; discretization decision-making

1. Introduction

In distributed hydrologic modeling, a watershed is treated as a number of small homogeneous units to address the spatial heterogeneity which results from variability of physical processes and physical character across a watershed (Singh & Frevert, 2005). This spatial heterogeneity is often attributed to the uneven distribution of a hydrological properties across a watershed (Anselin, 2010). The spatial discretization process, whereby we separate a watershed into homogeneous computational units for depiction in a hydrological model, is really the effort of determining how to characterize the inherent spatial heterogeneity found in a watershed. In general, spatial discretization should be detailed enough to capture the dominant processes and natural variability, while it also needs to be as concise as possible to save computation time and respect data availability (Booij, 2005). Excessively detailed spatial discretization increases model complexity (i.e., number of computational units) and thus increases model computation time. However, an overly coarse aggregation can lead to substantial information losses and give rise to increased model structural uncertainty, whose impacts on hydrological predictions are far more adverse than those of parameter and data uncertainty (Liu & Gupta, 2007; Ludwig et al., 2009). Therefore, defining an appropriate level of discretization is a critical task in distributed hydrologic modeling.

In order to investigate spatial discretization, it is necessary to first clarify the components of watershed discretization. For this paper, we will be examining the common subbasin-HRU discretization approach. In this approach, a watershed is discretized into a set of one or more subbasins, which can be further discretized into a number of contiguous or non-contiguous hydrological response units (HRUs), defined as areas with hydrologically unique response to meteorologic events. Subbasins are referred to by different names in the literature, including grid cell, subcatchment, and subwatershed (Tuppad, 2006). Here we recursively define a subbasin as the drainage area of a location on a stream network minus the drainage areas of one or more upstream subbasins which flow directly into the subbasin. Headwater subbasins are those which do not have any subbasins upstream, i.e., those whose drainage areas are equal to their subbasin area. An HRU is the basic computational unit of hydrological simulation and typically defined as a unique combination of hydrological response determinants such as soil, land cover, terrain type, and management policy (Flügel, 1995), often generated from readily available mapping products. The HRU is conceptually similar to other computational units such as the Representative Elementary Area (REA), Representative Elementary Watershed (REW), Grouped Response Unit (GRU), hydro-landscape unit, and field (Dehotin & Braud, 2008; Fenicia, Kavetski, Savenije, & Pfister, 2016; N Kouwen, Soulis, Pietroniro, Donald, & Harrington, 1993; Reggiani, Sivapalan, & Hassanizadeh, 1998; Wood, Sivapalan, Beven, & Band, 1988), and therefore the approach developed here will port over to models which are discretized using these alternative definitions of the smallest computational unit. In recent decades, the traditional approach for watershed discretization has been to use Geographic Information Systems (GISs) such as ESRI's ArcGIS software or ArcGIS-based toolkits such as Arc HYDRO, ArcSWAT, and HEC-GeoHMS (Doan, 2000; ESRI, 2014; Maidment, 2002; Winchell, Srinivasan, Di Luzio, & Arnold, 2007). While such automatic techniques make watershed discretization easy to practically implement, they do not have an explicit mechanism to account for, or assess, spatial input data information losses due to discretization choices. Here, information loss refers to the content change between candidate discretization schemes and the original, fully detailed, input data layers. Instead, modelers can only explicitly assess the model complexity under candidate discretization schemes based on the number of modelled homogeneous areas (subbasin or HRU computational units).

Haghnegahdar et al. (2015) claim that most modelers make discretization decisions in an ad hoc fashion. This approach is often based on the past experience of the modeler, rules of thumb or default discretization settings in specialized ArcGIS-based toolkits for creating a distributed hydrologic model (e.g., ArcSWAT (Winchell, et al., 2007)). The shortcoming with all ad hoc approaches is that there is no quantitative or formal justification of the selected discretization over other potential discretization choices. More sophisticated discretization approaches found in the literature use a cumbersome trial-and-error approach of building and then possibly calibrating multiple candidate models with different discretization levels in order to identify the most appropriate choice. For example, Arnold et al. (2010) compared the calibration and validation period flow simulation results of an enhanced SWAT model with four landscape delineations, and Petrucci and Bonhomme (2014) tested the calibration and validation period water quantity and water quality simulation results of six different discretization scenarios of the Stormwater

Management Model. Haghnegahdar et al. (2015) followed a similarly intensive but improved process except that they took into account the computational time spent for calibrating (calibration budget) and focused on the model performance in ungauged basins under four discretization schemes for a land-surface hydrologic modelling application. All of these approaches require model calibration in order to assess the quality of a given discretization scheme.

Given the above limitations, other studies have instead focused on designing *a priori* discretization error metrics to quantify the information loss incurred from spatial discretization. Such metrics are advantageous in that they do not require model runs. Haverkamp et al. (2002) provided an entropy based statistical tool, the Subwatershed Spatial Analysis Toll (SUSAT), to estimate the information loss for subwatershed and HRU discretization, respectively. Booij (2003) utilized the bias of the variance of aerially averaged variables under different correlation lengths to decide the appropriate modeling scale. Dehotin and Braud (2008) used Manhattan distance to measure the composition descriptor (e.g., histogram, mean, standard deviation, or matrix of co-occurrence) similarity between each mapping cell and the reference zones. There are three main shortcomings of the existing *a priori* discretization error metrics. First, the metrics do not directly correlate to the information required by hydrologic modeling applications, in particular for semi-distributed modeling. For example, entropy represents spatial disorder from the systematic perspective, but spatial heterogeneity essentially describes spatial pattern variability (Journel & Deutsch, 1993). Changes in system disorder cannot fully reflect the (more hydrologically important) changes in spatial heterogeneity and hence entropy is not a directly interpretable indicator for hydrologic modeling. Second, their property change identification process fails to refer to the original spatial input data in a complete way (i.e., cell-by-cell comparison). Instead, they use the overall heterogeneity statistics difference between a candidate discretization scheme and the original spatial input data as the information loss, which may lead to the equifinality problem. Finally, the existing *a priori* approaches are all aggregated (e.g., over the entire study watershed) and do not provide spatially distributed evaluations of candidate discretizations. The importance of evaluating distributed model behaviors rather than an integrated value (e.g., runoff at the watershed outlet) for distributed models has been highlighted by numerous researchers (Beven & Binley, 1992; Grayson, Blöschl, Moore, & Singh, 1995; Refsgaard, 1997; Shrestha & Rode, 2008). Just like multi-site calibration provides an efficient framework for spatially distributed evaluations (Madsen, 2003), multi-site discretization quality assessment is intrinsically valuable to reduce the prevalence of aggregation or compensation effects in distributed hydrologic modeling. With such shortcomings in mind, this study is focused on developing *a priori* discretization error metrics that are directly interpretable, spatially distributed, and hydrologically relevant, providing a direct measurement of information loss relative to the original spatial input data, where the original spatial data is presumed to have the highest information content.

In addition to the information loss induced by the extensively studied HRU discretization, another type of information loss occurs due to subbasin discretization which affects the routing processes of semi-distributed and distributed models, hereinafter called routing information loss. In a finely discretized fully distributed model, channel structure, channel roughness, and therefore network travel times can be well-respected. As the watershed is discretized into subbasins, stream network branches are implicitly merged, replaced, and shortened. As far as we know, in the published literature, the routing information loss has never been quantified though its significance has been highlighted by many studies. For example, Haverkamp (2002) indicates that the influences of the routing structure through subbasins to the watershed outlet should be considered in discretization evaluations when the effect of the routing on model results is not negligible. Dehotin and Braud (2008) emphasize the prospect of inclusion of linear discontinuities, including river reaches, hedges, ditches, and dikes, in order to properly describe networks in spatial discretization. Here, we address this need through the introduction of additional error metrics to estimate the routing information loss due to subbasin discretization.

The specific goals of this study are to (1) introduce *a priori* discretization error metrics to quantify the information loss due to subbasin and HRU discretization, respectively; (2) propose a two-step decision-making approach to identify an appropriate discretization scheme; (3) apply the error metrics and decision-making approach to the discretization of the Grand River watershed in Ontario, Canada. The simplicity of the error metrics allows for easy recoding and adoption into the preprocessing of a wide range of distributed models, including all semi-distributed models, such as HBV (Bergström, 1976, 1992), TOPMODEL (Beven & Kirkby, 1979), WATFLOOD (Nicholas Kouwen, 1988), the Soil and Water Assessment Tool (SWAT) (J. G. Arnold, Srinivasan, Muttiah, & Williams, 1998), and Modélisation Environmentale–Surface et Hydrologie (MESH) (Pietroniro et al., 2007). The error metrics may also be useful for fully distributed models, e.g., System Hydrologique Europeen (SHE) (Abbott, Bathurst, Cunge, O'Connell, & Rasmussen, 1986), TOPKAPI (Ciarapica & Todini, 2002), and Soil Moisture Distributed and Routing (SMDR) (Srinivasan, Gérard-Marchant, Veith, Gburek, & Steenhuis, 2005) when the model cell scales are greater than the resolution of original spatial input data.

The reminder of the paper is organized as follows. Section 2 describes in detail the *a priori* discretization error metrics and the two-step discretization decision-making approach. Section 3 explains the error metric applications to the Grand River watershed discretization. Section 4 provides an effective discussion of the proposed methods. Section 5 summarizes conclusions.

2. Methodology

2.1. Discretization Error Metrics

Our *a priori* discretization error metrics provide a novel and simple quantitative measurement of the information loss in the process of spatial discretization. They are introduced for the purpose of assessing candidate discretization schemes and finding an appropriate discretization level in data preprocessing without having to rely on computationally intensive hydrologic model building exercises. For each candidate discretization scheme, the metrics are designed to compare the user-defined key model input variable properties with that of a reference discretization scheme. The reference scheme is defined as a scheme that fully retains the information of the original spatial input data or, in special cases, the finest plausible discretization. Both a subbasin discretization error metric and a HRU discretization error metric are proposed.

2.1.1. Subbasin Discretization Error Metric

In general, the routing process has two components: in-catchment routing and in-channel routing. In-catchment routing occurs within a subbasin, and refers to the means of handling the delayed release of water from runoff, interflow, and baseflow to a subbasin outlet. This time delay is typically described by a unit hydrograph. In contrast, in-channel routing is the means by which water is exchanged downstream between subbasins and within the main channel of each subbasin. These definitions are applied by other models like ArcSWAT and HEC-GeoHMS (Doan, 2000; Winchell, et al., 2007). Our subbasin discretization assessment focuses on the influences of discretization only on in-channel routing. The approach assumes that in-channel routing is unidirectional (i.e., water moves downstream only through a branching stream network), each subbasin has one outlet and one main channel, headwater subbasins have no main channel for routing, and non-headwater subbasins have upstream subbasin flows added to the beginning of their respective main channels. Should any of these assumptions not hold in other modelling case studies, the error metric procedures detailed below would need to be adjusted accordingly.

Calculation of subbasin discretization errors requires a high resolution reference subbasin discretization scheme. For the drainage area upstream of a subbasin outlet, the in-channel routing length error (ΔL_s) equals to the in-channel routing length difference between the reference scheme (scheme 0) and the evaluated discretization (scheme s) as shown in Equation 1.

$$\Delta L_s = L_0 - L_s = \frac{\sum_{i=1}^{n} A_{i0} L_{i0}}{\sum_{i=1}^{n} A_{i0}} - \frac{\sum_{j=1}^{m} A_{js} L_{js}}{\sum_{j=1}^{m} A_{js}} \tag{1}$$

where L_0 and L_s are respectively the area-weighted in-channel routing length of scheme 0 and scheme s. For scheme 0, there are n subbasins within the evaluated drainage area and $i = 1,2,\cdots,n$ represents subbasin indices. A_{i0} is the area of subbasin i in scheme 0, and $\frac{\sum_{i=1}^{n} A_{i0} L_{i0}}{\sum_{i=1}^{n} A_{i0}}$ is the area-weighted sum of the in-channel routing length of subbasin i from the subbasin i outlet to the drainage area outlet of interest. For scheme s, there are m subbasins within the evaluated drainage area and $j = 1,2,\cdots,m$ represents subbasin indices. A_{js} is the area of subbasin j in scheme s, and $\frac{\sum_{j=1}^{m} A_{js}L_{js}}{\sum_{j=1}^{m} A_{js}}$ is the area-weighted sum of the in-channel routing length of subbasin j from the subbasin j outlet to the drainage area outlet of interest. The total area of the drainage area is $A = \sum_{i=1}^{n} A_{i0} = \sum_{j=1}^{m} A_{js}$.

The calculation of the in-channel routing length difference between schemes is best described in Figure 1 below with a visual example. The example in Figure 1 demonstrates the in-channel routing length difference (ΔL_s) between scheme 0 and scheme s as the difference in the thick routing arrows between the two discretization options. For example, in scheme 0, flows from headwater subbasins 1, 2 and 3 are all routed in the main channel of subbasin 7 for 2 km. In comparison, with the coarser discretization scheme *s*, the flows from this region of the watershed (subbasins 1, 2 and 3 in scheme 0) are no longer routed in-channel for this distance and thus treated as a discretization error. A similar error occurs for the subarea including subbasins 4, 5 and 6. In our metric, in-channel routing length errors are computed for subbasin outlets of interest and in this example, the 'outlet' is the site of interest in Figure 1. If all flows reaching the outlet had a 2 km shorter in-channel routing length in scheme *s* versus scheme 0, then ΔL_swould be 2 km at the outlet. This is not typically the case and so the representative change in routing length, ΔL_s, must account for this using area-weighting.

Figure 1. Here.

2.1.2. HRU Discretization Error Metric

As explained before, the information loss from spatial discretization is due to the diminished representation of spatial data content between a candidate discretization scheme and the original, fully detailed, input data layer. To quantify the relevant (case study specific) information loss derived from HRU discretization, the dominant hydrologic processes should first be identified by considering the modeling purpose, physiographic characteristics and management measures within the watershed. These dominant processes can be linked to dominant hydrologic model input variables derived from map inputs which will be used to evaluate information losses. For example, in rainfall-runoff modeling, if infiltration is identified as a critical process then the most relevant variables to compute information losses for can be hydraulic conductivity and/or available water content.

For a drainage area above an outlet, assume there are n HRUs in the reference scheme (scheme 0), and m HRUs in the evaluated discretization (scheme s), and thus $n \geqslant m$. In order to effectively consider the spatial pattern changes between the two schemes, the evaluated scheme layer needs to be overlaid with the reference scheme layer using vector overlay tools (e.g., union) for vector maps or raster overlay tools (i.e., weighted overlay) for raster maps in ArcGIS (ESRI, 2014). After overly, each polygon or cell of the output possesses both the evaluated and reference scheme HRU properties. Assume there are v polygons (cells) $(u = 1, \ldots, v)$ of the output. HRU discretization error metrics are designed to go through each polygon (cell) and measure the relative error of variable change between scheme s and scheme 0. Two different *a priori* discretization error metrics corresponding to nominal (categorized) and quantitative (continuous) data are developed.

Figure 2 shows an example of the overlay comparison process required for computing HRU discretization errors for an example subbasin, corresponding to subbasin 1 of scheme 0 in Figure 1, and uses a nominal variable (land cover) as an example. In scheme 0, there are four different land covers scattered over the entire subbasin (Figure 2a), but only two land covers remain in the coarser scheme s (Figure 2b). After overlay and property comparison, four cells show a property change as highlighted in Figure 2c, in which one cell of coniferous forest turns into deciduous forest, and one cell of coniferous forest and two cells of pasture turn into crop. The information loss due to recategorization is considered as a discretization error, expressed in terms of recategorized area (i.e., 4 km^2 in this example). For quantitative variables, the only difference is the absolute values of the property changes are utilized as shown in the following equations.

Figure 2. Here.

For nominal input variables (e.g., soil and land cover), the relative error equals to the sum of areas with property change from scheme 0 to scheme s divided by the total drainage area.

$$\delta_{HRUs} = \frac{\sum_{u=1}^{v} \Delta_u A_u}{\sum_{u=1}^{v} A_u} \tag{2}$$

$$\Delta_u = \begin{cases} 0, & if\ variable\ prorpty\ is\ unchanged\ relative\ to\ the\ reference\ scheme \\ 1, & if\ variable\ property\ is\ changed\ relative\ to\ the\ reference\ scheme \end{cases} \tag{3}$$

where δ_{HRUs} is relative error (0-1) of the evaluated scheme s describing the proportion of the drainage area where the variable property is changed and thus incorrect relative to the original spatial data. A_u is the area of the u^{th} polygon (cell) of the overlay output.

For quantitative input variables (e.g., hydraulic conductivity and available water content), the relative error equals to the area-weighted sum of the absolute values of input variable differences of all polygons (cells) between scheme s and scheme 0 divided by the area-weighted mean input variable value of scheme 0 within the drainage area. It is expressed as:

$$\delta_{HRUs} = \frac{\sum_{u=1}^{v} w_u |x_{us} - x_{u0}|}{\sum_{i=1}^{n} w_i x_{i0}} \quad (4)$$

where δ_{HRUs} is relative error (0-1) of the evaluated scheme s indicating the level of absolute input variable value change relative to the mean value of scheme 0. x_{us} and x_{u0} are the input variable values of the u^{th} polygon (cell) in scheme s and scheme 0, respectively. w_u is the area weight of the u^{th} polygon (cell) of the total drainage area. It is calculated by:

$$w_u = \frac{A_u}{\sum_{u=1}^{v} A_u} \quad (5)$$

where $\sum_{u=1}^{v} A_u$ is the total area of the evaluated drainage area.

The absolute value operation utilized in Equation (4) is to properly track all spatial heterogeneity changes once the input variable property differs from the original spatial input data. In other words, compensation effects (two errors cancelling each other) are not allowed.

2.2. Sensitivity of Hydrologic Model Simulation Results to Discretization Error Metrics

To validate the impact of the *a priori* error metrics on hydrologic model simulation results, multiple hydrologic models were built (one for each candidate discretization scheme). The only difference between these models exists in discretization. We chose to build our simulation models for different discretization levels in the Raven hydrological modeling framework (Craig et al., 2016). All the models are semi-distributed with two buckets and simulate water transfer between soil (upper and lower layers) and atmosphere through a series of hydrologic processes. The models simulate on an hourly time step and in-channel routing is based on a non-linear level pool routing approach using Manning's equation. Specific details of the hydrologic model are provided in Appendix A.1 of this paper.

Similar to discretization error metrics, hydrologic simulation results are assessed relative to a reference simulation result. The reference simulation result corresponds to the model using the reference discretization scheme (scheme 0). All other model simulation results are compared relative to the reference result using error indices such as the peak flow rate error, the peak flow timing error, and the cumulative flow volume error. The peak flow rate error is computed as the absolute peak flow rate difference between scheme s and scheme 0 divided by the peak flow rate of scheme 0. The peak flow timing error is the time of peak flow occurrence with scheme 0 minus the time of peak flow occurrence with scheme s. The cumulative flow volume error is the absolute cumulative flow volume difference between scheme s and scheme 0 divided by the cumulative flow volume of scheme 0. Non-zero values for these indices are the direct result of different discretization choices.

The relationship between discretization errors and model errors is estimated by the Spearman's rank correlation coefficient (r_s) which ranges from -1 to +1. The objective of this analysis is to validate that changes in our proposed error metrics indeed impact hydrologic model simulation results. Note that our analysis necessarily avoids the issue of model calibration and validation decisions confounding the analysis. A future larger scale, multi-basin study would be required to properly validate the role discretization errors have in terms of their net impact on model predictive accuracy.

2.3. Discretization Decision-Making Approach

We demonstrate one of many ways modelers can utilize the proposed *a priori* error metrics by using them within a structured two-step approach to watershed discretization decision-making. The two-step approach is applicable to both subbasin and HRU discretization decisions and is described in the following two sections.

2.3.1. Subbasin Discretization Decision-Making Approach

Step 1: Select a subbasin scheme from candidate discretization schemes (Candidacy step).
Candidate subbasin schemes would typically first be generated by placing subbasin outlets at the sites of interest within the watershed (e.g., gauge stations and/or reservoirs) and at stream junctions, with subbasin boundaries determined using standard terrain analysis algorithms. The subbasin boundaries will vary depending on stream network resolution. Here, we generate the stream network and junctions based on a flow accumulation threshold as done in ArcSWAT (Winchell, et al., 2007). Other approaches to junction generation could be used, for example, truncating the stream network based upon Strahler stream order. The relationships between the flow accumulation threshold and the coarseness of the stream network are monotonic – as the accumulation threshold increases, stream network becomes less detailed and fewer subbasins are included. In this step, typically users should vary the spatially consistent flow accumulation threshold (uniformly applied for the entire watershed) and assess the resulting routing length errors.

A routing length error threshold (referred to as the preliminary error threshold) is then specified to select a subbasin scheme from candidates. The selected scheme meets the criteria that all sites of interest satisfy the preliminary error threshold at the minimum discretization complexity cost (i.e., the total number of subbasins) among all candidate schemes. Setting the preliminary error threshold to a very large value would function to select the most coarsely defined candidate scheme among the candidates.

Step 2: Refine subbasin discretization for the areas with extreme discretization errors (Polishing step).

This step is used to refine the candidate subbasin discretization selected in Step 1 for the areas with the most extreme discretization errors. It can also be used to focus on minimizing discretization errors at modeler-specified critical sites of interest where smaller discretization errors are desired for some reason. Functionally speaking, this step is optional. If utilized, this step involves specifying a second, stricter routing length error threshold (referred to as extreme error threshold) and requires the stream junction locations of other finer resolution candidate schemes. Given a subbasin scheme from *Step 1*, the complete process of *Step 2* is demonstrated by Figure 3.

Figure 3. Here.

Step 2a: Identify the sites of interest with extreme discretization errors.

Sites of interest with discretization errors not satisfying the extreme error threshold are identified. These sites are referred to as extreme sites.

Step 2b: Replace junctions in the upstream refinement areas of extreme sites with those of the nearest, more detailed satisfactory discretization scheme.

There are three cases in identifying the upstream refinement area for each extreme site:

- Case 1. If the extreme site has no upstream sites of interest, increased resolution of the stream network is applied to the whole drainage area above the extreme site.
- Case 2. If the extreme site has satisfactory (non-extreme) upstream site(s) of interest, increased network resolution is only applied to the intermediate area between upstream site(s) of interest and the extreme site.
- Case 3. If the extreme site has an upstream extreme site(s), the network is not refined. What will happen in this case is that the upstream extreme site(s) will first be refined (under Case 1) and then in a future discretization refinement iteration, the intermediate area(s) will only be refined if the new discretization error(s) for the site in question remains extreme (the extreme site will be re-categorized into Case 2).

Once the upstream refinement area is determined, replace the junctions within it with those of the nearest more detailed satisfactory scheme. More detailed alternate candidate schemes would typically be available from the candidacy selection step (Step 1) but if not, the modeler would be required to generate one or more detailed schemes (e.g., by decreasing the flow accumulation threshold). It is worth explaining the reason why there is no need to replace junctions for the extreme sites of Case 3. In Case 3, the influence of the upstream refinement on the downstream error metric result is unclear unless the new errors are recalculated. If the extreme site located downstream can take the advantage of upstream refinement and obtain a satisfactory error result without junction replacements, this will be the most cost-effective solution in terms of model complexity.

Step2c: Re-discretize subbasins and re-calculate errors for the sites of interest.

In order to get the systematic upstream-downstream flow path relation among subbasins, re-discretize the watershed with the updated junctions and re-calculate the error metric results. The detailed re-discretization processes are provided in the Appendix A.2 of this paper.

- If the new error metric results in all the previously extreme sites are satisfactory (less than the extreme error threshold), adopt these junctions. *Step 2* ends.
- If some extreme sites do not satisfy the extreme error threshold, return to *Step 2b*. Iterate *Step 2b* and *Step 2c* until all the extreme sites are satisfactory.

Because the polishing step introduces non-uniformity to the discretization scheme (i.e., the refined areas have finer subbasin discretization than the non-refined areas), we refer to this discretization scheme as a non-uniform scheme.

2.3.2. HRU Discretization Decision-Making Approach

Similar to subbasin discretization decision-making, modelers can also choose an appropriate HRU discretization following the two-step decision-making approach outlined in Section 2.3.1. *Step 1* is selecting a uniform HRU scheme from candidates based on some predefined uniform HRU discretization preliminary error threshold(s). As with subbasin discretization, the candidate HRU discretization schemes should each be based on some uniform level of detail across the watershed. As described in Section 2.3.1, we identified candidate HRU schemes by varying an

HRU size threshold, below which the small HRUs in that subbasin are merged and replaced with more dominant HRU types. Again, the relationship between this size threshold and the model complexity is monotonic. Unlike the subbasin discretization step, there may be multiple hydrologic model input variables for which a modeler wishes to compute HRU discretization errors. In this case, the metric results of multiple input variables can be treated equally or assigned different weights based on their importance in decision-making.

Step 2 is polishing HRU discretization. The only difference from subbasin discretization refinement is that, in *Step 2b*, HRUs can be directly replaced without junction replacement. *Step 2c* simply involves merging all resultant HRUs into an output layer and re-calculating errors for the sites of interest.

3. Results of Discretization Error Metrics Application

This study is conducted in the Grand River watershed in southwestern Ontario, Canada. With drainage area of 6704 km^2, the Grand River flows south to Lake Erie and is mainly covered by agricultural land. The applications are presented in two sections. Section 3.1 shows the application of the subbasin discretization error metric, and Section 3.2 shows the application of the HRU discretization error metric.

3.1. Subbasin Discretization Error Metric Application

3.1.1. Candidate Subbasin Discretization Schemes

In this study, subbasins were represented in subwatershed format and derived from $10m \times 10m$ digital elevation model (DEM) data. Subbasins were discretized based on the ArcSWAT (Winchell, et al., 2007) flow accumulation threshold approach as described in Section 2.3.1. Research shows that, reducing the flow accumulation threshold below 0.5% of the maximum flow accumulation doesn't improve model performance but complicates remaining preprocessing, whereas increasing it significantly above 1% might lead to performance ramifications (Djokic, 2008). According to these findings, we took the percentage of the maximum flow accumulation across the entire watershed as the subbasin discretization threshold and treated 0.5% as the minimum flow accumulation threshold value. Therefore, twelve candidate subbasin schemes were generated corresponding to twelve successively increasing flow accumulation thresholds. The detailed subbasin discretization results are listed in Table 1.

Scheme 0 was defined as the reference scheme because subbasin discretization with threshold 0.5% is the finest scheme of all the candidates and we assume the channel information loss between the real full channel scheme (i.e., one channel for each DEM cell) and scheme 0 is irremediable. Scheme Max only used the 32 sites of interest as subbasin outlets. The 32 sites include 24 gauge stations, 7 dams, and the watershed outlet, and their detailed information has been listed in Table 2.

Table 1. Candidate subbasin discretization schemes

Scheme	Flow accumulation threshold (%)	Number of subbasins
0	0.5	130
1	0.6	110
2	0.7	100
3	0.8	94
4	0.9	92
5	1.0	90
6	2.0	60
7	3.0	46
8	5.0	44
9	6.0	40
10	10.0	38
Max	Only sites of interest	32

Table 2. Details of 32 sites of interest and their drainage areas

Site of interest	Site name	Drainage area (km^2)	Site of interest	Site name	Drainage area (km^2)
1	02GA041	66	17	02GA015	565
2	Luther Dam	45	18	02GA038	313
3	02GA014	654	19	Laurel Creek Dam	31
4	02GA039	272	20	02GA024	59
5	Shand Dam	775	21	02GA047	757
6	02GA016	776	22	02GA048	2477
7	Conestogo Dam	559	23	Shades Mill Dam	96
8	02GA028	564	24	02GA018	536
9	02GA040	178	25	02GA003	3490
10	Woolwich Dam	60	26	02GA010	1028
11	Guelph Dam	241	27	02GB006	157
12	02GA034	1148	28	02GB007	384
13	02GA031	40	29	02GB001	4784
14	02GA023	113	30	02GB008	378
15	02GA029	226	31	02GB010	170
16	02GA006	769	32	Watershed outlet	6704

In this study, we consider all 32 sites of interest as locations where the discretization error metrics will be assessed. Each drainage area is the combined total upstream area draining to the site as illustrated in Figure 4. For instance, drainage area 3 is defined to include subbasins 1, 2 and 3.

Figure 4. Here.

3.1.2. Subbasin Discretization Error Metric Results

In distributed hydrologic modeling applications, most of the time modelers will only pay attention to the information loss at the sites of interest. Moreover, it is unnecessary to analyze error metric results for the sites above which candidate subbasin discretizations are always as fine as the reference one because in this situation the error metric result is always zero. As a result, we limited the subbasin error metric results analysis to the 32 sites as introduced in Section 3.1 and then excluded the 13 sites whose upstream subbasins do not change from scheme 0 to scheme Max. The remaining 19 sites for analysis are sites 3, 5, 6, 7, 8, 9, 11, 12, 16, 17, 18, 21, 22, 24, 25, 26, 28, 29, 32, and their error metric results for the twelve discretization schemes were computed. For brevity, only the results from nine representative subbasin schemes are shown in Figure 5.

Figure 5. Here.

In each subplot of Figure 5, the routing length errors of the 19 sites are plotted versus their drainage areas. Figure 5(a) shows that when discretization is detailed at the reference scheme level, no error exists. Then in Figure 5(b-i), as subbasin discretization gets coarser, the number of subbasins within a drainage area decreases, and the routing length error increases. This is reflected by the ranges of error values of Figure 5(b-i). Moreover, in each subplot, the downstream sites with the largest drainage areas typically have intermediate error values rather than the maximum value of all the errors at the 19 sites of interest. For example, moving downstream in the Grand River watershed, site 22 (drainage area 2477 km^2), site 25 (drainage area 3490 km^2), and site 29 (drainage area 4784 km^2) all get intermediate error values for all the subbasin schemes. This trend can be explained by the fact that, for in-channel routing, the downstream error integrates all its upstream errors in an area-weighted fashion (see Equation 1), so the drainage area outlet is not necessarily the point that has the largest information loss. This implies that if modelers are concerned about the multi-site discretization quality or the multi-site hydrologic model performance, multiple sites rather than just the watershed outlet are worth considering in subbasin discretization evaluation.

3.1.3. Sensitivity of Hydrologic Model Simulation Results to Subbasin Discretization Error Metric

To access the sensitivity of model simulation results to the proposed subbasin error metric, we built twelve hydrologic models corresponding to all the subbasin schemes of Table 1, in which their only difference is subbasin discretization and the connectivity between subbasins. We focused the analysis on a short period (Jan 4 – Jan 20, 2008) of peak or near peak measured flows over the last ~15 year period across the Grand River watershed. The reference simulation result corresponds to the model using the reference discretization scheme (scheme 0 of Table 1) and all simulation model results were compared relative to the reference result using the peak flow rate error and peak flow timing error.

Taking the watershed outlet as an example, Figure 6 summarizes the relationship between the *a priori* routing length error metric and the hydrologic model error indices where each data corresponds to one of the eleven candidate subbasin discretization schemes. As the routing length error increases, both model error indices increase (almost monotonically) to practically significant levels. Correlation (r_s) between the routing length error and the peak flow rate error is 0.99, and correlation (r_s) between the routing length error and the peak flow timing error is also 0.99. This strong correlation is observed for the majority of sites of interest (e.g., considering the correlation between the routing length error and the peak flow rate error, 15 sites show r_s values of 0.8 or more).

Figure 6. Here.

3.1.4. Subbasin Discretization Decision-making

Based on the error metric results of all candidate subbasin discretization schemes, we applied the two-step decision-making approach to get an appropriate subbasin discretization scheme. It was assumed that all of the 19 sites of interest are equally important, and 21 km is selected as the preliminary routing length error threshold. The subjective value of 21 km was selected for demonstration purposes and based on balancing travel time error implications (assuming a reference velocity of 1 m/s) and computational complexity (limiting number of subbasins).

Step 1: Select a subbasin scheme from candidate discretization schemes

Scheme 6 (number of subbasins=60) was chosen as the uniform threshold subbasin scheme because the error metric values of all the 19 sites of scheme 6 are satisfactory (less than 21 km) and the number of subbasins is the minimum among all the satisfactory schemes (schemes 1-6).

Step 2: Refine subbasin discretization for the areas with extreme discretization errors

- Step 2a: Identify the sites of interest with extreme discretization errors (extreme sites).

  The extreme error threshold was 10.7 km, defined as the 90th percentile of the error distribution of scheme 6, and the resultant extreme sites that have the highest 10% errors were sites 26 and 28, which are highlighted in Figure 7a and Figure 7b.

- Step 2b: Replace junctions in the upstream refinement areas of extreme sites with those of the nearest, more detailed satisfactory discretization scheme. Specifically, different sites have different upstream refinement areas:

  Case 1: Site 28 has no upstream sites of interest, thus junction replacement is applicable to the whole drainage area above site 28. Since the error of site 28 in scheme 5 is 4.2 km (less than 10.7 km), scheme 5 is the nearest satisfactory scheme compared with scheme 6.

  Case 2: Site 26 has a satisfactory upstream site of interest, site 24, so junction replacement only takes place in the intermediate area between the site 24 and site 26. Since the error of site 26 in scheme 5 is 5.0 km (less than 10.7 km), scheme 5 is also the nearest satisfactory scheme relative to scheme 6.

- Step2c: Re-discretize subbasins and re-calculate errors for the sites of interest.

  After re-discretization, the subbasin compositions within the upstream refinement areas were changed to the new more detailed subbasins as shown in Figure 7c. Meanwhile, the total number of subbasins for the entire Grand River watershed increased from 60 to 66. The routing length errors of sites 26 and 28 became satisfactory (less than 10.7 km as shown in Table 3).

Figure 7. Here.

Table 3 shows the routing length errors of scheme 6, refined scheme 6, and scheme*. Scheme* has the same number of subbasins as refined scheme 6 but was generated with a uniform flow accumulation threshold of 1.55%. In addition to the purposeful reduction of routing errors at the two extreme sites, Table 3 also shows the substantial error decrease of all the associated downstream sites (e.g., sites 29 and 32) in refined scheme 6. Moreover, comparing refined scheme 6 with scheme*, the error mean and standard deviation of refined scheme 6 are lower than those of scheme*. This indicates that the refined subbasin discretization better represents the in-channel routing structure than the uniform discretization under the same number of computational (subbasin) units.

Table 3. Subbasin discretization error metric results for three subbasin discretization schemes. Scheme 6 is based on a flow accumulation threshold of 2.0%, while Scheme* is based on a threshold of 1.55%. Sites of interest that are discretized the same way under all three schemes are not included. Highlighted errors for refined scheme 6 are lower than corresponding errors in one or both of Scheme 6 and Scheme*. Note that site 32 corresponds to the watershed outlet.

Site of interest	Scheme 6		Refined scheme 6		Scheme*	
	Number of subbasins	Error (km)	Number of subbasins	Error (km)	Number of subbasins	Error (km)
7	4	4.0	4	4.0	6	0.9
8	5	4.0	5	4.0	7	0.9
16	6	6.4	6	6.4	2	3.9
17	7	1.7	7	1.7	8	4.1
18	3	0.0	3	0.0	7	1.7
22	25	5.9	25	5.9	27	5.2
25	37	4.7	37	4.7	39	4.2
26[e]	5	20.7	9	5.0	5	20.7
28[e]	1	20.4	3	4.2	3	4.2
29	47	8.0	51	4.6	49	7.6
32	60	8.5	66	5.2	66	7.0
Error mean		7.7		4.2		5.5
Error St. deviation		6.8		1.8		5.5
Error 90^{th} percentile[f]		10.7[f]				

[e] denotes an extreme site under scheme 6 based on exceeding the 90^{th} percentiles of the error metric. The subbasin discretization within this site's drainage area is refined based on *Step2*.
[f] The 90^{th} percentile computed based on errors across all 19 sites considered (see Section 3.1.2).

3.2. HRU Discretization Error Metric Application

3.2.1. Candidate HRU Discretization Schemes

In this study, HRU is discretized after subbasin, and an HRU is defined as the unique combination of subbasin and soil and land cover categories. Subbasin input was one of the candidate subbasin schemes generated in Section 3.1. Soil spatial input data was from the Canadian Soil Information Service (CANSIS) available from Agriculture and Agri-Food Canada (2013) and subdivided into fourteen classes in terms of soil profile. Each soil profile except water is built up by a unique soil horizon combination from three mineral horizons A, B, C, and an organic horizon O. Soil profile A-B-C covers more than 70% of the Grand River watershed (Table 4a). Land cover spatial input data was from Canada's National Land Cover Database available from Natural Resources Canada (2014) and subdivided in seven classes, in which cropland is dominant across the watershed (Table 4b). Soil and land cover inputs used here are vector coverages derived from 1:20,000 to 1:60,000 scale county-level soil maps attained from CANSIS and 1:50,000 scale land cover maps from Canada's National Land Cover Database.

The map obtained by the overlay (union) of the above subbasin, soil, and land cover layers defines the reference HRU scheme (scheme 0). Since the map algebra union operation usually leads to a very fragmented set of sliver HRUs, these sliver HRUs can be suppressed for aggregation based on certain HRU size threshold. Here, the HRU size threshold was defined as the HRU area percentage of its affiliated subbasin. The HRU whose area percentage is less than the size threshold was merged with its neighboring HRU sharing the longest border within the same subbasin. In order to investigate the influence of the subbasin discretization input on HRU discretization, we chose two representative subbasin schemes (scheme 5 and scheme Max) as subbasin inputs to discretize HRUs, respectively. The generated candidate HRU schemes are listed in Table 5. For the HRU candidates under 90 subbasins, HRU scheme 0 (number of HRUs=2706) is the reference scheme; while for the HRU candidates under 32 subbasins, HRU scheme 0 (number of HRUs=1232) is the reference scheme. Each reference scheme retains 100% of land cover and soil data as the reference scheme does not eliminate/aggregate sliver HRUs. In HRU scheme Max, each subbasin is represented by the dominant HRU. Table 5 shows that subbasin discretization choice significantly affects HRU discretization complexity (i.e., the number of HRUs) because under the same HRU size threshold, the number of HRUs with 90 subbasins input is always two to three times more than that with 32 subbasins input.

Table 4. Grand River watershed (a) Soil classes (b) Land cover classes and their percent coverage of the watershed.

Soil class	Area percentage (%)
A B C	72.29
Water	8.17
A B BC C	7.76
O B	3.40
A B	3.32
A AB B C	2.51
A B AB B C	1.13
AB	0.64
C	0.27
A C	0.25
O C	0.12
A	0.09
C A C	0.04
A AB C	0.03

Land cover class	Area percentage (%)
Annual Cropland	40.70
Perennial Cropland and Pasture	33.91
Deciduous Forest	14.74
Urban	5.43
Mixed Forest	2.98
Wetland	1.24
Water	1.00

Table 5. Candidate HRU discretization schemes with two subbasin discretization schemes (90 and 32 subbasins)

HRU Scheme	HRU size threshold (% of subbasin area)	Number of HRUs	
		Number of subbasins=90	Number of subbasins=32
0	0	2706	1232
1	1	852	333
2	2	625	234
3	3	502	190
4	4	433	156
5	5	385	135
6	6	346	121
7	7	318	109
8	8	290	99
9	9	252	90
10	10	234	84
Max	One HRU per subbasin	90	32

3.2.2. HRU Discretization Error Metric Results

In this study, infiltration and evapotranspiration were identified as the two dominant hydrological processes, thus vertical hydraulic conductivity (Kz), available water content (AWC), and land cover were defined as the key hydrologic model input variables of interest. For each soil class of Table 4a, Kz and AWC are the weighted harmonic mean values of the Kz and AWC of its soil horizon components. The detailed soil horizon information is available from Agriculture and Agri-Food Canada (2013). The area-weighted mean values of Kz and AWC of the entire watershed are 0.9 cm/h and 12.6% (except the soil class water), respectively. Figure 8 demonstrates the discretization error metric results of Kz, AWC, and land cover at the watershed outlet versus HRU size thresholds. As the HRU size threshold increases, discretization gets coarser, meanwhile the relative errors of all the three variables increase. However, the same HRU size threshold imposes different impacts on the information losses of different variables. For example, under the same HRU schemes (before HRU scheme Max), the relative errors of Kz and land cover are always similar in magnitude (Figure 8a, Figure 8c), but the relative errors of AWC are comparatively smaller (less than 0.05 in Figure 8b). In HRU scheme Max, land cover error jumps to 0.55, while Kz and AWC errors are 0.15 and 0.05, respectively. Land cover errors jump to much higher values compared to Kz and AWC because some merged HRUs only experience land cover changes but no change in soil properties. The results show that, unsurprisingly, relative discretization errors are positively correlated with HRU size threshold.

The subbasin discretization decision between 90 or 32 subbasins has a substantial influence on HRU discretization complexity (100%-200% increase in number of HRUs seen in Table 5). However, this decision does not make a big difference for information loss as Figure 8 indicates that two error metric results (AWC and land cover) of the three variables are almost identical and only one variable (Kz) obtains slightly different error metric results under different subbasin inputs.

Figure 8. Here.

Figure 8 supports how a modeler might make decisions based on a single watershed outlet. However, in distributed or semi-distributed modelling applications where distributed watershed responses are of interest, discretization errors should be assessed at multiple sites beyond just the outlet. Figure 9 is a more robust comparative approach than Figure 8 as it compares discretization errors at all the 32 sites of interest across the Grand River watershed under subbasin scheme 5 (number of subbasins = 90). The interesting pattern in Figure 9 is that for all the three variables of interest (Kz, AWC, and Land cover), the largest discretization errors (and the highest variance) appear in the relatively small drainage areas, and as drainage area increases, errors approach some constant level. Therefore, while errors for the watershed outlet might be sufficiently small, they can be unacceptably large in some small upstream subbasins. Although results are not shown, this pattern persists across all HRU discretization levels.

Figure 9. Here.

3.2.3. Sensitivity of Hydrologic Model Simulation Results to HRU Discretization Error Metrics

Similar to the sensitivity analysis in Section 3.1.3, we checked the sensitivity of hydrologic model simulation results to the proposed HRU error metrics based on twelve hydrologic models. These models correspond to all the HRU schemes under 90 subbasins of Table 5, and the only difference between these models is the property of HRUs. The model output with scheme 0 (Number of HRUs =2706) is the reference simulation result in model errors calculation. The peak flow rate error and cumulative flow volume error were computed.

Figure 10 presents the relationship between the *a priori* HRU discretization error metrics and the model error indices where each data corresponds to one of the eleven candidate HRU discretization schemes at the watershed outlet (subbasin 32 outlet). The two model errors are plotted versus the HRU discretization errors of Kz, AWC, and land cover. Clearly, both model errors indices monotonically increase with the HRU discretization errors of the three variables. Correlations (r_s) between the three HRU discretization errors (Kz, AWC, and land cover) and the peak flow rate error are all 0.99. Similarly, correlations (r_s) between the three HRU discretization errors and the cumulative flow volume error are also 0.99. This strong correlation also shows up in most sites of interest (e.g., considering the correlation between the land cover error metric and the peak flow rate error, 23 sites show r_s values of 0.8 or more).

Figure 10. Here

Figure 11 provides a more complete description of hydrologic simulation responses by plotting all sites of interest model errors against their drainage areas under the same three representative HRU schemes of Figure 9. The upstream sites with relatively small drainage areas obtain a high variance of model errors, in which some of them have three or more times errors than their downstream sites. This observation appears in both the peak flow rate error and the cumulative flow volume error and is consistent with results from Figure 9 (indicating the largest HRU discretization errors are also associated with small drainage areas).

Figure 11. Here

3.2.4. HRU Discretization Decision-making

An alternative to the commonly applied uniform discretization framework demonstrated above is to make discretization decisions differently in different parts of the watershed, in response to excessively high error metric values. This relies on the two-step HRU discretization decision-making approach (see Section 2.3.2) where different subareas can use different HRU delineation thresholds. To demonstrate, assume subbasin scheme 5 (number of subbasins=90) is the subbasin input for HRU discretization; all the 32 sites of interest and all the three hydrologic model input variables of interest are equivalently important in HRU scheme decision-making; and 0.40 is the preliminary error threshold for all the three variables. The subjective value of 0.40 was selected for demonstration purposes only and selected with the goal of generating a modest number of HRUs relative to the range of candidate HRU discretizations.

Step 1: Select an HRU scheme from candidate discretization schemes.

HRU scheme 10 (number of HRUs=234) was chosen as the uniform HRU scheme because the relative errors of all the sites of interest in scheme 10 are satisfactory (less than 0.40) and the number of HRUs is minimum among all the satisfactory schemes (schemes 1-10).

Step 2: Refine HRU discretization for the areas with extreme discretization errors.

- Step 2a: Identify the sites of interest with extreme discretization metrics (extreme sites).

The extreme error thresholds were defined as the 90th percentiles of the error distributions of the three variables (0.13, 0.06, and 0.31 for Kz, AWC, and land cover, respectively). As a result, the sites having the highest 10% Kz, AWC, or land cover errors were identified as the extreme sites of interest to have their discretization refined (i.e., sites 10, 13, 15, 19, 20, 23, 28, and 31). The drainage areas above sites 19 and 20 are highlighted for discretization refinement demonstration in Figure 12.

- Step 2b: Replace HRUs in the upstream refinement areas of extreme sites with those of the nearest, more detailed satisfactory discretization scheme, in which different extreme sites have different upstream refinement areas.

Case 1: Extreme sites 10, 13, 19, 23, 28, and 31 have no upstream sites of interest, so the HRU refinement areas cover the whole drainage areas above these sites.

Case 3: Extreme sites 15 and 20 have extreme upstream sites of interest (site 13 and 19, respectively), and it is unnecessary to replace HRUs across their entire drainage area in the first refinement iteration.

Then, only Case 1 sites had the HRUs within them replaced with those of the nearest more detailed satisfactory HRU scheme relative to HRU scheme 10. This replacement step was applied independently for each of the refined extreme sites. The detailed HRU replacement results are summarized in Table 6.

Table 6. HRU replacement results for the extreme sites in the first HRU discretization refinement iteration

HRU replacement area	Original number of HRUs	Nearest satisfactory HRU Scheme	New number of HRUs
Drainage area above site 10	2	HRU scheme 1	10
Drainage area above site 13	4	HRU scheme 9	5
Drainage area above site 19	4	HRU scheme 5	8
Drainage area above site 23	2	HRU scheme 7	5
Drainage area above site 28	10	HRU scheme 5	16
Drainage area above site 31	3	HRU scheme 3	7

- Step 2c: Merge all resultant HRUs into an output layer and re-calculate discretization errors for the sites of interest.

After the first refinement iteration, it was found that all Case 1 sites became satisfactory, but some errors of sites 15 and 20 were still extreme. Therefore, *Step 2b* needed to be repeated to replace HRUs for sites 15 and 20.

- Step 2b: Replace some or all HRUs in the upstream refinement areas of extreme sites with those of the nearest, more detailed satisfactory discretization scheme.

  Case 2: Extreme sites 15 and 20 became Case 2 after the first refinement iteration, and thus the intermediate area between sites 13 and 15 and the intermediate area between sites 19 and 20 were identified as the HRU replacement areas in the second refinement iteration. The HRUs within these intermediate areas were replaced with those of the nearest satisfactory schemes relative to HRU scheme 10. The detailed HRU replacement results are summarized in Table 7.

Table 7. HRU replacement results for the extreme sites in the second HRU discretization refinement iteration

HRU replacement area	Original number of HRUs	Nearest satisfactory HRU Scheme	New number of HRUs
Intermediate area 13-15[i]	10	HRU scheme 8	16
Intermediate area 19-20	1	HRU scheme 4	3

[i] Intermediate area 13-15 means the intermediate area between site 13 and site 15. This also applies to intermediate area 19-20.

- Step 2c: Merge all resultant HRUs into an output layer and re-calculate errors across the watershed.

After the second iteration, the errors of all the originally identified extreme sites became satisfactory, thus the refinement process ended and this scheme was the refined HRU scheme. Figure 12 provides a visual comparison for the HRUs before and after refinement of the drainage areas of sites 19 and 20 under subbasin scheme 5 (90 subbasins).

Figure 12. Here.

Table 8 shows the error metric results of HRU scheme 10, refined scheme 10, and scheme*. Scheme* has the same number of HRUs as refined scheme 10 (number of HRUs=271), but was generated with a uniform HRU size threshold of 8.4%. Through discretization refinement, the extreme errors identified in Step 2b above are reduced, and the discretization quality for site 32 representing the entire watershed is also improved for all the three variables. Moreover, the discretization error means and standard deviations of the three variables across all the sites of interest of the refined scheme also decrease in contrast with scheme*. Therefore, the non-uniform discretization functions to retain more input data information than the uniform discretization under the same discretization complexity. In addition, to get a sense of how non-uniform the HRU discretization is in refined scheme 10, the average HRU sizes of the uniformly discretized areas and the non-uniformly discretized areas within the watershed were respectively calculated as 28.8 km^2 and 13.6 km^2. The latter is more than 50% smaller than the former, which means the HRUs within the refined areas are obviously finer than those of the uniformly discretized areas.

Table 8. Discretization error metric results for three HRU discretization schemes (using 90 subbasins). Scheme 10 is based on an HRU size threshold of 10%, while Scheme* is based on a threshold of 8.4%. Note that site 32 corresponds to the watershed outlet and sites of interest 1, 9, 11, 18, 24, 27 and 30 are not included because they are discretized the same way under all three schemes. Highlighted errors for Refined scheme 10 are lower than corresponding errors in one or both of Scheme 10 and Scheme*.

Site of interest	Scheme 10				Refined scheme 10				Scheme*			
	Number of HRUs	Kz	AWC	Land cover	Number of HRUs	Kz	AWC	Land cover	Number of HRUs	Kz	AWC	Land cover
2	3	0.06	0.02	0.25	3	0.06	0.02	0.25	4	0.02	0.01	0.22
3	17	0.06	0.03	0.20	17	0.06	0.03	0.20	22	0.06	0.02	0.14
4	7	0.02	0.01	0.12	7	0.02	0.01	0.12	8	0.02	0.01	0.07
5	20	0.06	0.03	0.22	20	0.06	0.03	0.22	25	0.05	0.02	0.17
6	22	0.06	0.03	0.22	22	0.06	0.03	0.22	28	0.05	0.02	0.17
7	15	0.02	0.01	0.10	15	0.02	0.01	0.10	16	0.02	0.01	0.07
8	18	0.02	0.01	0.10	18	0.02	0.01	0.10	19	0.02	0.01	0.07
10[e]	2	0.11	0.06	0.11	10	0.06	0.02	0.02	2	0.11	0.06	0.11
12	29	0.06	0.03	0.19	29	0.06	0.03	0.19	35	0.06	0.02	0.15
13[e]	4	0.02	0.00	0.31	5	0.01	0.01	0.22	6	0.02	0.00	0.14
14	4	0.12	0.05	0.14	12	0.10	0.03	0.08	4	0.12	0.05	0.14
15[e]	14	0.03	0.01	0.36	21	0.03	0.01	0.26	20	0.03	0.01	0.30
16	24	0.07	0.01	0.09	24	0.07	0.01	0.09	26	0.06	0.01	0.08
17	33	0.05	0.02	0.27	40	0.05	0.02	0.23	40	0.05	0.02	0.23
19[e]	4	0.23	0.03	0.35	8	0.13	0.01	0.17	4	0.23	0.03	0.35
20[e]	5	0.23	0.03	0.34	11	0.13	0.02	0.17	5	0.23	0.03	0.34
21	36	0.07	0.03	0.26	43	0.07	0.03	0.23	43	0.07	0.03	0.23
22	89	0.08	0.02	0.15	103	0.08	0.02	0.15	102	0.08	0.02	0.12
23[e]	2	0.13	0.07	0.39	8	0.03	0.01	0.07	5	0.05	0.02	0.18
25	141	0.08	0.03	0.19	168	0.08	0.02	0.17	166	0.08	0.02	0.16
26	19	0.12	0.03	0.16	19	0.12	0.03	0.16	20	0.12	0.02	0.16
28[e]	10	0.21	0.06	0.13	16	0.12	0.03	0.08	11	0.20	0.05	0.13
29	176	0.09	0.03	0.19	203	0.09	0.02	0.17	207	0.09	0.02	0.16
31[e]	3	0.24	0.13	0.04	7	0.06	0.04	0.05	3	0.24	0.13	0.04
32	234	0.12	0.04	0.16	271	0.10	0.03	0.15	271	0.11	0.04	0.14
Error mean		0.09	0.03	0.20		0.07	0.02	0.15		0.09	0.03	0.16
Error Std. deviation		0.07	0.03	0.09		0.04	0.01	0.07		0.07	0.03	0.08
Error 90^{th} percentile [f]		0.13	0.06	0.31								

[e] denotes an extreme site under scheme 10 based on exceeding the 90^{th} percentiles of the error metrics. The HRU discretization within this site's drainage area is refined based on *Step2*.

[f] The 90^{th} percentile computed based on errors across all 32 sites of interest.

4. Discussion

4.1. Reference Discretization Scheme Determination

The reference scheme is defined as a scheme that fully retains the information of the original spatial input data or, in special cases, the finest plausible discretization. The implication is that the modeler is interested in quantifying how much information is lost relative to the reference scheme.

Our subbasin reference scheme was defined based on a subjective flow accumulation threshold to determine reference main channel lengths. Alternatively, the real full flow path information (i.e., flow path of each cell in the DEM) can be obtained, for example, by the flow length tool of ArcGIS, and the corresponding discretization could be used as the reference scheme. For HRU discretization, our reference scheme retained all raw input spatial data and thus avoided any subjective decisions. Alternatively, the reference HRU scheme could be subjectively defined as a discretization that addresses some numerical and topological problems if this discretization is the one that modelers will practically apply and want relative errors computed against (Sanzana et al., 2013). While absolute discretization error metric values will be impacted by what can be a subjective reference scheme choice, the relative error values among candidate discretization choices should not change significantly.

4.2. Discretization Error Metrics

The subbasin discretization error metric estimates the in-channel routing length difference relative to the reference scheme. An improved approach would be to instead consider travel time error by using a reference flow velocity. Assuming the reference flow velocity as a constant is an easy and common method for practical purposes (De Lavenne, Boudhraâ, & Cudennec, 2015; Rigon, Bancheri, Formetta, & de Lavenne, 2016; Sanzana, et al., 2013). However, this assumption is questionable as typical watersheds have faster velocity upstream reaches compared to lower velocity downstream reaches. As such, a travel time error could instead be based on a spatially variable reference flow velocity. In addition, other available roughness, geometry, channel slope information can be incorporated into the routing information loss estimation by being linked to flow velocity (e.g., with Manning's Equation).

The *a priori* metrics (both nominal and quantitative) are able to provide directly meaningful descriptions on information loss because they explicitly characterize how much area or value of the hydrologic model input variable is changed after discretization. Moreover, they are unique as compared to the existing *a priori* metrics in the way they identify the property change. Haverkamp et al.(2002) , Booij (2003), and Dehotin and Braud (2008) all define discretization information loss as the overall statistics difference between the candidate scheme and the reference scheme, failing to conduct the cell-by-cell comparison with the original spatial input data. In contrast, the metrics proposed here correspond one-to-one with information loss during discretization. The overlay comparison process is a straightforward technique and is feasible for both raster and vector spatial input data. This enables other hydrologic variables of interest such as land surface slope and aspect to be analyzed with similar *a priori* discretization error metrics.

Figure 5 and Figure 9 show that discretization errors are highest in smaller upstream subbasins while Figure 11 shows that hydrologic model error indices (for peak flow and cumulative volume) are also highest in smaller upstream subbasins. This observation explains to some extent the modelling difficulties associated with small upstream subbasins in semi-distributed modelling. Although past studies such as Andersen (2001) and Tuppad (2006) have attributed the poor relative performance of calibrated upstream gauges to calibrated downstream locations to factors like more uncertain rainfall, our observation reveals that relatively poor performance in the smaller upstream subbasins of our case study can be expected since the discretization errors (and hydrologic model error indices) of these subbasins have a high variance and can be three times larger than the corresponding errors of the downstream larger drainage areas in the uniform threshold discretization framework. This demonstrates the utility of multi-site discretization evaluation in distributed modelling applications, and also suggests that a non-homogenous approach to watershed discretization decision-making would be beneficial.

Our HRU error metric approach for nominal input data did not disaggregate the individual area changes of the different categories of nominal data. For example, the area changes of the crop land or the deciduous forest land. However, modelers may only care about the area change of a certain category in their watershed (e.g., the change from forest to suburban may be of consequence but the change from wetland to swamp may be immaterial). Although not demonstrated in this work, the error metric for nominal variables (Equation 2) can be readily modified to assess the relative error of a specific category of nominal input data.

4.3. Variations to Discretization Approach

Our approach first generated all candidate subbasin schemes by ArcSWAT, and then generated candidate HRU schemes by sliver area aggregation. Any other candidate schemes generated by different discretization methods can also be evaluated by our proposed *a priori* discretization error metrics. Additional checks could be added to the subbasin discretization step, for example, checking the reference scheme against additional data such as orthophotos or hydrographic survey maps. Another variation is related to handling the small but potentially important sliver HRUs in HRU discretization simplification. For instance, in periurban areas where the land cover is very heterogeneous some small HRUs can be meaningful in terms of hydrology, thus such HRUs should be protected from merging in discretization simplification. One approach to preserve these key HRUs is to introduce an importance factor that would artificially increase the areas of key HRUs so that they would exceed the HRU discretization threshold used to aggregate small HRUs.

5. Conclusions

This study proposed *a priori* discretization error metrics that can estimate the information loss for any candidate discretization scheme. These metrics do not require model simulation, are independent of any specific modelling software, provide modelers with directly interpretable information on discretization quality, and allow for multi-site and multi-variable discretization evaluations prior to model development. In particular, the subbasin error metric provides the first attempt at quantifying the routing information loss from discretization; the HRU error metrics improves upon the existing *a priori* metrics in variable property change identification by the overlay comparison process. The proposed error metrics are straightforward to understand and easy to recode into the preprocessing of any semi-distributed hydrologic models and the fully distributed models using spatial input data aggregation. As a potential application of the proposed *a priori* discretization error metrics, a two-step decision-making approach was formulated to help modelers to get the appropriate subbasin and HRU discretization schemes, respectively. The approach does not only allow choosing a traditional spatially uniform-threshold discretization scheme based on the modeler-defined error threshold(s), but also enables compressing extreme errors to satisfy the modeler-specified discretization error targets.

These *a priori* discretization error metrics were applied to the discretization of the Grand River watershed. Results indicated that the discretization-induced information loss as measured by our discretization error metrics monotonically increases as discretization gets coarser. Hydrologic modeling under candidate discretization schemes validates the strong correlation between our discretization error metrics and model predictions (peak flow rate, cumulative flow and peak flow timing). Discretization evaluation results show that model accuracy moving from larger downstream locations to smaller upstream locations would be expected to increase since the largest discretization errors and highest error variability occur in smaller upstream locations. This pattern is also evident when changes in hydrologic model outputs were used in place of HRU discretization error metrics. Finally, results show that the common and convenient approach of applying uniform discretization across the watershed domain performs worse compared with the metrics-informed non-uniform discretization approach as the latter is able to preserve more input data information using the same number of computational units. However, the influence of non-uniform discretization on hydrologic model outputs should be further studied using a number of hydrologic models and case studies.

In applying the proposed *a priori* discretization error metrics to discretization decision-making, accounting for input forcing data (e.g., precipitation and temperature) resolution is also an important future consideration. This will require comparing the spatial and temporal distributions of the forcing input data under candidate schemes and those under the reference scheme. Beyond the application in discretization decision-making, future studies can utilize the discretization error metrics in other ways. For instance, the discretization error metrics may be useful in trying to account for the uncertainty induced by watershed discretization decisions which is commonly ignored. Furthermore, the discretization error metrics should prove useful even when they are not calculated *a priori* in that they could serve an important role in diagnosing the causes of model prediction errors in distributed modeling applications.

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