

Topological relationships-based flow direction modeling: mesh-independent river networks representation

Chang Liao¹, Tian Zhou¹, Donghui Xu¹, Matt Cooper¹, Darren Engwirda², Hong-Yi Li³,
and L Ruby Leung¹

¹Pacific Northwest National Laboratory

²Los Alamos National Laboratory

³University of Houston

November 22, 2022

Abstract

River networks are important features in surface hydrology. However, accurately representing river networks in spatially distributed hydrologic and Earth system models is often sensitive to the model's spatial resolution. Specifically, river networks are often misrepresented because of the mismatch between the model's spatial resolution and river network details, resulting in significant uncertainty in the projected flow direction. In this study, we developed a topological relationships-based river network representation method for spatially distributed hydrologic models. This novel method uses (1) graph theory algorithms to simplify real-world vector-based river networks and assist in mesh generation; and (2) a topological relationship-based method to reconstruct conceptual river networks. The main advantages of our method are that (1) it combines the strengths of vector-based and DEM raster-based river network extraction methods; and (2) it is mesh-independent and can be applied to both structured and unstructured meshes. This method paves a path for advanced terrain analysis and hydrologic modeling across different scales.

1 **Topological relationships-based flow direction modeling:**
2 **mesh-independent river networks representation**

3 **Chang Liao¹, Tian Zhou¹, Donghui Xu¹, Matt Cooper¹, Darren Engwirda²,**
4 **Hong-Yi Li³, L. Ruby Leung¹**

5 ¹Atmospheric Sciences and Global Change, Pacific Northwest National Laboratory, Richland, WA, USA

6 ²T-3 Fluid Dynamics and Solid Mechanics Group, Los Alamos National Laboratory, Los Alamos, NM,

7 USA

8 ³University of Houston, Houston, TX, USA

9 **Key Points:**

- 10 • We use graph theory algorithms to simplify real-world river networks.
11 • Topological relationships are reconstructed from simplified river networks and mesh
12 intersections.
13 • Topological relationships can be used to model flow direction field and flow rout-
14 ing parameters.

Corresponding author: Chang Liao, chang.liao@pnnl.gov

15 Abstract

16 River networks are important features in surface hydrology. However, accurately
17 representing river networks in spatially distributed hydrologic and Earth system mod-
18 els is often sensitive to the model's spatial resolution. Specifically, river networks are of-
19 ten misrepresented because of the mismatch between the model's spatial resolution and
20 river network details, resulting in significant uncertainty in the projected flow direction.
21 In this study, we developed a topological relationships-based river network representa-
22 tion method for spatially distributed hydrologic models. This novel method uses (1) graph
23 theory algorithms to simplify real-world vector-based river networks and assist in mesh
24 generation; and (2) a topological relationship-based method to reconstruct conceptual
25 river networks. The main advantages of our method are that (1) it combines the strengths
26 of vector-based and DEM raster-based river network extraction methods; and (2) it is
27 mesh-independent and can be applied to both structured and unstructured meshes. This
28 method paves a path for advanced terrain analysis and hydrologic modeling across dif-
29 ferent scales.

30 Plain Language Summary

31 Representing rivers in hydrologic models is difficult because river networks are of-
32 ten very complex. Existing methods generally rely on elevation differences between land
33 and rivers or image processing to define river networks in computer models. In this study,
34 we combine the strengths of two existing methods and develop a topology-based method.
35 This follows river channels and defines river networks in a way that works for any grid
36 system and spatial resolution. The products of this method can be used to improve hy-
37 drologic models.

38 1 Introduction

39 River networks are important features in hydrologic and Earth system modeling(Jolley
40 & Wheeler, 1997; Wu et al., 2012; Liao et al., 2019). Real-world river networks are com-
41 plex, depending on landscape features such as elevation, aspect, and lithology. Moreover,
42 the fractal nature of river networks means that they are approximately scale-free(Tarboton
43 et al., 1988) without a well-defined spatial resolution at which they should be represented(Davies
44 & Bell, 2009; Yamazaki et al., 2009). As a result, hydrologic models often use a concep-
45 tual representation of river networks. To date, there are mainly three methods for rep-
46 resenting river networks, each with its own advantages and disadvantages. However, lim-
47 itations remain when representing river networks due to the resolution mismatch and their
48 interactions with other hydrologic features (e.g., ocean).

49 There are two methods useful at the watershed/regional scale, the first of which
50 is the vector-based river networks analysis method. This method uses vector datasets
51 to represent the river networks and their topological relationships(Mizukami et al., 2016;
52 Lin et al., 2018). Vector datasets are often provided by public agencies, e.g., the United
53 States Geological Survey (USGS), or are digitized from satellite image processing, e.g.,
54 vectorization-based river channel extraction. Various graph theory algorithms are then
55 used to perform quality control and network analysis based on the vector river networks(Lindsay
56 et al., 2019). Lindsay, et al. reviewed several potential issues in existing vector river net-
57 works datasets: (1) the vertex coordinates of river flowlines may not exactly overlap with
58 the actual locations due to digitization error and floating-point rounding error. (2) the
59 starting and ending-vertices of a river flowline may be reversed during spatial analysis,
60 resulting in an opposite flow direction. (3) vector datasets obtained from different sources
61 generally use different spatial references and cannot be used or combined directly. Even
62 without these issues, vector datasets still require other pre-processing before use. For ex-
63 ample, braided rivers are not universally supported in hydrologic models as multiple flow

104 directions are not always supported. Although the vector-based river networks representation method is computationally efficient and scale-independent, it has limitations. First, 105 the resulting vector networks are not explicitly linked with the rectangle mesh system 106 commonly used in hydrologic models. As a result, the vector-based river networks method 107 is limited to flow routing and cannot be easily coupled with other hydrologic processes. 108 Second, this method can only be applied to areas with vector datasets unless it's combined 109 with advanced terrain analysis. 110

111 The second method is the raster digital elevation model (DEM)-based river networks 112 extraction method (Tarboton, 2003; Esri Water Resources Team, 2011; Yamazaki 113 et al., 2019). This method generally involves several steps: (1) calculation of cell-to-cell 114 flow direction for each raster cell based on elevation differences (e.g., D4/D8 algorithm); 115 (2) calculation of flow accumulation based on flow direction; and (3) definition of river 116 cells using an accumulation threshold. Because of local depressions in the DEM, a depression- 117 filling operation is often required before step 1 to guarantee that water can flow out of 118 each cell. The raster DEM-based river networks extraction method is widely used with 119 a few limitations. First, this method is very sensitive to the spatial resolution and accuracy 120 of the DEM. In general, it only performs well for high-resolution (< 1 km) DEMs (Goulden 121 et al., 2014; Sood & Smakhtin, 2015). Second, because the derived flow direction in step 1 122 relies on elevation differences, it is less accurate in flat areas with fewer topographic 123 variations. As a result, obtaining unrealistic river networks is common. To address these 124 limitations, the “stream burning” technique (also called “DEM reconditioning”) is often 125 used to lower elevations within and near river channels so that water always flows into 126 the river cells (Hellweger & Maidment, 1997; Lindsay, 2016a). This technique requires 127 an additional river network dataset, typically in vector format. The user-provided river 128 networks dataset is often converted into a binary mask with the same spatial resolution 129 as the DEM (Lindsay, 2016b). Because the binary mask does not describe the upstream- 130 downstream topological relationships between mesh cells, it cannot accurately capture 131 the meander, confluence, and parallel river. In this study, we define parallel rivers as rivers 132 running in adjacent mesh cells side by side. As a result, it often produces incorrect flow 133 directions in these locations (Figures S1-S6). The extensive modifications to the elevations 134 of river networks and riparian-zone can result in large biases in slope calculations 135 (river channel slope and riparian zone slope), which will significantly impact the flow routing 136 and flooding processes in hydrologic models (Shelef & Hilley, 2013). To remediate this, 137 slopes are sometimes calculated from the original DEM (Lindsay, 2016b), but this requires 138 additional adjustments to consider local depressions. Similar issues also arise in the terrain 139 analysis depression filling process. Several studies used additional topological information 140 in the hybrid breaching-filling algorithm to minimize modifications to elevation (Lindsay, 141 2016a). However, this hybrid approach is not readily available and is not used in most 142 Geographic Information System (GIS) or hydrologic models. The raster DEM-based method 143 is often not directly used at large spatial domains due to the computational cost. Instead, 144 the study domain is often separated into small tiles, which are merged together after applying 145 the method.

146 The third method is used on a continental to global scale. Because the target spatial 147 resolution (around 10 km to 200 km) is much coarser compared to regional-scale applications 148 (Sood & Smakhtin, 2015), this method often assumes that there is always one major river channel 149 and many tributaries within each mesh cell (Wu et al., 2011). Due to the resolution 150 mismatch between fine-scale river networks and mesh cell size, their topological relationships 151 are even more complex (Shaw et al., 2005). For example, multiple major rivers may 152 run in the same cell or in parallel. To maintain the large-scale flow pattern, many models 153 use high spatial resolution datasets (e.g., results from the raster DEM-based method) 154 as guidance to define the coarse resolution cell-to-cell flow direction (Fekete et al., 2001; 155 Davies & Bell, 2009; Wu et al., 2011). This type of method is also often referred to as 156 the upscaling method. For example, the Cell Outlet Tracing with an Area Threshold (COTAT) 157 (Reed, 2003) and Network Tracing Method (NTM) (Wu et al., 2012) use either high-resolution

118 raster or vector-based river networks to guide their coarse resolution flow directions. With-
119 out increasing the mesh resolution, the upscale method often needs to modify the ma-
120 jor river locations to avoid aforementioned issues(Wu et al., 2012; Eilander et al., 2021;
121 Munier & Decharme, 2022). Although this method captures the flowlines, the shift of
122 locations can result in unrealistic spatial distribution of model outputs, for example, when
123 floodplain inundation is of particular interest(Yamazaki et al., 2011; Decharme et al., 2012;
124 Luo et al., 2017; Mao et al., 2019; Zhou et al., 2020). One possible solution is to use an
125 unstructured mesh with regional refinement for the regions with complex river networks;
126 however, all existing model implementations only support the structured rectangle meshes.
127 Taken together, the existing three methods have different advantages and disadvantages,
128 and they are often used in different scales, applications, and hydrologic communities (Ta-
129 ble S1).

130 To date, all the spatially-distributed flow routing models (except vector-based) are
131 limited to the structured rectangle meshes, and cannot be seamlessly coupled with other
132 unstructured mesh-based numerical models. Moreover, existing methods mainly focus
133 on projecting existing river networks onto prescribed structured rectangle meshes. Less
134 attention has been paid to unstructured meshes, which allow certain hydrologic features,
135 such as river networks, to be burnt into the meshes. Many studies have attempted to “burn”
136 river networks into meshes, with most using the Triangular Irregular Network (TIN) approach(Kreveld
137 & Silveira, 2011; Coon et al., 2019). However, existing TIN-based methods do not gen-
138 erally incorporate stream burning or depression filling methods(Ivanov et al., 2004; Coon
139 et al., 2019). As a result, there is still uncertainty in flow direction and slope calcula-
140 tions.

141 In recent years, model development based on unstructured meshes is an emerging
142 area of interest in hydrologic and Earth system models because it provides several advantages(Engwirda
143 & Liao, 2021): (1) unstructured mesh refinement can be used to define specific regions
144 of interest (ROIs). Because hydrologic features such as river networks, dams, and coastal
145 lines do not align well with the rectangle meshes used in numerical models, spatial in-
146 terpolation and approximation are often needed. In contrast, unstructured meshes pro-
147 vide the flexibility to represent these features reasonably well through variable size and
148 rotation, resulting in reduced model uncertainty. (2) spatial interpolation will be signif-
149 icantly reduced or removed in a unified unstructured mesh framework that includes all
150 the model components, e.g., ocean, land, and river. These components can exchange fluxes
151 seamlessly at their interfaces(Liao et al., 2022). (3) unstructured meshes can be used to
152 balance spatial resolution and computational cost through variable resolution, critical
153 for large-scale hydrologic and Earth system models.

154 To the authors’ knowledge, there is no river networks representation method de-
155 signed for the unstructured mesh system(Paz & Collischonn, 2007; Sood & Smakhtin,
156 2015; de Azeredo Freitas et al., 2016; Hyvaluoma, 2017; Hsu, 2020). For hydrologic mod-
157 els and Earth system models, this requires a new river networks representation and flow
158 direction method that supports unstructured meshes. In this two-part study, we intro-
159 duce a novel method that combines the strengths of existing methods to produce river
160 networks and flow direction for any mesh system. In part 1, we mainly focus on the topo-
161 logical relationship-based river network representation model (PyFlowline)(Liao & Cooper,
162 2022). In part 2, we will demonstrate how to use the topological relationship in depres-
163 sion filling and flow direction modeling in the HexWatershed model(Liao et al., 2020, 2022).
164 Part 1 of the study is organized as follows. We first introduce the model algorithms. Then
165 we apply this model to a coastal watershed, the Susquehanna river basin (SRB), using
166 different model configurations, and evaluate the model performance against real-world
167 river networks using several metrics including river length and area of differences. Last,
168 we discuss the limitations and future applications in hydrologic and Earth system mod-
169 els.

170 **2 Methods**

171 **2.1 Overview**

172 Conceptually, any river channel can be represented using three basic graph elements:
 173 vertex, edge, and flowline (Figure S7). River networks can be viewed as collections of
 174 these three elements. After converting existing river network datasets into these basic
 175 elements, we can then use graph algorithms to extract topological relationships includ-
 176 ing connectivity and direction. For notation, a single letter/number will be used for the
 177 vertex (e.g., vertex A) and a sequence of letters/numbers will be used for the directed
 178 edge and flowline (e.g., edge A->B). The essence of our method is that in the simplest
 179 scenario, in any type of mesh system, a river channel always intersects (enters and ex-
 180 its) a mesh cell on two different edges (or, less likely, its vertices) (Figure 1), unless it
 181 is either a headwater or river mouth in which either the starting or ending vertex lies
 182 within the mesh cell.

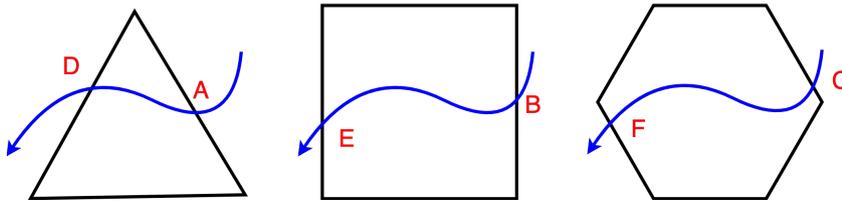


Figure 1. Illustration of a river channel entering and exiting a mesh cell from its edges. Blue curves are river channels. Black polygons are mesh cells (triangle, square, and hexagon). Regardless of the cell type, the intersection between a river channel and a mesh cell always results in two vertices on mesh cell edges, such as A/D, B/E, and C/F pairs, and a directed flowline within, such as A->D, B->E, and C->F.

183 Based on the intersections between the river channels and mesh system, real-world
 184 river networks can be represented digitally as collections of the individual “reach” within
 185 each mesh cell (e.g., flowline A->D and B->E in Figure 1). Based on the intersections,
 186 topological relationships (e.g., which cells are upstream of the current cell) between mesh
 187 cells can be built. As a result, river networks can be consistently preserved in any mesh
 188 system. To achieve this, our method consists of several major steps, illustrated in Fig-
 189 ure 2 and described in detail in the following sections.

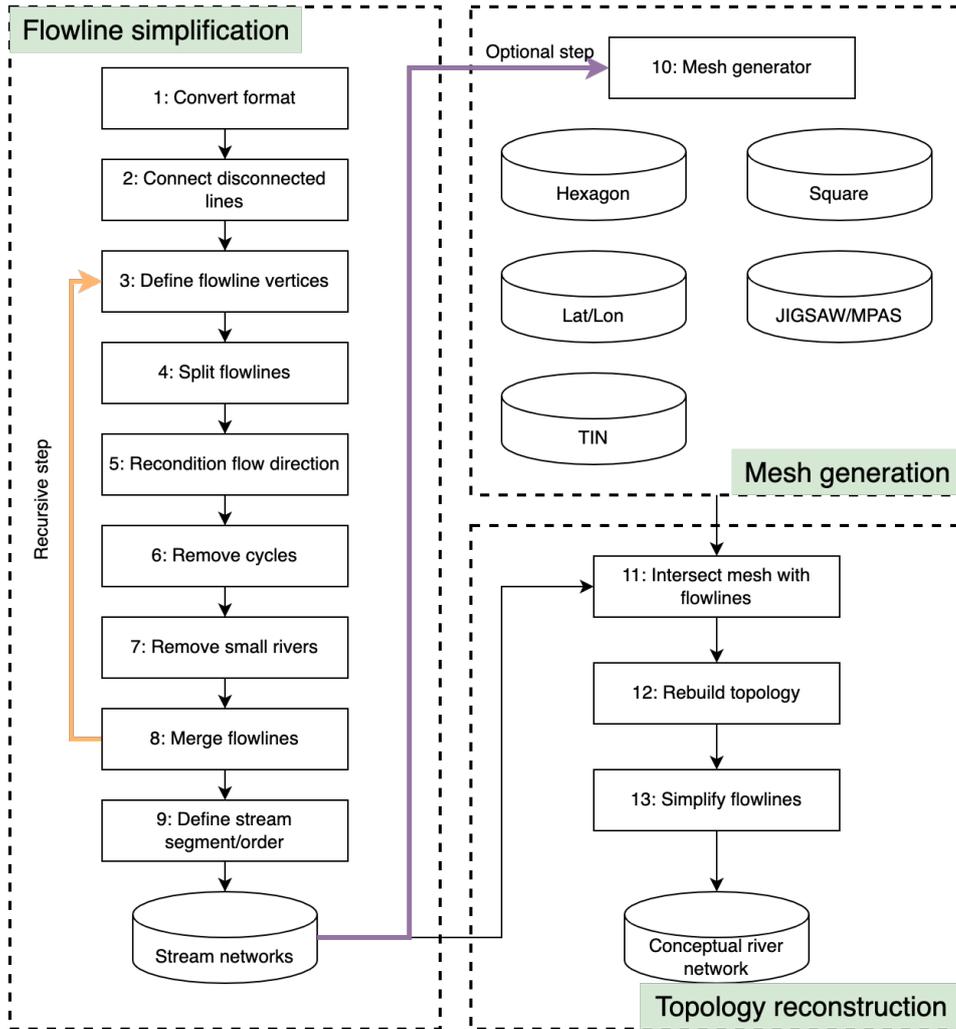


Figure 2. The workflow of the topological relationship-based river networks representation method. The workflow includes three major components: flowline simplification, mesh generation, and intersection-based topology reconstruction. Each component contains one or more steps with indices. In flowline simplification, several steps (highlighted by the yellow arrow) may be run recursively. The output from flowline simplification can be optionally used for mesh generation (purple arrow). Both structured (e.g., rectangle lat-lon and hexagon) and unstructured meshes (e.g., MPAS mesh) are supported. Step 13 is a combination of several steps from Step 3 to 9.

190 Besides, because our method is completely built upon the geodesic coordinate system
 191 (Text S1), it can be applied to both regional and global scales.

192 2.2 Flowline simplification

193 To address potential issues in existing vector datasets, we developed a list of al-
 194 gorithms (Steps 1 to 9 in Figure 2) to pre-process the vector flowlines. In practice, these
 195 algorithms may be run in different combinations and orders depending on the datasets.
 196 From now on flowline pre-processing, as either individual steps or a collection of several
 197 steps, is referred to as flowline simplification. And the outputs from flowline simplifica-
 198 tion are referred to as simplified flowlines. Details of the algorithms in Steps 1 to 9 are

199 provided in the supplementary materials (Text S2). Additionally, our method provides
 200 the option to burn dams and associated flowlines in the workflow. For flowline simpli-
 201 fication, this means that other than the prescribed high-order flowlines, the model also
 202 includes all the downstream flowlines of the user-provided dams.

203 **2.3 Mesh generation**

204 Mesh generation is the process that defines the spatial domain discretization(Liao
 205 et al., 2020). Structured meshes such as the geographic coordinate system (GCS) rect-
 206 angle mesh (latitude-longitude), projected coordination system (PCS) rectangle mesh
 207 (square), and hexagonal mesh, can be generated using various GIS computer programs
 208 (e.g., QGIS MMQGIS)(Minn, 2015) or with Python scripting(Liao et al., 2022). This
 209 usually involves the following steps: (1) obtaining the spatial extent of the study domain;
 210 (2) setting the lower-left or upper-left corner as the origin; (3) calculating the number
 211 of rows and columns based on the desired resolution and spatial extent; (4) calculating
 212 the vertex coordinates of each mesh cell; and (5) exporting all the mesh cells to a GIS
 213 file format.

214 For unstructured meshes such as the TIN or the Model for Prediction Across Scales
 215 (MPAS) mesh (Text S3)(Ringler et al., 2013), advanced mesh generators such as JIG-
 216 SAW are available(Engwirda, 2014; Sahr, 2015). These mesh generators can generally
 217 apply mesh refinement near some ROIs, such as river networks and/or coastal areas. Some
 218 generators also allow mesh grid centers to align with predefined polylines (e.g., river flow-
 219 lines or coastal lines) and points (e.g., dams) to satisfy particular modeling needs. In our
 220 study, we mainly used the JIGSAW mesh generator to produce an MPAS mesh. Specif-
 221 ically, we used simplified flowlines, dam locations, and coastal lines during the mesh re-
 222 finement process so that the MPAS mesh cells align with these hydrologic features(Engwirda,
 223 2017).

To maintain consistency, we use “equivalent” resolution which is the square root
 of the mesh cell spherical sector area, to define mesh resolution (Equation 1, and Text
 S1)(Liao et al., 2022). For a structured GCS rectangle mesh, the equivalent resolution
 changes with latitude. For unstructured variable resolution meshes such as TIN and MPAS
 meshes, the equivalent resolution only applies to a certain mesh cell.

$$\text{Res}_c = \sqrt{\text{Area}_c} \quad (1)$$

224 where Res_c is the “equivalent” resolution (m); and Area_c is the mesh cell spherical sec-
 225 tor area (m^2).

226 Mesh generation is not the focus of this study and has been extensively explored
 227 in relevant communities(Minn, 2015; Sahr, 2015; Engwirda, 2017). In this study, we use
 228 relatively simple meshes and existing mesh generators as test cases to demonstrate our
 229 new method.

230 **2.4 Topological relationships reconstruction**

231 Intersecting the simplified flowlines and meshes breaks stream segments into stream
 232 reaches. For simplicity, we redefine the simplified flowlines using stream segments and
 233 stream reaches (Figure S12). Because both the stream segment index and stream order
 234 information are defined during the flowline simplification step (Step 9 in Figure 2), they
 235 are directly assigned to each stream reach. A mesh cell may contain one or more inter-
 236 nal reaches if it intersects with the simplified flowlines.

237 Reconstruction of the mesh cell topological relationships starts from the user-provided
 238 approximate outlet location (latitude and longitude coordinates) and searches from the
 239 outlet to upstream headwater in reverse. Figure 3 illustrates this process in the simplest
 240 scenario with only three stream segments in a rectangle mesh. The model also allows a

241 segment to take a “shortcut” (Red dashed edge F->I in Figure 3) when it passes a mesh
 242 cell in a short distance (Reach 3->2 within cell E), which produces the classical D8 di-
 243 agonal travel path (only in the rectangle mesh). This short distance is defined as a “short-
 244 cut” threshold parameter (Table S2). The resulting topological relationships are stored
 245 and expressed as conceptual flowlines, which connect one cell center to another (blue and
 246 red dashed arrows/edges).

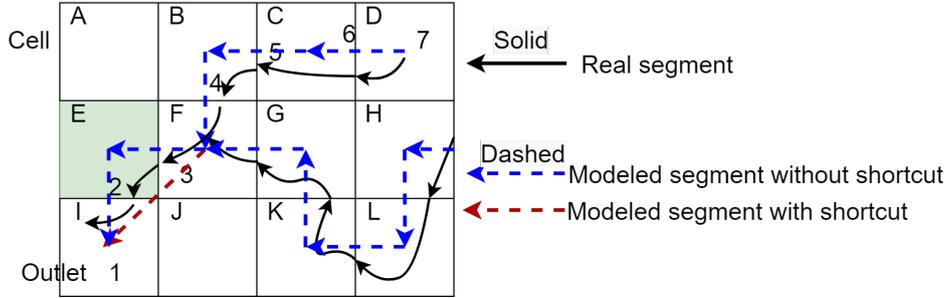


Figure 3. Illustration of the topological relationships reconstruction in a 3-row by 4-column rectangle mesh. The letters in the top-left corner of each cell, from A to L, represent mesh cell IDs. The numbers from 1 to 7 represent the start, end, and intersected vertices. Colored solid arrows are intersected real stream reaches within each mesh cell. Starting from outlet vertex 1, the algorithm searches reversely and reconstructs the cell topological relationships as D->C->B->F, H->L->K->G->F, and F->E->I in blue dashed arrows. Optionally, if the D8 diagonal path is turned on because the reach (3->2) length within grid E is less than the user-provided threshold, the algorithm omits the grid E and takes a shortcut (red dashed arrow). Because the algorithm strictly follows topology relationships, it precisely captures confluence (Grid F), parallel river (C->B and G->F), and meander (H->L->K->G).

247 With these capabilities, the model can represent the river meander, confluence, and
 248 parallel river in any mesh system (Figures S4-S6). In some cases, a stream segment may
 249 enter and exit a mesh cell multiple times on the same cell edge, which results in a “cy-
 250 cling” effect (e.g., F->E->B->E->D in Figure S10). To address this issue, the cycling
 251 removal algorithm (Step 6 in Figure 2) is applied again to remove the loop (e.g., the fi-
 252 nal topological relationships are F->E->D). It is also possible that multiple conceptual
 253 flowlines enter and exit the same cell. Therefore, some flowline simplification algorithms
 254 are reused (Step 13 in Figure 2).

255 3 Model application

256 3.1 Study area

257 The Susquehanna river basin (SRB) is a major river basin located in the Mid-Atlantic
 258 region of the United States. The total drainage area of the SRB is about 7.1×10^4 km².
 259 Its surface elevation ranges from 0 m to more than 900 m. It contains both relatively mild
 260 and steep surface slopes, ranging to 30 degrees in some areas (Figure 4). Spatial datasets
 261 and maps were produced using the Python packages including Matplotlib and GDAL(Hunter,
 262 2007; Gillies & others, 2007; GDAL/OGR contributors, 2019; Liao, 2022).

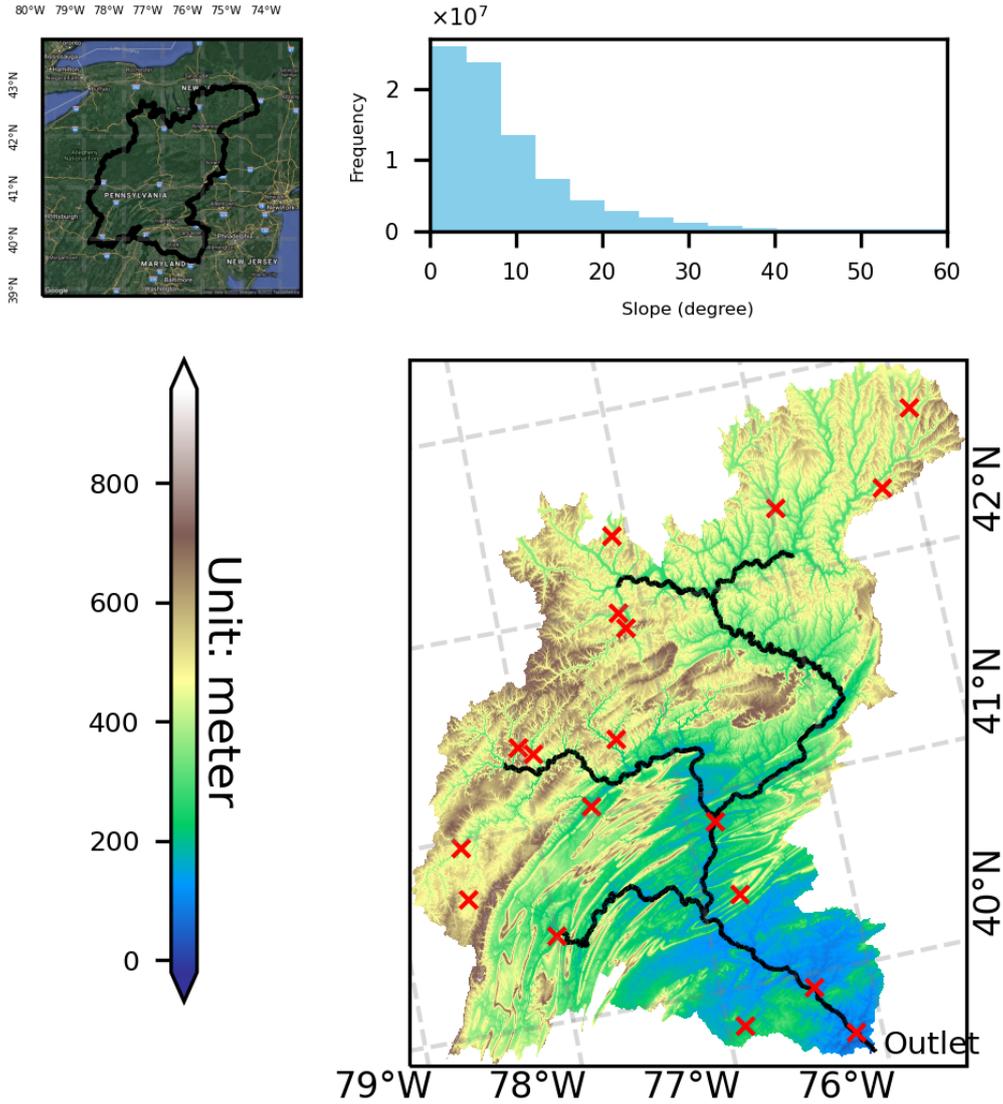


Figure 4. The spatial location, surface elevation, and surface slope distribution (based on DEM) of the Susquehanna river basin. The upper left red polygon is the Watershed Boundary Dataset watershed boundary on Google Maps; the upper right is the histogram of surface slope (degree), and the bottom is the topographic map (m). In the topographic map, the black lines are major river channels. The red crosses are major dams. The outlet is in the lower right corner.

263 Because the river outlet of the SRB is into Delaware Bay, the study area is prone
 264 to sea-level rise, storm surge, and other extreme event-induced flooding. Due to the res-
 265 olution mismatch and mesh differences between the land, river, and ocean in Earth system
 266 models, the study area is generally poorly represented, especially near the coastal
 267 lines (Feng et al., 2022).

268

3.2 Data

269

270

271

272

273

We collected river networks, watershed boundary, and dam locations from the United States National Hydrography Dataset Plus High Resolution (NHD Plus HR) and Watershed Boundary Dataset (USGS, 2013). Because NHDPlus HR contains more than 10,000 flowlines in the SRB (Figure 5), we used stream order (higher and equal to 6 or 7) to reduce the number to 120 (Figure 5) (Tarboton et al., 1991).

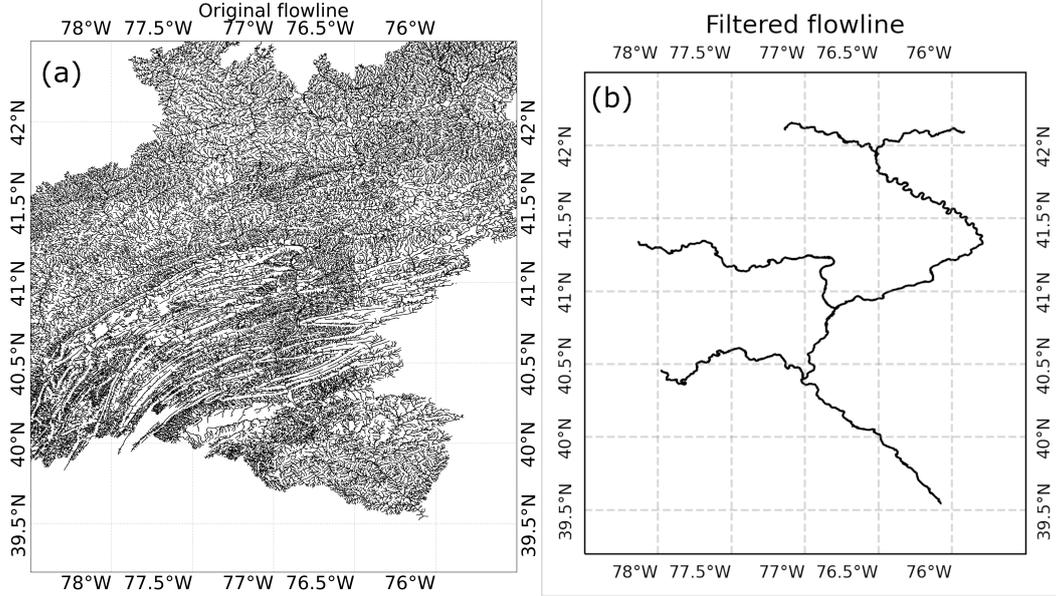


Figure 5. The spatial distribution of river flowlines from NHDPlus HR for the Susquehanna river basin. (a) is the raw data with all flowlines (more than 10k flowlines) and (b) shows filtered flowlines with stream orders higher or equal to 7. A total of 120 river flowlines are retained.

274

3.3 Model setup

275

276

277

Major model configuration parameters are listed in Table S2. To evaluate the sensitivity of model performance to spatial resolution and meshes, we ran the model with different configurations with case indices used for illustrations (Table 1).

Table 1. Simulation configurations with case indices. The illustrations and analyses all use the same indices.

Mesh/Resolution	50 km	10 km	5 km
Lat-lon	1	2	3
Square	4	5	6
Hexagon	7	8	9
MPAS	10/11/12		

278 For the structured meshes, i.e., GCS rectangle mesh (lat-lon), PCS rectangle mesh
279 (square), hexagon, we ran 3 different spatial resolutions (50 km, 10 km, and 5 km) with
280 the same stream order threshold 7. The square mesh Case 9 results are used for com-
281 parison with the traditional raster DEM-based method (Text S4, Figure S13).

282 For the unstructured variable resolution (3 ~ 10 km) MPAS mesh, we ran 3 cases:
283 (1) Case 10 with stream order threshold 7 (the same with structured-mesh cases); (2)
284 Case 11 with stream order threshold 6. This case is used to evaluate the performance
285 at different levels of flowline details; (3) Case 12 with stream order threshold 7 and ad-
286 ditional dams burnt in the flowlines and mesh. This case is used to illustrate the dam
287 burning capability.

288 **3.4 Results and analysis**

289 ***3.4.1 Flowline simplification***

290 After model simulation, the river flowlines were substantially simplified. First, the
291 total number of flowlines is reduced from 120 to 7, with 4 headwater vertices, 3 conflu-
292 ence vertices, and 1 outlet vertex (Figure 6). Second, all the small rivers with lengths
293 less than the threshold were removed (Figure 7). Third, all braided rivers were removed
294 (Figure 7). Flowline simplification results are the same from Cases 1 to 10.

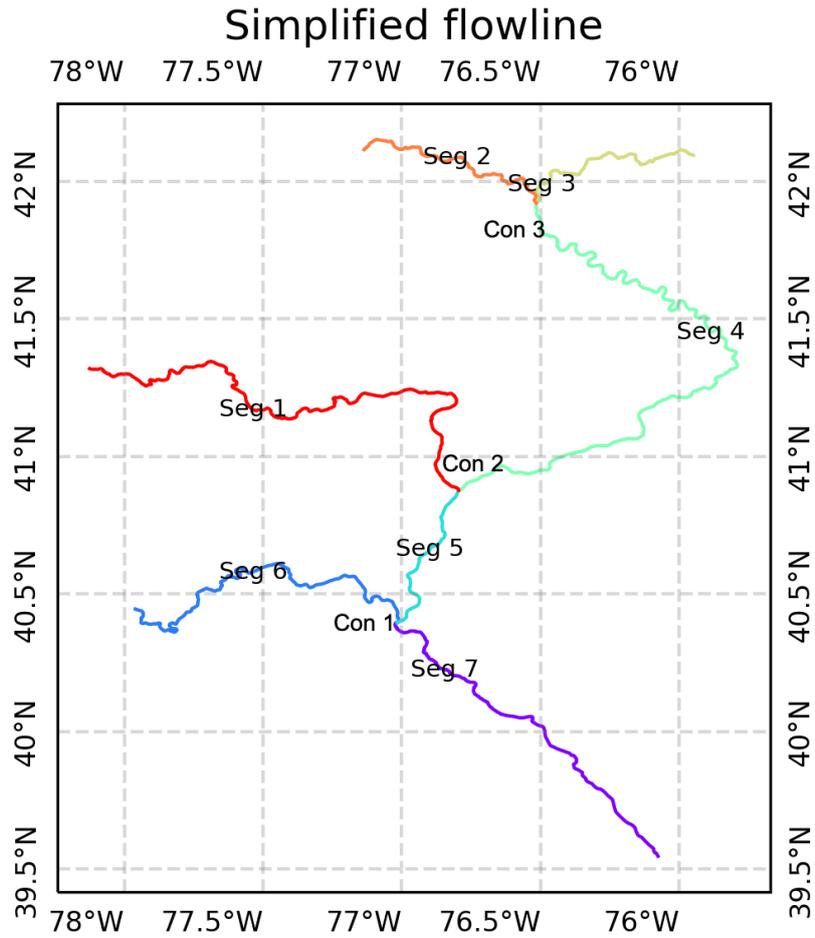


Figure 6. The spatial distribution of flowlines after flowline simplification. (a) Colored line features are 7 flowlines after simplification. Segments 1 to 7 are segment indices. Confluences 1 to 3 are confluence indices.

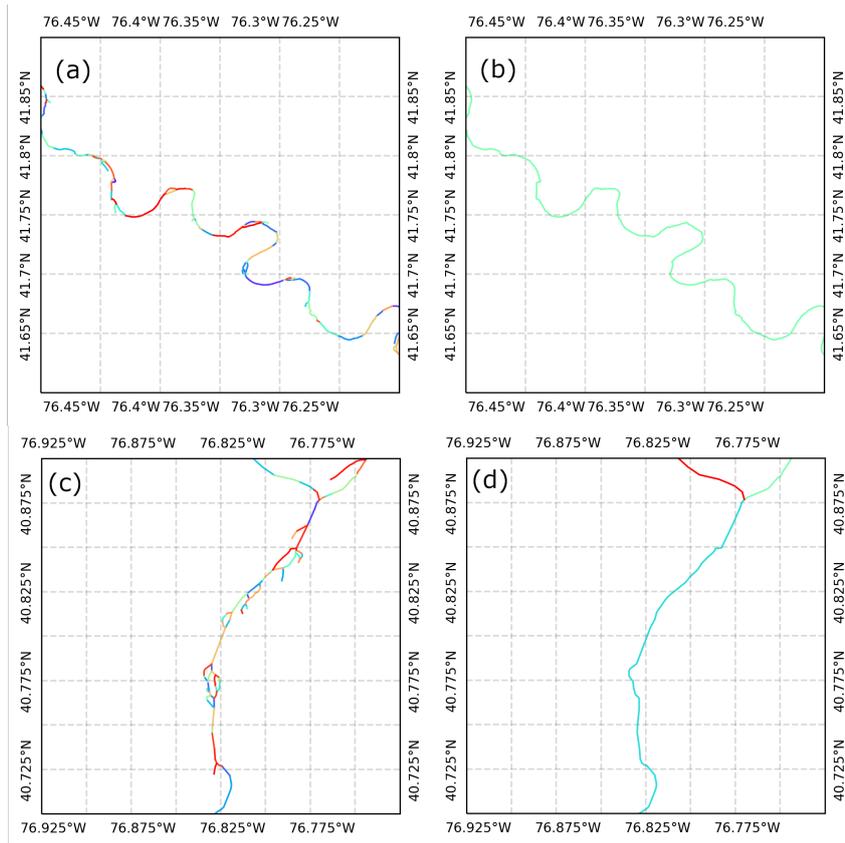


Figure 7. Before and after flowline simplification comparisons. (a) and (b) are zoomed-in views where small rivers are removed near the river meanders; (c) and (d) are zoomed-in views where braided and small rivers are removed.

295 After removing small and braided rivers, the total length of the flowlines decreased
 296 10.0% (dashed red and blue lines in Figure 8).

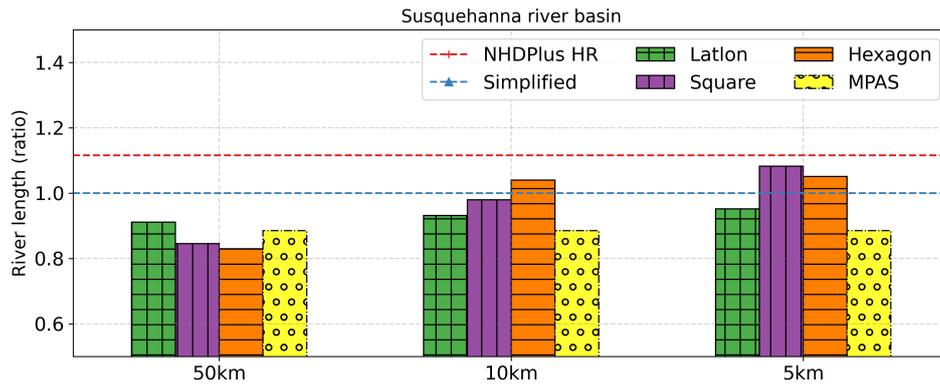


Figure 8. Comparison of the total flowline length from different model configurations. The X-axis is the spatial resolution and the Y-axis is the ratio between modeled and simplified river length. The dashed red and blue lines are the NHDPlus HR and simplified total flowline length. Colored (green, purple, orange, and yellow) bars with textures represent different model configurations.

297 Depending on user needs, a combination of stream order and dam information can
 298 be used in PyFlowline to preserve different levels of details (e.g., tributaries). For ex-
 299 ample, the simplified flowlines from Cases 11 and 12 are illustrated in Figure S11.

300 **3.4.2 Mesh generation**

301 The generated structured GCS rectangle lat-lon, PCS square, and PCS hexagon
 302 meshes are illustrated in Figure 9.

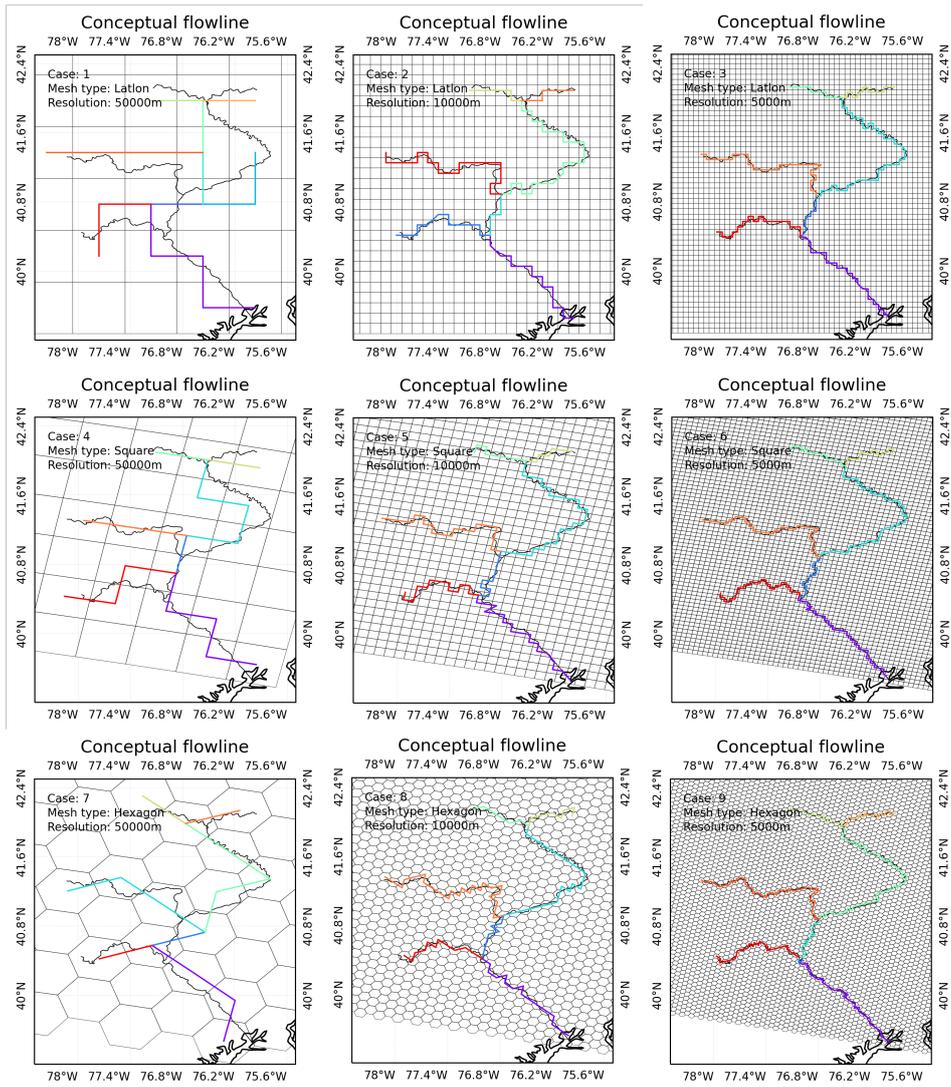


Figure 9. The spatial distributions of modeled conceptual flowlines on the lat-lon, square, and hexagon meshes at multiple spatial resolutions. The layout of the figures and Case indices from 1 to 9 is the same as Table 1. Black line features represent the simplified flowlines. Colored line features represent the conceptual flowlines.

303 The generated MPAS mesh is illustrated in Figure 10. Because both the small and
 304 braided rivers were removed, JIGSAW successfully aligned cell centers following the sim-
 305 plified flowlines at the desired resolution. JIGSAW also varies cell resolution by consid-
 306 ering the distance of the cell center to the simplified flowlines (as well as the coastal lines)
 307 through a density function. In this case, a coastal-resolving mesh spacing function is adopted
 308 to cluster high model resolution near coastlines. Mesh resolution varies between 3 km
 309 near the river outlet/coastal line and 10 km near the domain boundary.

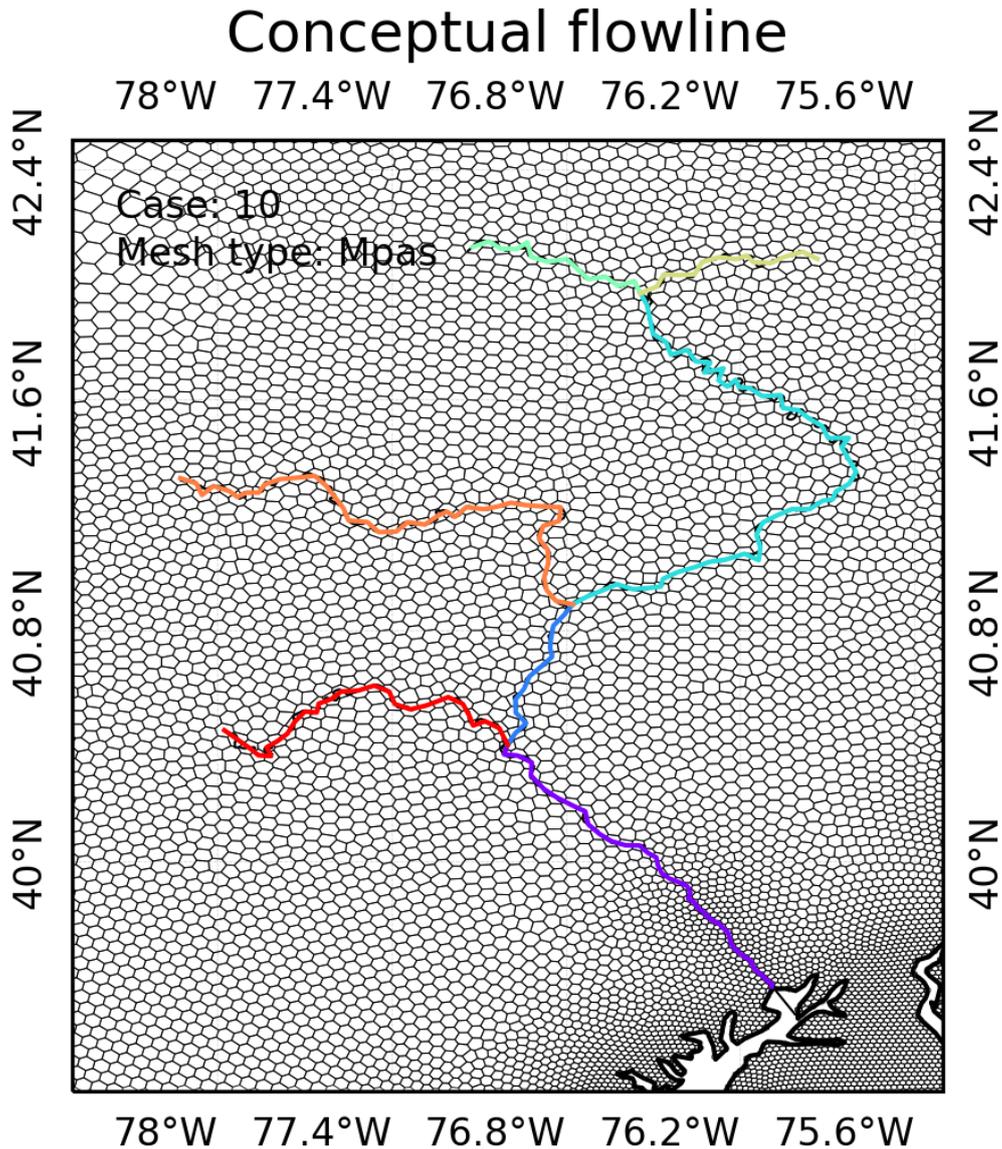


Figure 10. Modeled flowline-guided MPAS mesh from Case 10 (clipped to the study domain) (Table 1). Because the JIGSAW mesh generator considers the simplified flowlines in its density function, the mesh cell center locations align with the flowlines and cell resolutions are higher (~ 3 km) near the flowline than away from it (~ 10 km).

310 *3.4.3 Topological relationship reconstruction*

311 In general, on the structured meshes, the spatial patterns of modeled conceptual
312 flowlines are similar to the simplified flowlines at different spatial resolutions (Figure 9).

313 The model is able to separate parallel flowlines such as Segments 1 and 6 (Figure
314 6). It also captures all the river confluences. As the spatial resolution increases, the model
315 can capture more spatial details. At 5 km resolution, the modeled conceptual flowlines

316 can accurately describe the river confluences. The shortcut algorithm also works well,
 317 as it produces the classical D8 diagonal paths in many scenarios (e.g., Cases 2 and 5).

318 On the unstructured MPAS mesh, the modeled conceptual flowlines closely follow
 319 the provided simplified flowlines (Figures 10 and 11). The model's performance varies
 320 with the complexity of the simplified flowline and mesh cell resolution. For example, at
 321 moderate resolution (~ 6 km) the modeled conceptual flowline follows the overall pat-
 322 tern and captures the sharp U-turn near the river meander (Figure 11). Near Conflu-
 323 ence 1 and the outlet (~ 3 km), the modeled conceptual flowlines almost overlap with
 324 the provided simplified flowlines (Figure 11). The modeled MPAS mesh-based concep-
 325 tual flowlines are closer to the simplified flowlines than the modeled structured meshes-
 326 based conceptual flowlines (Section 3.5.2). This improved fidelity is a result of the en-
 327 hanced flexibility of a fully unstructured mesh representation. This allows for the close
 328 alignment of mesh cells with stream features during the mesh generation phase, which
 329 in turn significantly improves the accuracy of the reconstructed river flowlines.

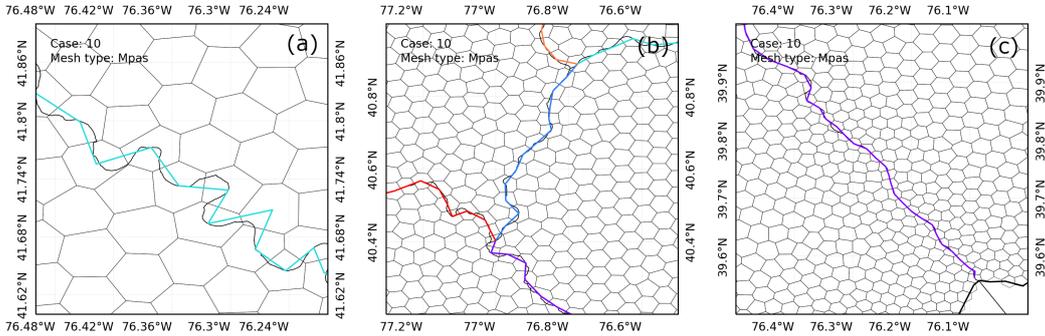


Figure 11. The zoom-in views of the spatial distributions of modeled conceptual flowlines on the MPAS mesh from Case 10 (Table 1). (a), (b), and (c), are the zoomed-in views near the river meander, river confluence, and river outlet, respectively. Black line features are the simplified flowlines. Colored line features are the conceptual flowlines.

330 With increased flowline details, i.e., stream order 6 or dam burnt in, the model is
 331 still able to capture the river networks (Figure S11).

332 3.5 Metrics analysis

333 For metrics analysis, we only focus on Cases 1 to 10 as they have the same level
 334 of flowline details.

335 3.5.1 Flowline length

336 The modeled cell center-based conceptual flowline length, although not always used
 337 in hydrologic or Earth system models (Paz & Collischonn, 2007), reflects the closeness
 338 between the modeled and real river networks. For structured meshes, the total flowline
 339 length increases as the spatial resolution increases (Figure 8). At the same spatial res-
 340 olution, the differences between different meshes are around 10.0%. The total length from
 341 the MPAS mesh-based flowlines is shorter than the results from equivalent structured
 342 meshes (Figure 8). Differences between different segments are mainly influenced by river
 343 meander features (Section 3.5.4).

344 Because the MPAS mesh is designed to follow flowlines whenever possible, its length
 345 and area of difference (Section 3.5.2) are the smallest. In contrast, the structured mesh-
 346 based flowlines usually generate a “zig-zag” effect, which produces a larger length and
 347 area of difference (Figure 12).

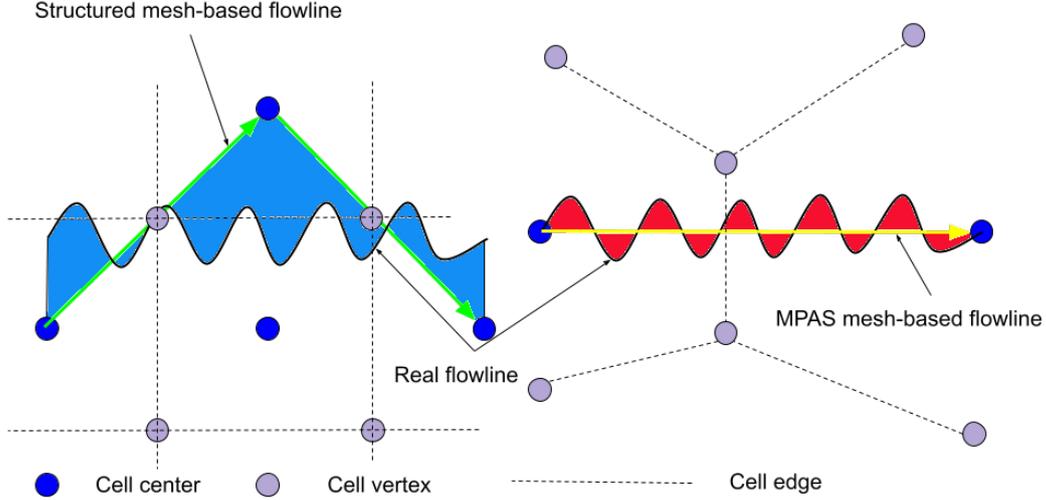


Figure 12. Illustration of the conceptual length and area of difference. The dashed black lines are the cell edges. The blue and purple dots are cell centers and vertices, respectively. The black/green/yellow lines are the real, structured mesh-based, and MPAS mesh-based flowlines. Because the structured mesh-based flowlines (green lines) do not closely follow the real flowlines (black lines), their total length is larger than the MPAS mesh-based flowline (yellow line). The structured mesh-based area of difference (light blue polygons) is larger than the MPAS mesh-based area of difference (red polygons).

348 *3.5.2 Area of difference*

349 Similar to our earlier study (Liao et al., 2022), we compared the area of difference
 350 formed by flowline intersections. In this method, we used area to represent line feature
 351 discrepancies. If two or more line features intersect, the intersected segments can be used
 352 to create enclosed polygons. In general, the smaller the total area, the closer the line fea-
 353 tures. The area of difference is illustrated in Figure 12. Area of differences can be cal-
 354 culated using Python scripting in the following steps:

- 355 1. Convert modeled conceptual flowlines into edge-based flowlines A;
- 356 2. Intersect the edge-based flowlines A with the simplified flowlines B to obtain all
 357 the vertices list C;
- 358 3. Classify the vertices C into different types of vertices (Text S2);
- 359 4. Split both A and B using C to obtain a list of flowlines D;
- 360 5. Build all the polygons enclosed by connected flowlines in D using a cycling algo-
 361 rithm and calculate their areas;
- 362 6. Sum up the areas to obtain the total area of difference.

363 For structured meshes, the area of difference decreases as the spatial resolution in-
 364 creases. At the same spatial resolution, the hexagon mesh-based area of difference is the

365 smallest except at the 50 km spatial resolution. For the unstructured mesh, the MPAS
366 mesh-based area of difference is smaller than its equivalent structured mesh results (Fig-
367 ures 13 and 14).

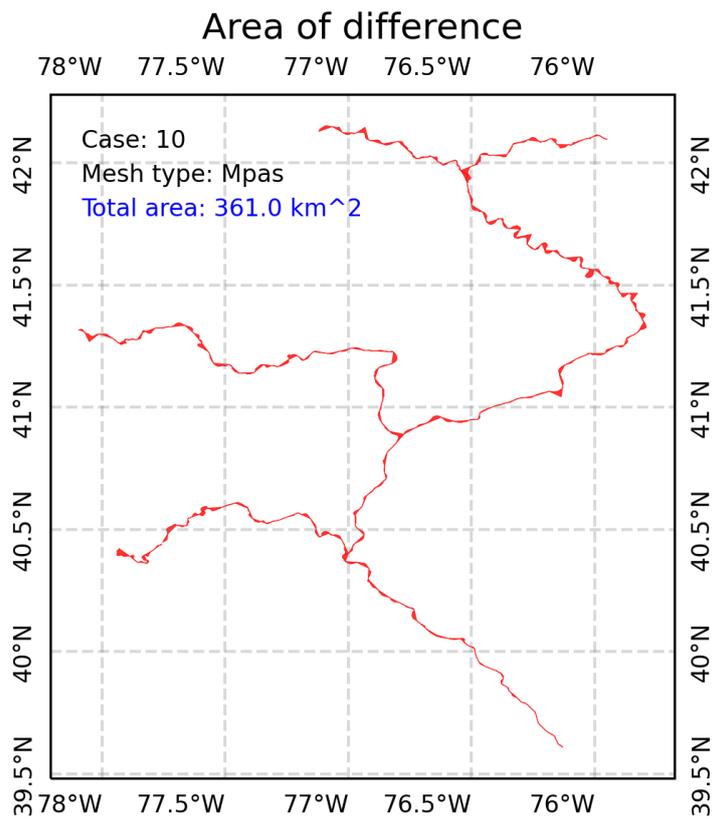


Figure 13. The enclosed area of difference between modeled river networks and simplified NHDPlus flowlines from the MPAS mesh.

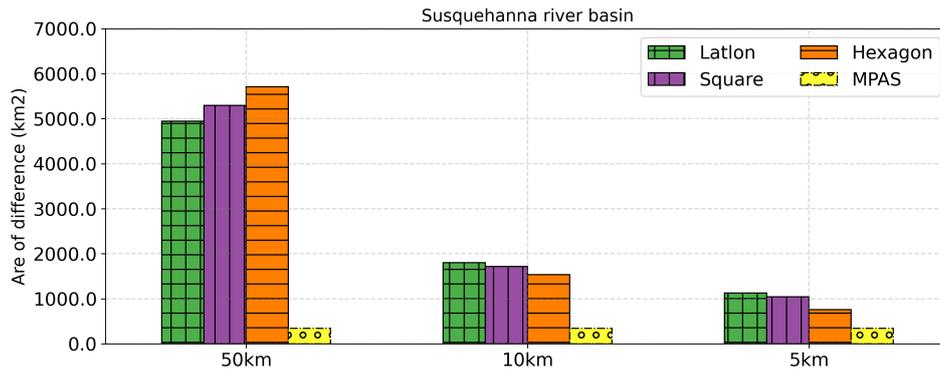


Figure 14. Comparison of the area-of-difference for modeled conceptual flowlines from different model configurations. The X-axis is the spatial resolution and the Y-axis is the area of difference (km^2).

368

3.5.3 Branching angle

369

370

371

372

373

374

375

376

The ramification angle, or branching angle (Text S1), is another important characteristic of river networks (Devauchelle et al., 2012). This metric is calculated using the last incoming flowline edges of a confluence. The results show that conceptual flowlines generally cannot capture the branching angles well, especially at the 50 km spatial resolution. For example, the branching angles at Confluence 2 are all 180 degrees from the structured meshes (Figures 9 and 15). This is because only a limited number of branching angles are supported by the structured meshes. In contrast, the branching angles from the MPAS mesh are more flexible because the mesh provides flexible rotations.

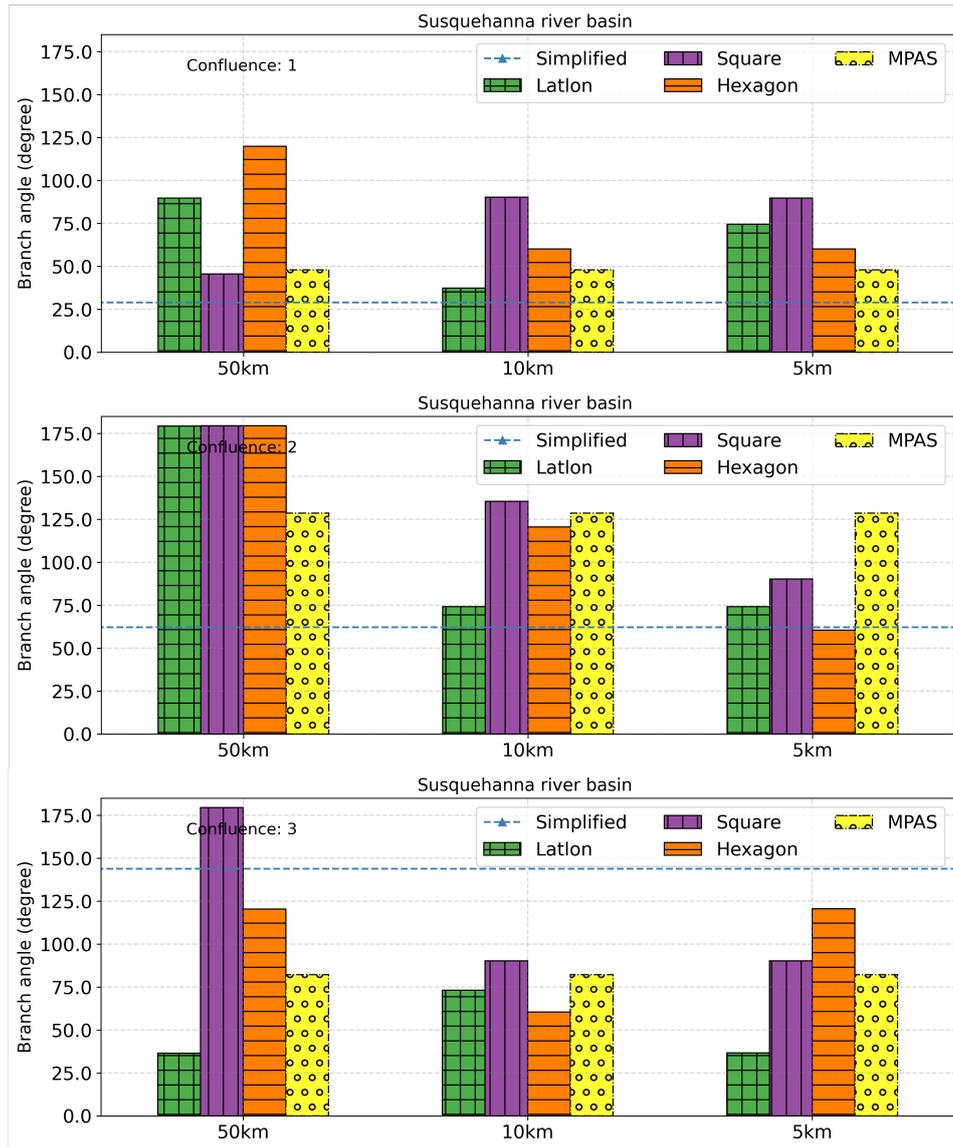


Figure 15. Comparison of the river branch angle from different model configurations for Confluence 1 to 3. The X-axis is the spatial resolution and the Y-axis is the branch angle (degree). The dashed blue line represents results from the simplified flowlines, used as the reference.

377

3.5.4 River sinuosity

378

379

380

381

382

383

River sinuosity is the ratio between flowline length and valley length (the distance between the starting and ending vertices of a flowline). For example, all the models underestimate river sinuosity for Segment 4, which exhibits many meander features (Figure 16). In contrast, the modeled river sinuosity is much closer to the reference for Segment 7, especially at the 5 km high spatial resolution in part because there are fewer meander features (Figure 16).

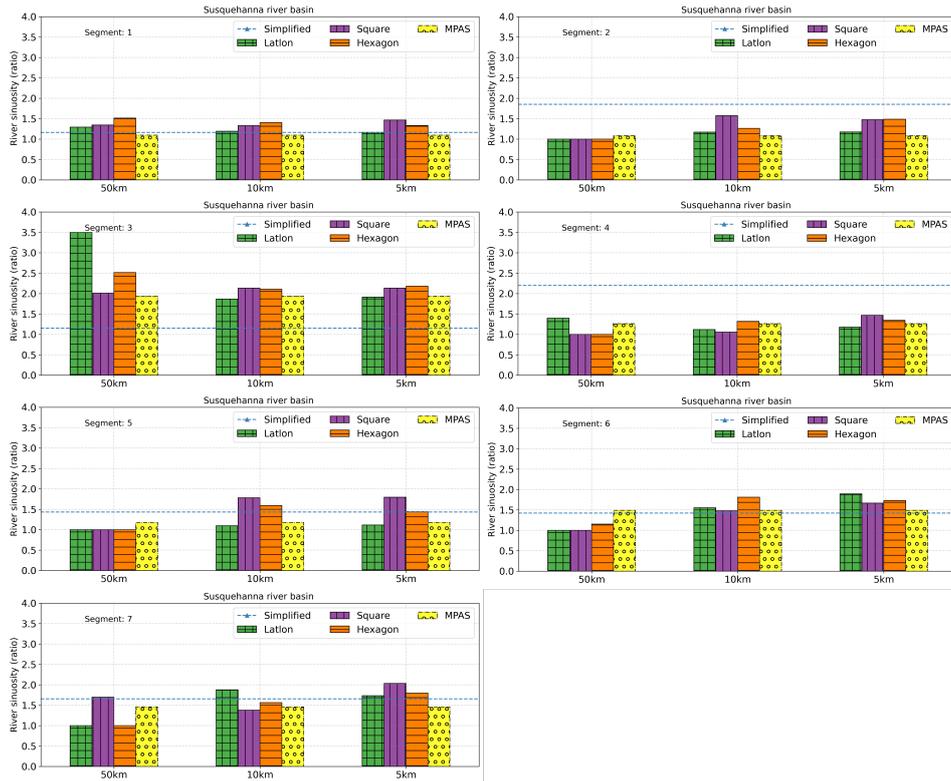


Figure 16. Comparison of river sinuosity for Segment 1 to 7 from different model configurations. The X-axis is the spatial resolution and the Y-axis is the sinuosity (ratio). The dashed blue line is the simplified flowline, used as the reference. Colored (green, purple, orange, and yellow) bars with textures represent different model configurations.

384 **4 Discussion**

385 **4.1 Thresholds**

386 **4.1.1 Stream order**

387 The stream order used to filter out small rivers from the original NHDPlus HR datasets
 388 determines the level of details the model can preserve (Figure 5). This threshold should
 389 be tested based on the mesh spatial resolution and hydrologic model application. For
 390 example, if low-order rivers are included during the data preparation step, they may be
 391 still removed by the small river removal algorithm.

392 Because stream order is based on the topological relationship between stream seg-
 393 ments, it may not reflect the actual drainage area of a river channel. For this reason, the
 394 drainage area should also be considered to filter out small rivers.

395 **4.1.2 Small river removal**

396 The “small river” threshold (Table S2) is an important parameter for removing river
 397 channels with relatively short lengths. It should be configured considering the mesh spa-
 398 tial resolution. User-provided flowlines may be too fragmented, causing the model to ex-
 399 cessively remove flowlines. For this reason, a visual inspection of the raw flowlines is im-
 400 portant.

4.1.3 Shortcut path length

Although the “shortcut path” algorithm allows the model to reproduce the classical D8 diagonal travel path in the rectangle meshes, its impact on the topological relationship reconstruction process is not trivial. The structured rectangle mesh particularly exemplifies the effects of the "shortcut path" algorithm because it produces a diagonal travel path that goes through the mesh cell vertex. In contrast, the shortcut remains on the mesh cell edge instead of vertex for the structured hexagon and unstructured MPAS meshes. Thus, the structured hexagon and unstructured MPAS meshes are preferred for coupled surface and subsurface hydrologic simulations because they are more compatible with hydrologic models that assume the flux exchange occur through the cell faces (Liao et al., 2022).

Similar to the small river removal algorithm, this parameter should consider the mesh spatial resolution. Therefore, a fraction between 0.0 and 1.0 of the mesh cell resolution is preferred.

In our model, the flowline length is used to determine whether the conceptual flowline should take a shortcut. Other studies also suggest that the distance from the flowline to the mesh cell center should also be considered (Lindsay, 2016b). A combined approach considering both length and distance may produce even more robust results.

4.2 Quality of modeled conceptual flowlines

In general, the quality of modeled conceptual flowlines increases as the spatial resolution increases. For structured meshes, the model performances are very close and the hexagon mesh is potentially better (Figure 14), which is constant with our earlier study (Liao et al., 2020). The MPAS mesh-based conceptual flowlines are the closest to the real flowlines.

Although the center-to-center flowline length often leads to reduced river length, the length decrease is offset by the “zig-zag” effect (Figure 12). This explains why the total length can be higher than the simplified flowlines from the structured meshes-based results (Figure 8). Because the MPAS mesh cells align with the simplified flowlines, they have a minimized offset effect and the shortest total length (Figure 16).

The area of difference comparison shows that the MPAS mesh produces the closest conceptual flowlines to the simplified flowlines in terms of area followed by the hexagon mesh. Its performance is even better than structured meshes at higher resolution 5 km (Figure 14).

Branching angle analysis shows that the structured meshes generally cannot capture the confluence ramification feature well because they only support a limited number of angles. The MPAS mesh has the potential to resolve this issue, but requires a high-quality mesh (Figure 15).

4.3 Importance of topological relationships

Compared with the vector-based or raster DEM-based river networks extraction methods, our topological relationship-based method overcomes several existing limitations. It precisely follows river channels near river meander and confluence, producing high-quality conceptual river networks.

Given the explicit topological relationships, advanced stream-burning algorithms can be implemented to remove the depressions within river channels. Traditionally, stream burning algorithms blindly lower river channel elevations significantly to force the flow direction. More recently, adaptive stream-burning algorithms can adjust river channel elevations using a hybrid breaching and filling approach (Lindsay, 2016b). However, the

breaching algorithm requires topological relationships, especially near river confluences, to avoid incorrect breaching directions(Liao et al., 2022). Therefore, the topological relationships produced from our method provide an opportunity to use the fully hybrid breaching and filling method to minimize modifications to both land and river elevations.

4.4 Implication for hydrologic and Earth system models

Representing river networks is key to hydrologic models. Our study achieves this through two major considerations. First, the flowline simplification guarantees that the most important river information is preserved while keeping river flowlines in their simplest formats. Second, the topological relationship-based conceptual flowlines further preserve the river network structures while linking them with the mesh system. In this way, the model is able to consistently capture the spatial pattern of river networks.

The support for non-rectangle meshes further improves model performance and demonstrates the advantage of using unstructured meshes in hydrologic and Earth system models. Instead of projecting existing hydrologic features onto the rectangle meshes, we can now directly generate meshes that explicitly define these features. For example, in this study, we burnt flowlines in the MPAS mesh through the JIGSAW density function and in the conceptual flowlines through the topological relationship reconstruction. Our method also burnt dams through the workflow (Figure S11). In the future, we can include other hydrologic features such as lakes and wetlands. This enables us to much more precisely define the geometry of hydrologic features, resulting in improved hydrologic and Earth system models(Liao et al., 2022).

Our method produces high-quality river routing parameters other than the spatial pattern. For example, it keeps track of both actual and conceptual flowline length throughout the processes. However, when the “shortcut” occurs, the corresponding flowline length can be merged into the upstream/downstream, or ignored. More importantly, the topological relationships can be used to minimize the modifications to both land and river elevations in the fully adaptive hybrid breaching and filling method, generating more realistic slopes in both rivers and riparian zones. Because both river length and slope are important river routing parameters, the results from our method can be used to improve flow routing models.

4.5 Limitations

There are several limitations to the current model. First, unlike the small river removal and shortcut path length parameters that can be configured to consider the mesh resolution, the stream order threshold used to filter out small rivers is not directly associated with any physical attribute. Alternatively, drainage area should be a more meaningful metric to filter out small rivers.

Second, the model does not use additional information in the cycling detection algorithm to decide which channel should be preserved if they have the same stream order. River channel width or length may be included to capture the dominant river channel.

Third, our current method only considers rivers in the workflow. Other hydrologic features (e.g., lake and reservoir) are not fully considered. In a complex landscape, these features should also be included so the final flow routing map is consistent for hydrologic and Earth system models.

Last, our model currently only relies on the topological relationship to reconstruct conceptual river networks. It is possible to combine our method with other upscaling methods to consider more complex scenarios. In this case, a more dedicated mesh cell topol-

495 ogy algorithm is needed because unstructured meshes often do not have the parent-child
496 hierarchical structure.

497 5 Conclusions

498 In this study, we developed a mesh-independent topological relationships-based river
499 networks representation model (PyFlowline). We applied the model to the Susquehanna
500 river basin with different configurations. The model evaluation shows that the model per-
501 forms well and the modeled conceptual river networks are consistent with the real-world
502 river networks. The outputs of our model, especially the topological relationships, should
503 be used for advanced terrain analysis and hydrologic models.

504 Acknowledgments

505 This work was supported by the Earth System Model Development program area of the
506 U.S. Department of Energy, Office of Science, Office of Biological and Environmental Re-
507 search as part of the multi-program, collaborative Integrated Coastal Modeling (ICoM)
508 project. The data used for model simulations can be downloaded through the USGS web-
509 site (<https://www.usgs.gov/national-hydrography>). The PyFlowline model can be
510 installed as a Python package (<https://github.com/changliao1025/pyflowline>). The
511 data and code used in this paper is available from [https://github.com/DOE-ICoM/liao-
512 -etal_2022_pyflowline_james](https://github.com/DOE-ICoM/liao-etal_2022_pyflowline_james). A portion of this research was performed using PNNL
513 Research Computing at Pacific Northwest National Laboratory. PNNL is operated for
514 DOE by Battelle Memorial Institute under contract DE-AC05-76RL01830.

515 Conflict of Interest

516 The authors certify that they have NO affiliations with or involvement in any or-
517 ganization or entity with any financial interest (such as honoraria; educational grants;
518 participation in speakers' bureaus; membership, employment, consultancies, stock own-
519 ership, or other equity interest; and expert testimony or patent-licensing arrangements),
520 or non-financial interest (such as personal or professional relationships, affiliations, knowl-
521 edge or beliefs) in the subject matter or materials discussed in this manuscript.

522 References

- 523 Coon, E., Svyatsky, D., Jan, A., Kikinzon, E., Berndt, M., Atchley, A., ...
524 Molins, S. (2019, 9). *Advanced Terrestrial Simulator*. [Computer Soft-
525 ware] \url{https://doi.org/10.11578/dc.20190911.1}. Retrieved from
526 <https://doi.org/10.11578/dc.20190911.1> doi: 10.11578/dc.20190911.1
- 527 Davies, H. N., & Bell, V. A. (2009). Assessment of methods for extracting low-
528 resolution river networks from high-resolution digital data. *Hydrological Sci-
529 ences Journal*, *54*(1), 17–28. doi: 10.1623/hysj.54.1.17
- 530 de Azeredo Freitas, H. R., da Costa Freitas, C., Rosim, S., & de Freitas Oliveira,
531 J. R. (2016). Drainage networks and watersheds delineation derived from
532 TIN-based digital elevation models. *Computers & Geosciences*, *92*, 21–37.
- 533 Decharme, B., Alkama, R., Papa, F., Faroux, S., Douville, H., & Prigent, C. (2012).
534 Global off-line evaluation of the ISBA-TRIP flood model. *Climate Dynamics*,
535 *38*(7), 1389–1412.
- 536 Devauchelle, O., Petroff, A. P., Seybold, H. F., & Rothman, D. H. (2012). Rami-
537 fication of stream networks. *Proceedings of the National Academy of Sciences*,
538 *109*(51), 20832–20836.
- 539 Eilander, D., Van Verseveld, W., Yamazaki, D., Weerts, A., Winsemius, H. C., &
540 Ward, P. J. (2021). A hydrography upscaling method for scale-invariant

- 541 parametrization of distributed hydrological models. *Hydrology and Earth*
 542 *System Sciences*, 25(9), 5287–5313.
- 543 Engwirda, D. (2014). Locally optimal Delaunay-refinement and optimisation-based
 544 mesh generation.
- 545 Engwirda, D. (2017). JIGSAW-GEO (1.0): locally orthogonal staggered unstruc-
 546 tured grid generation for general circulation modelling on the sphere. *Geosci-*
 547 *entific Model Development*, 10(6), 2117–2140.
- 548 Engwirda, D., & Liao, C. (2021, 10). 'Unified' Laguerre-Power Meshes for Cou-
 549 pled Earth System Modelling. *Zenodo*. Retrieved from [https://zenodo.org/](https://zenodo.org/record/5558988)
 550 [record/5558988](https://zenodo.org/record/5558988) doi: 10.5281/ZENODO.5558988
- 551 Esri Water Resources Team. (2011). *Arc Hydro Tools - Tutorial* (Tech. Rep.).
- 552 Fekete, B. M., Vorosmarty, C. J., & Lammers, R. B. (2001). Scaling gridded river
 553 networks for macroscale hydrology: Development, analysis, and control of
 554 error. *Water Resources Research*, 37(7), 1955–1967.
- 555 Feng, D., Tan, Z., Engwirda, D., Liao, C., Xu, D., Bisht, G., . . . Leung, R.
 556 (2022). Investigating coastal backwater effects and flooding in the coastal
 557 zone using a global river transport model on an unstructured mesh. *Hy-*
 558 *drology and Earth System Sciences Discussions*, 2022, 1–31. Retrieved
 559 from <https://hess.copernicus.org/preprints/hess-2022-251/> doi:
 560 10.5194/hess-2022-251
- 561 GDAL/OGR contributors. (2019). *Geospatial Data Abstraction software Library*.
 562 Retrieved from <https://gdal.org>
- 563 Gillies, S., & others. (2007). *Shapely: manipulation and analysis of geometric ob-*
 564 *jects*. Retrieved from <https://github.com/Toblerity/Shapely>
- 565 Goulden, T., Hopkinson, C., Jamieson, R., & Sterling, S. (2014). Sensitivity of
 566 watershed attributes to spatial resolution and interpolation method of LiDAR
 567 DEMs in three distinct landscapes. *Water Resources Research*, 50(3), 1908–
 568 1927. doi: 10.1002/2013WR013846
- 569 Hellweger, F., & Maidment, D. (1997). AGREE-DEM surface
 570 reconditioning system. *Online at http://www.ce.utexas.edu/prof/maidment/gishydro/ferdi/research/agree/agree.html (last accessed*
 571 *March 3, 2005)*.
- 572
- 573 Hsu, S.-C. (2020). Hex-Urban: Investigating the adoption of hexagonal grids to rep-
 574 resent the total urban water cycle within a distributed water balance model.
- 575 Hunter, J. D. (2007). Matplotlib: A 2D graphics environment. *Computing in Science*
 576 *and Engineering*, 9(3), 90–95. doi: 10.1109/MCSE.2007.55
- 577 Hyvaluoma, J. (2017). Reducing the grid orientation dependence of flow routing on
 578 square-grid digital elevation models. *International Journal of Geographical In-*
 579 *formation Science*, 31(11), 2272–2285.
- 580 Ivanov, V. Y., Vivoni, E. R., Bras, R. L., & Entekhabi, D. (2004). Catchment hy-
 581 drologic response with a fully distributed triangulated irregular network model.
 582 *Water Resources Research*, 40(11). doi: 10.1029/2004WR003218
- 583 Jolley, T. J., & Wheeler, H. S. (1997). The introduction of runoff routing into large-
 584 scale hydrological models. *Hydrological processes*, 11(15), 1917–1926.
- 585 Kreveld, M. v., & Silveira, R. I. (2011). Embedding rivers in triangulated irregular
 586 networks with linear programming. *International Journal of Geographical In-*
 587 *formation Science*, 25(4), 615–631.
- 588 Liao, C. (2022, 3). *A lightweight Python package for Earth science*. *Zenodo*. Re-
 589 trieved from <https://zenodo.org/record/6368652> doi: 10.5281/ZENODO
 590 .6368652
- 591 Liao, C., & Cooper, M. (2022, 4). *Pyflowline a mesh-independent river network gen-*
 592 *erator for hydrologic models*. *Zenodo*. Retrieved from [https://doi.org/10](https://doi.org/10.5281/zenodo.6407299)
 593 [.5281/zenodo.6407299](https://doi.org/10.5281/zenodo.6407299) doi: 10.5281/zenodo.6407299
- 594 Liao, C., Tesfa, T., Duan, Z., & Leung, L. R. (2020). Watershed delineation on
 595 a hexagonal mesh grid. *Environmental Modelling & Software*, 128, 104702.

- 596 Retrieved from [http://www.sciencedirect.com/science/article/pii/](http://www.sciencedirect.com/science/article/pii/S1364815219308278)
597 S1364815219308278 doi: 10.1016/j.envsoft.2020.104702
- 598 Liao, C., Zhou, T., Xu, D., Barnes, R., Bisht, G., Li, H.-Y., ... Engwirda, D.
599 (2022). Advances in hexagon mesh-based flow direction modeling. *Advances in*
600 *Water Resources*, 104099. doi: 10.1016/j.advwatres.2021.104099
- 601 Liao, C., Zhuang, Q., Leung, L. R., & Guo, L. (2019). Quantifying Dissolved Or-
602 ganic Carbon Dynamics Using a Three-Dimensional Terrestrial Ecosystem
603 Model at High Spatial-Temporal Resolutions. *Journal of Advances in Modeling*
604 *Earth Systems*, 11(12), 4489–4512. doi: 10.1029/2019MS001792
- 605 Lin, P., Yang, Z.-L., Gochis, D. J., Yu, W., Maidment, D. R., Somos-Valenzuela,
606 M. A., & David, C. H. (2018). Implementation of a vector-based river network
607 routing scheme in the community WRF-Hydro modeling framework for flood
608 discharge simulation. *Environmental Modelling & Software*, 107, 1–11.
- 609 Lindsay, J. B. (2016a). Efficient hybrid breaching-filling sink removal methods for
610 flow path enforcement in digital elevation models. *Hydrological Processes*,
611 30(6), 846–857. doi: 10.1002/hyp.10648
- 612 Lindsay, J. B. (2016b). The practice of DEM stream burning revisited. *Earth Sur-*
613 *face Processes and Landforms*, 41(5), 658–668. doi: 10.1002/esp.3888
- 614 Lindsay, J. B., Yang, W., & Hornby, D. D. (2019). Drainage network analysis and
615 structuring of topologically noisy vector stream data. *ISPRS International*
616 *Journal of Geo-Information*, 8(9), 422.
- 617 Luo, X., Hong-Yi, L., Leung, L. R., Tesfa, T. K., Getirana, A., Papa, F., & Hess,
618 L. L. (2017). Modeling surface water dynamics in the Amazon Basin using
619 MOSART-Inundation v1.0: impacts of geomorphological parameters and river
620 flow representation. *Geoscientific Model Development*, 10(3), 1233.
- 621 Mao, Y., Zhou, T., Leung, L. R., Tesfa, T. K., Li, H., Wang, K., ... Getirana,
622 A. (2019). Flood inundation generation mechanisms and their changes in
623 1953–2004 in global major river basins. *Journal of Geophysical Research:*
624 *Atmospheres*, 124(22), 11672–11692.
- 625 Minn, M. (2015). MMQGIS for QGIS Geographic Information System. *Open Source*
626 *Geospatial Foundation Project.* [(accessed on 17 May 2018)].
- 627 Mizukami, N., Clark, M. P., Sampson, K., Nijssen, B., Mao, Y., McMillan, H., ...
628 Woods, R. (2016). mizuRoute version 1: a river network routing tool for a
629 continental domain water resources applications. *Geoscientific Model Develop-*
630 *ment*, 9(6), 2223–2238.
- 631 Munier, S., & Decharme, B. (2022). River network and hydro-geomorphological pa-
632 rameters at 1 / 12 resolution for global hydrological and climate studies. *Earth*
633 *System Science Data*, 14(5), 2239–2258.
- 634 Paz, A. R., & Collischonn, W. (2007). River reach length and slope estimates for
635 large-scale hydrological models based on a relatively high-resolution digital
636 elevation model. *Journal of Hydrology*, 343(3-4), 127–139.
- 637 Reed, S. M. (2003). Deriving flow directions for coarse-resolution (1–4 km) gridded
638 hydrologic modeling. *Water resources research*, 39(9).
- 639 Ringler, T., Petersen, M., Higdon, R. L., Jacobsen, D., Jones, P. W., & Maltrud,
640 M. (2013). A multi-resolution approach to global ocean modeling. *Ocean*
641 *Modelling*, 69, 211–232. doi: 10.1016/j.ocemod.2013.04.010
- 642 Sahr, K. (2015). *DGGRID version 6.2 b: User documentation for discrete global grid*
643 *software*.
- 644 Shaw, D. A., Martz, L. W., & Pietroniro, A. (2005). A methodology for preserving
645 channel flow networks and connectivity patterns in large-scale distributed hy-
646 drological models. *Hydrological Processes: An International Journal*, 19(1),
647 149–168.
- 648 Shelef, E., & Hilley, G. E. (2013). Impact of flow routing on catchment area calcu-
649 lations, slope estimates, and numerical simulations of landscape development.
650 *Journal of Geophysical Research: Earth Surface*, 118(4), 2105–2123.

- 651 Sood, A., & Smakhtin, V. (2015). Global hydrological models: a review. *Hydrological*
652 *Sciences Journal*, *60*(4), 549–565. doi: 10.1080/02626667.2014.950580
- 653 Tarboton, D. G. (2003). Terrain analysis using digital elevation models in hydrology. In *23rd esri international users conference, san diego, california* (Vol. 14).
654 Citeseer.
- 655 Tarboton, D. G., Bras, R. L., & Rodriguez-Iturbe, I. (1988). The fractal nature of
656 river networks. *Water Resources Research*, *24*(8), 1317–1322.
- 657 Tarboton, D. G., Bras, R. L., & Rodriguez-Iturbe, I. (1991). On the extraction of
658 channel networks from digital elevation data. *Hydrological processes*, *5*(1), 81–
659 100. doi: 10.1002/hyp.3360050107
- 660 USGS. (2013). *National Hydrography Geodatabase: The National Map*
661 *viewer available on the World Wide Web, accessed [June 02, 2015], at url*
662 *[<http://viewer.nationalmap.gov/viewer/nhd.html?p=nhd>]. Retrieved from*
663 *<http://viewer.nationalmap.gov/viewer/nhd.html?p=nhd>*
- 664 Wu, H., Kimball, J. S., Li, H., Huang, M., Leung, L. R., & Adler, R. F. (2012). A
665 new global river network database for macroscale hydrologic modeling. *Water*
666 *resources research*, *48*(9). doi: 10.1029/2012WR012313
- 667 Wu, H., Kimball, J. S., Mantua, N., & Stanford, J. (2011). Automated upscaling
668 of river networks for macroscale hydrological modeling. *Water Resources Re-*
669 *search*, *47*(3). doi: 10.1029/2009WR008871
- 670 Yamazaki, D., Ikeshima, D., Sosa, J., Bates, P. D., Allen, G. H., & Pavelsky, T. M.
671 (2019). MERIT Hydro: A high-resolution global hydrography map based on
672 latest topography dataset. *Water Resources Research*, *55*(6), 5053–5073. doi:
673 10.1029/2019WR024873
- 674 Yamazaki, D., Kanae, S., Kim, H., & Oki, T. (2011). A physically based descrip-
675 tion of floodplain inundation dynamics in a global river routing model. *Water*
676 *Resources Research*, *47*(4).
- 677 Yamazaki, D., Oki, T., & Kanae, S. (2009). Deriving a global river network map
678 and its sub-grid topographic characteristics from a fine-resolution flow direc-
679 tion map. *Hydrology and Earth System Sciences*, *13*(11), 2241–2251. doi:
680 10.5194/hess-13-2241-2009
- 681 Zhou, T., Leung, L. R., Leng, G., Voisin, N., Li, H., Craig, A. P., . . . Mao, Y.
682 (2020). Global irrigation characteristics and effects simulated by fully cou-
683 pled land surface, river, and water management models in E3SM. *Journal of*
684 *Advances in Modeling Earth Systems*, *12*(10), e2020MS002069.
- 685

Supporting Information for "Topological relationships-based flow direction modeling: mesh-independent river networks representation"

Chang Liao¹, Tian Zhou¹, Donghui Xu¹, Matt Cooper¹, Darren Engwirda²,

Hong-Yi Li³, L. Ruby Leung¹

¹Atmospheric Sciences and Global Change, Pacific Northwest National Laboratory, Richland, WA, USA

²T-3 Fluid Dynamics and Solid Mechanics Group, Los Alamos National Laboratory, Los Alamos, NM, USA

³University of Houston, Houston, TX, USA

Contents of this file

1. Text S1 to S4
2. Figures S1 to S13
3. Tables S1 to S2

Introduction

This supplementary information includes details of the following topics.

1. Spatial reference and computational geometry (Text S1)
2. River network simplification algorithm (Text S2, Figures S8-S10)
3. MPAS mesh and additional results (Text S3, Figure S11)
4. Comparison with the raster DEM-based (with stream burning) method (Text S4, Figure S13)

5. Advantages of topological relationship-based method on the rectangle and hexagon meshes (Figures S1-S6)

6. Data model and definition (Figures S7 and S12)

7. Comparisons of existing river network representation methods at watershed and global scales (Table S1)

8. Major model configurations (Table S2)

Text S1.

Because different grid/mesh systems use different types of spatial references, computing and visualizing several metrics (e.g., distance and area) under the same framework is not straightforward. Therefore, we converted all meshes into the geographic coordinate system (GCS) spatial reference and implemented geometric algorithms based on the GCS framework. For example, the original structured square and hexagon meshes use the projected coordinate system (PCS) system. During the mesh generation process, all the coordinates were re-projected to the GCS system.

Geodesic distance

We assume the Earth surface is a perfect sphere. We define the great-circle length, the distance between two vertices on a curved surface, as the vertex distance.

Geodesic area

We define the spherical sector area, the area enclosed by more than two vertices on a curved surface, as the mesh cell area.

Geodesic angle

We define the geodesic angle, the vector angle in a three-dimensional sphere, as the river confluence branching angle.

Text S2.**Step 1 format conversion**

This step converts the user provided vector-based river networks into the model framework, i.e., GCS-based flowline.

Step 2 connect disconnected flowlines

This step connects two flowlines separated due to digitization error.

Step 3 define flowline vertices

A vertex classification algorithm was developed to classify all the vertices into headwater/outlet vertex, middle vertex, and confluence vertex depending on the associated number of flowlines. For example, in Figure S8a, vertices A, C, and F are defined as headwater/outlet vertices because they are associated with just one flowline. Vertices B and E are defined as middle vertices because B is connected to both flowline A->B and B->E and E is connected to both flowline B->E and E->F. Vertex D is initially defined as a headwater/outlet vertex because it is the end vertex of flowline C->D. However, after the split-by-vertex algorithm, flowline A->B splits into A->D and D->B, which redefines D as a confluence vertex because it is now connected to three flowlines.

Step 4 and 8 flowlines split and merge

Based on vertex classification, the flowlines are split or merged recursively until the network cannot be further simplified (Figure S8).

Step 5 recondition flowline

This step corrects flowline direction using the user-provided outlet location. The algorithm recursively searches from the river outlet. For example, if the starting-vertex of a flowline is the same as the outlet vertex, this flowline direction is then reversed.

Step 6 cycle removal

A cycling detection algorithm was developed to identify and simplify braided river flowlines. This algorithm scans the network and finds braided rivers. If a vertex has multiple downstream flowlines, it only keeps the one with the highest stream order as the dominant flowline (Figure S9).

Step 7 small river removal

Small headwater flowlines can be optionally removed using a user-provided length threshold. This step may be run multiple times because the previous iteration may convert non-headwaters into headwaters.

Step 9 flowline indexing

After flowline simplification, the individual flowline is considered a stream segment (Flowline A->D, C->D, and D->F in Figure S8c). Both stream segment index and stream order (Strahler) are re-calculated(USGS, 2013; Liao et al., 2022). This information is used by the topological relationships reconstruction algorithm.

Text S3.

The Model for Prediction Across Scales (MPAS) mesh is an unstructured mesh widely used by the Earth system model community to provide a unified modeling framework for atmosphere, ocean, and other earth-system components(Ringler et al., 2013). It offers a gradual refinement of horizontal resolution to resolve several numerical difficulties in nested-domain modeling applications. It is based on Spherical Centroidal Voronoi Tessellations (SCVTs) and is composed of an irregular mesh of polygons (mostly hexagons). MPAS mesh can be generated by the JIGSAW mesh generator(Engwirda, 2017).

Text S4.

Because our method is an extension of our earlier studies(Liao et al., 2020, 2022), the results of this study are comparable to both large-scale flow direction datasets(Wu et al., 2012) and regional/watershed scale raster DEM-based (with stream burning) results depending on the model configurations. The full flow direction comparison will be provided in our part 2 study. Below we provide the comparison between our method and the raster DEM-based (with stream burning) method.

Because the raster DEM-based method is very sensitive to the DEM spatial resolution, we used the configuration with the highest resolution (5km) for comparison. Specifically, we compared the PCS rectangle mesh (square)-based results from Case 7 with the existing raster DEM-based method(Winchell et al., 2007). We first resampled the USGS National Elevation Dataset (NED) high resolution 30 m DEM to 5km, then ran the method using the resampled DEM and user-provided river networks.

Because the raster DEM-based method relies on flow accumulation, the final modeled flowlines are different from the user-provided flowlines. Our comparison only focuses on the flowlines produced by both methods.

At 5 km spatial resolution, the spatial patterns from both methods are very close (Figure S13). However, there are two major differences. First, some mesh cells that contain user-provided flowlines are excluded in the raster DEM-based method because their flow accumulations are smaller than the accumulation threshold. Therefore the DEM-based method cannot capture the river meander in many locations and produces a much shorter total length of modeled flowlines. In contrast, the topology-based method mostly preserves these mesh cells and generates a much longer total length (Figure S13). Second, the DEM-based method often produces shifted river confluence locations. In contrast, the topology-based method can capture river confluences in most cases. However, the topology-based method can also produce incorrect confluences due to the cycle removal algorithm.

Figure S1.

Figure S2.

Figure S3.

Figure S4.

Figure S5.

Figure S6.

Figure S7.

Figure S8.

Figure S9.

Figure S10.

Figure S11.

Figure S12.

Figure S13.

Table S1

Table S2

Table S1. Comparisons of existing river network representation methods at watershed and global scales.

	Watershed scale		Global scale
	Vector	Raster DEM (stream burning)	e.g., COTAT/NTM
Inputs	Vector flowline	Raster DEM + vector flowline	Vector flowline + Cartesian mesh
Recommended resolution	High + moderate	High	Coarse
Flat area	Not sensitive	Less sensitive	Not sensitive
Support unstructured mesh	Not applicable	No	No
Small river removal	Optional	Optional	Automate
Braided river removal	Automate	Require pre-processing	Automate
Coverage	Only river	Entire domain	Entire domain
Impact on slope	Not applicable	High	Low
Impact on mesh generation	Not applicable	Not applicable	Not applicable

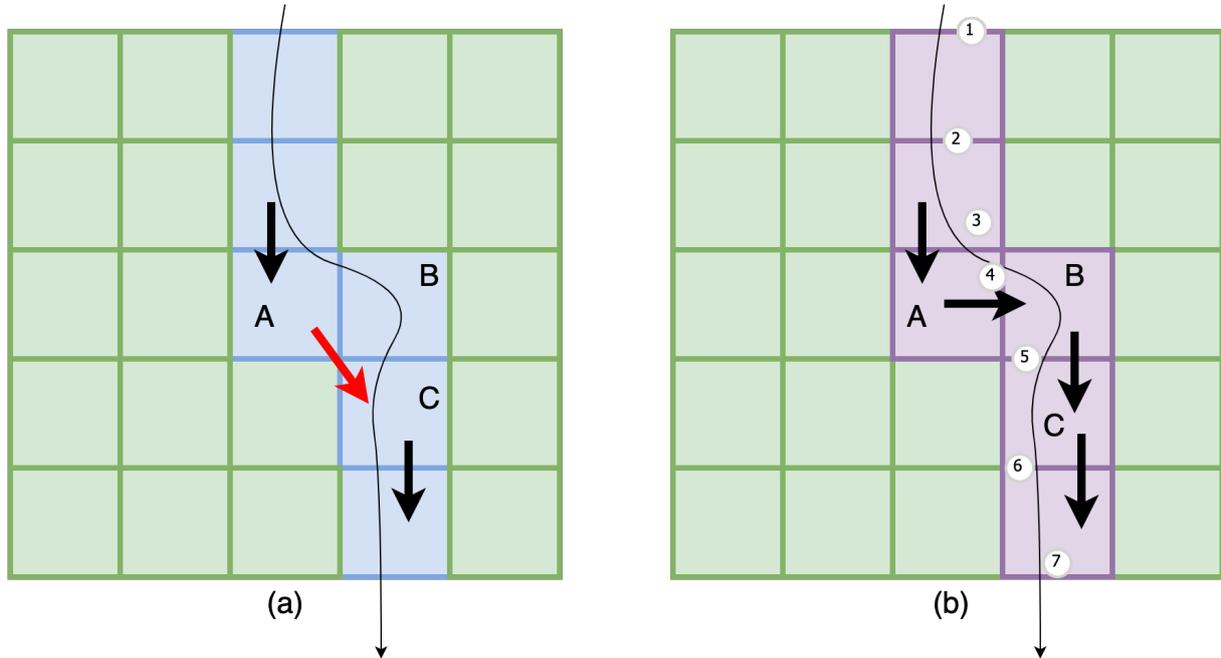


Figure S1. Illustration of flow direction on a rectangle mesh (a) without and (b) with the topological relationship at river meanders. Green mesh cells are land cells. Light blue and purple mesh cells (A, B, and C) are river cells. The black lines are the stream segments. Red arrow (A->C) and black arrows (A->B and B->C) are incorrect and correct flow directions, respectively. Circles with indices (1, 2, ..., 7) are vertices where a segment intersects with cell edges.

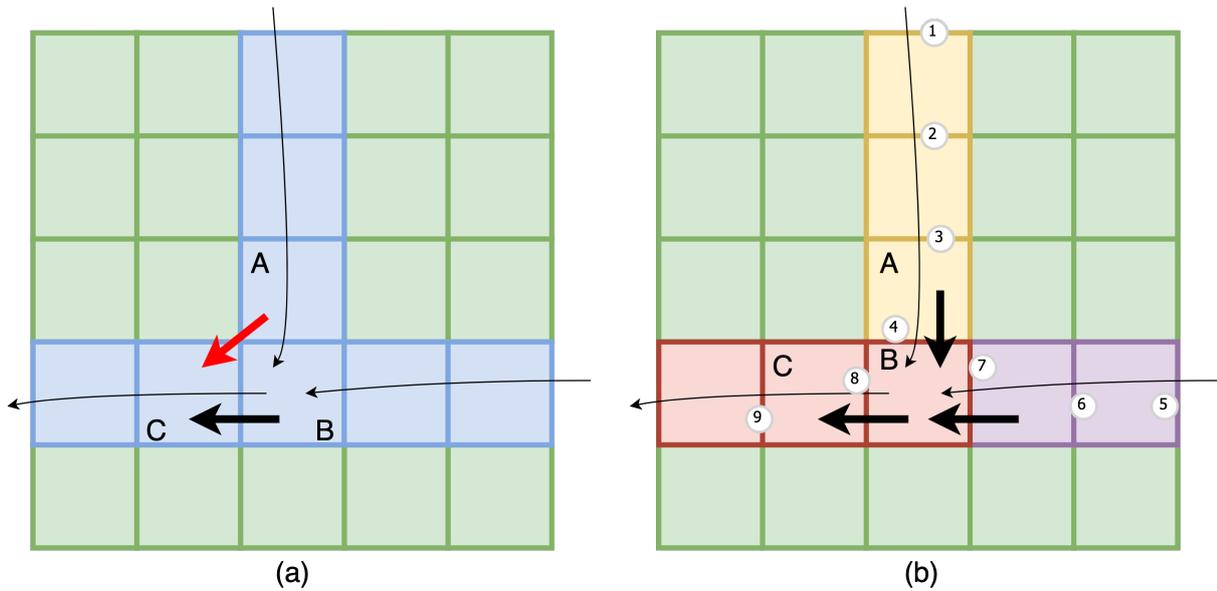


Figure S2. Illustration of flow direction on a rectangle mesh (a) without and (b) with the topological relationship at river confluence. Green cells are land. Light blue, yellow, red, and purple cells (A, B, and C) are river cells. Black lines are the stream segments. Red arrow (A->C) and black arrows (A->B and B->C) are incorrect and correct flow directions, respectively. Circles with indices (1, 2, ..., 9) are vertices where segments intersect with cell edges or each other.

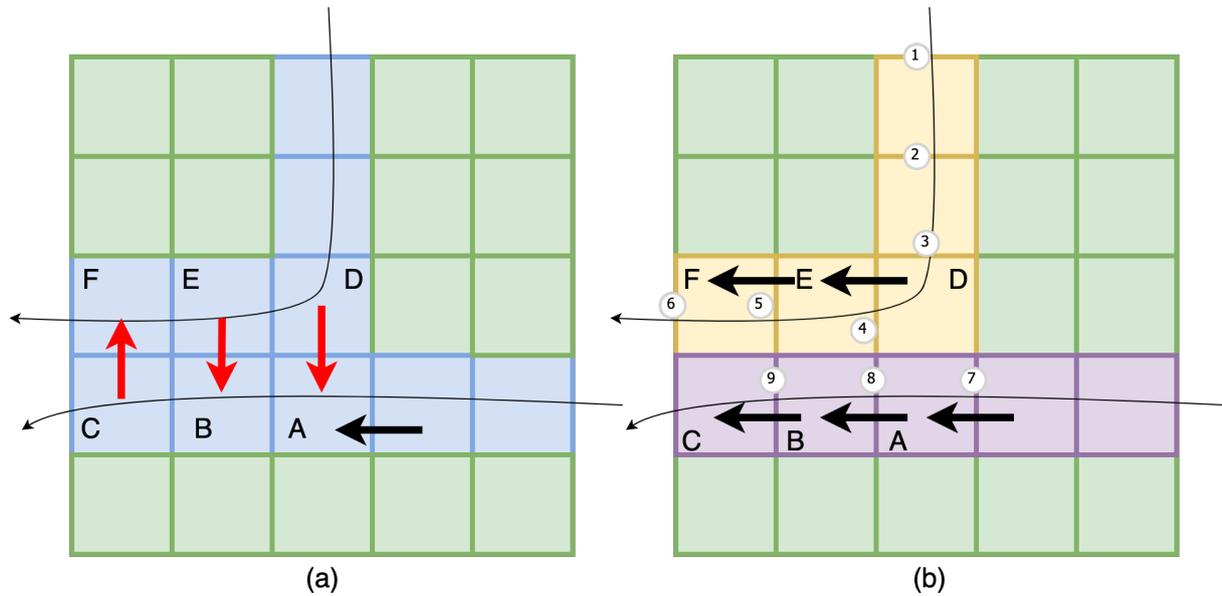


Figure S3. Illustration of flow direction on a rectangle mesh (a) without and (b) with the topological relationship when two rivers run in parallel. Green mesh cells are land cells. Light blue, yellow, and purple mesh cells (A, B,..., and F) are river cells. Black lines are the stream channels. Red arrows (D->A, B->E, and C->F) and black arrows (A->B, B->C, D->E, and E->F) are incorrect and correct flow directions, respectively. Circles with indices (1, 2, ..., 9) are vertices where river channels intersect with mesh cell edges.

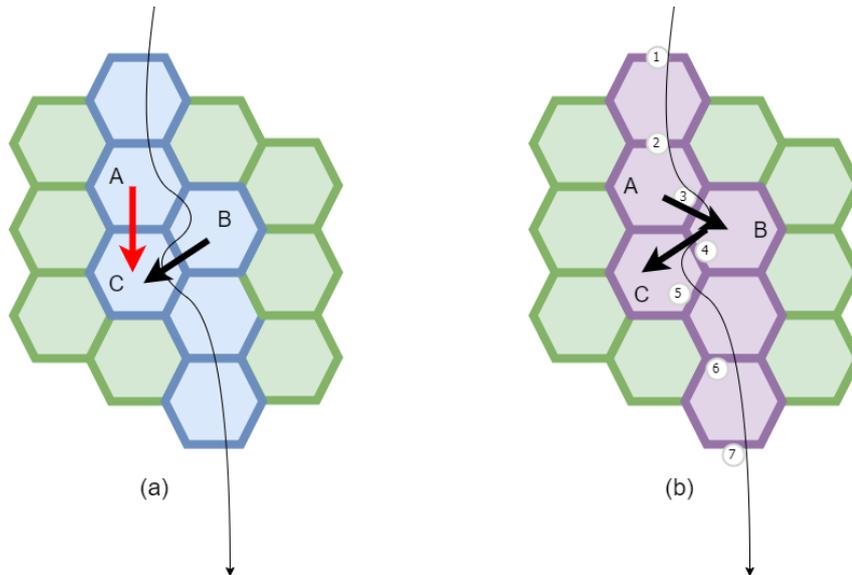


Figure S4. Illustration of flow direction on a hexagon mesh (a) without and (b) with the topological relationship when river meanders. Green mesh cells are land cells. Light blue and purple mesh cells (A, B, and C) are river cells. Black lines are the stream segments. Red and black arrows are incorrect ($A \rightarrow C$) and correct ($A \rightarrow B$ and $B \rightarrow C$) flow directions, respectively. Circles with indices (1, 2, ..., 7) are vertices where segment intersects with cell edges.

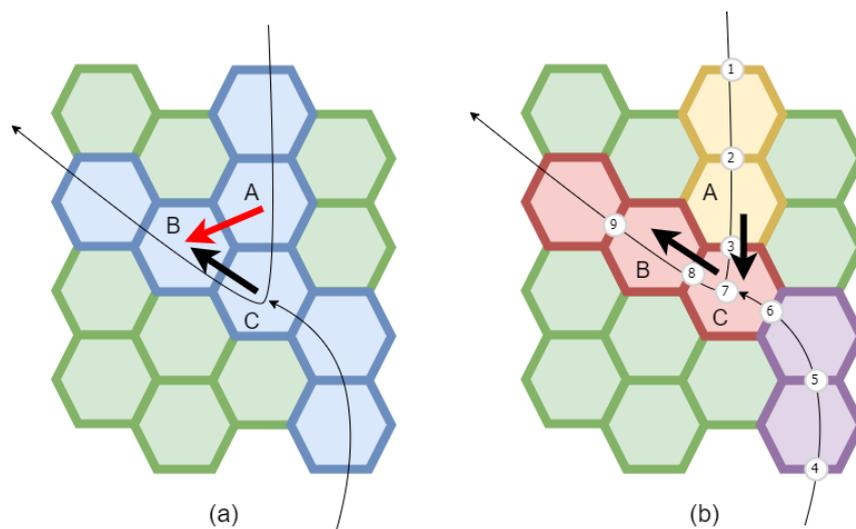


Figure S5. Illustration of flow direction on a hexagon mesh (a) without and (b) with the topological relationship at a river confluence. Green cells are land. Light blue, yellow, red, and purple cells (A, B, and C) are river cells. Black lines are the stream segments. Red and black arrows are incorrect (A->B) and correct (A->C and C->B) flow directions, respectively. Circles with indices (1, 2, ..., 9) are vertices where segments intersect with cell edges or each other.

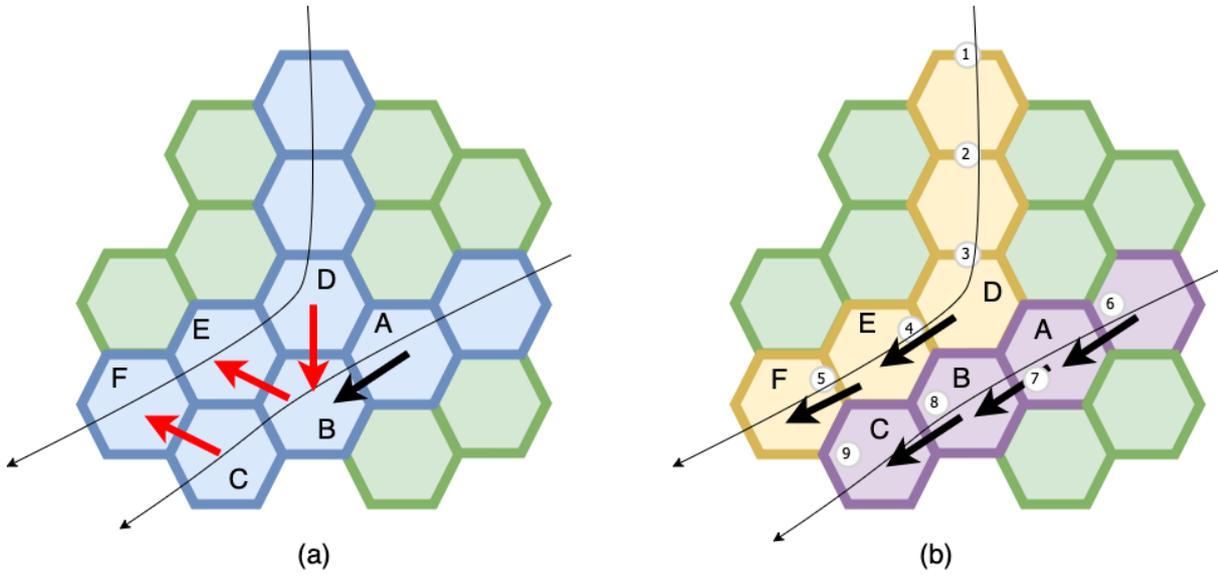


Figure S6. Illustration of flow direction on a hexagon mesh (a) without and (b) with the topological relationship when two rivers run in parallel. Green mesh cells are land cells. Light blue, yellow, and purple mesh cells (A, B,..., and F) are river cells. Black lines are the stream channels. Red and black arrows are incorrect (D->B, B->E, and C->F) and correct (A->B, B->C, D->E, and E->F) flow directions, respectively. Circles with indices (1, 2, ..., 9) are vertices where river channels intersect with mesh cell edges.

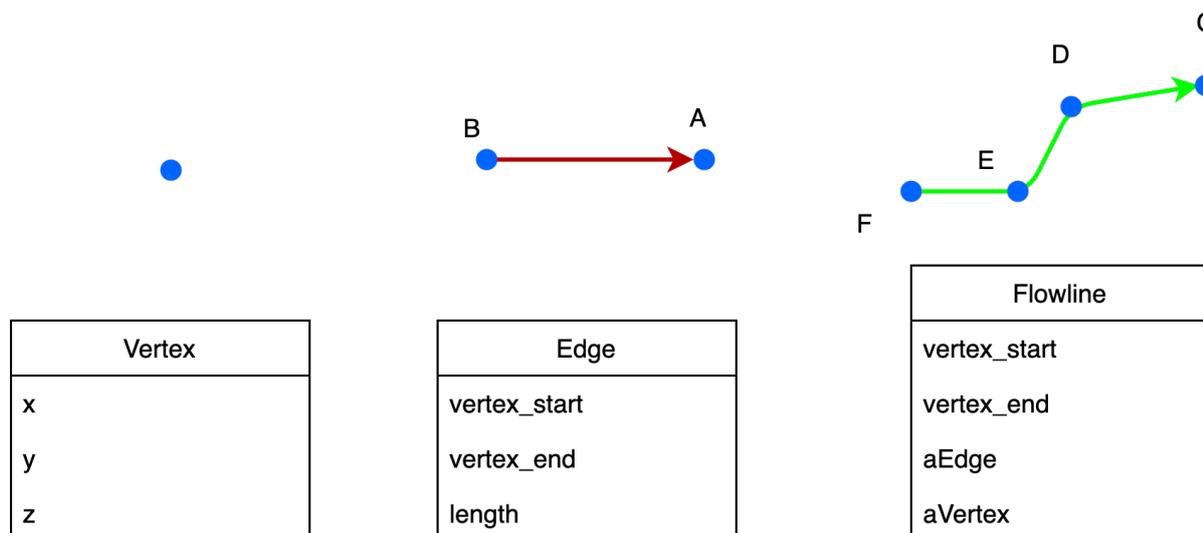


Figure S7. Illustration of the three basic elements (with attributes) used to represent a river channel. A vertex is a point with location attributes (x, y, and z). A directed edge is a link connecting two vertices (start and end). It also has the length attribute. A flowline is a list of connected edges (an edge is also a single-edge flowline). It has both start and end vertices. Its length is the sum of all member edges. For notation, a single letter/number will be used for a vertex (e.g., vertex A), two letters/numbers will be used for a directed edge (e.g., B->A), and multiple letters/numbers will be used for a directed flowline (e.g., F->E->D->C).

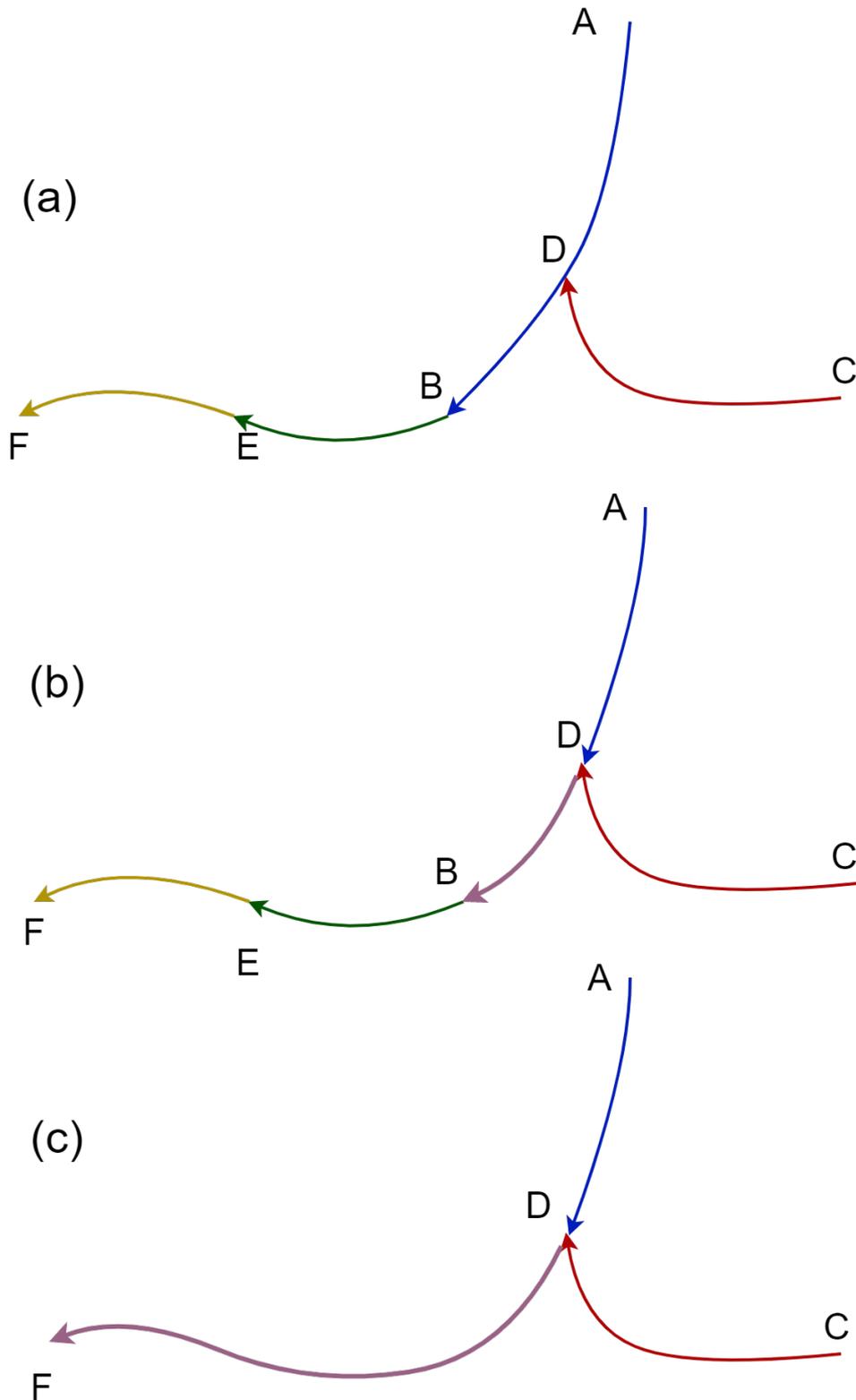


Figure S8. Illustration of flowline split and merge algorithms. The original river networks have 4 flowlines (colored lines A->B, B->E, E->F, and C->D). First, the split-by-vertex algorithm splits A->B using all vertices to obtain 5 flowlines (A->D, C->D, D->B, B->E, and E->F). Second, vertex D is left as a reference vertex. Third, the algorithm merges flowlines D->B, B->E, and E->F because vertex B and E are middle vertices. In the end, only 3 flowlines, A->D, C->D, and D->F, are defined.

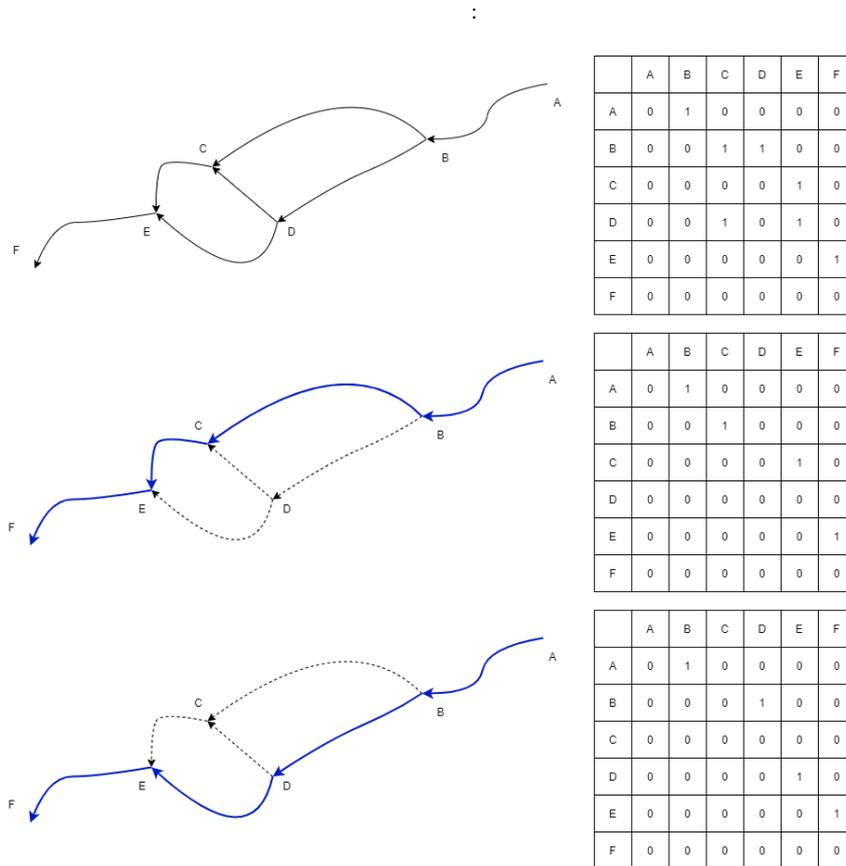


Figure S9. Illustration of braided river simplification using the cycling detection algorithm. On the left, black lines are original river flowlines, blue flowlines are 2 out of 3 candidate simplified flowlines ($A \rightarrow B \rightarrow C \rightarrow E \rightarrow F$ or $A \rightarrow B \rightarrow D \rightarrow E \rightarrow F$). Dashed flowlines are removed flowlines. On the right, each matrix is the corresponding network matrix with 0 and 1 representing no flow and flow, respectively. In a directed network, a braided river occurs when a vertex is the starting vertex of more than one flowline. Correspondingly, its network matrix has multiple 1s on the same row.

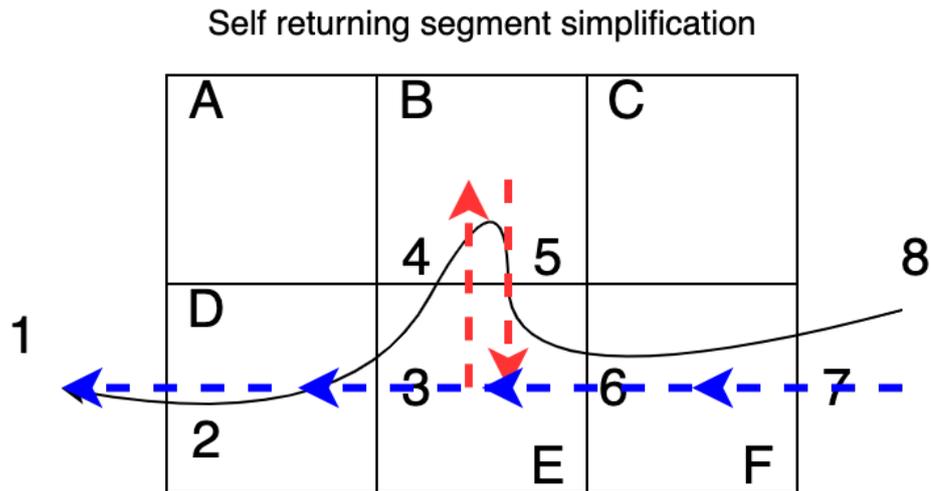


Figure S10. Illustration of the self-returning stream segment simplification in a 2-row by 3-column Cartesian mesh. Letters on the top left corner from A to F represent the mesh cells. Numbers from 1 to 8 represent the start, end, and intersected vertices. Black line is the actual flowline. Because it enters and exits the edge between grid B and E twice, the grid topological relationships $F \rightarrow E \rightarrow B \rightarrow E \rightarrow D$ (red dashed arrows in the loop) demonstrate cycling. The algorithm detects and removes cycling and the final topological relationships are $F \rightarrow E \rightarrow D$ (blue dashed arrows).

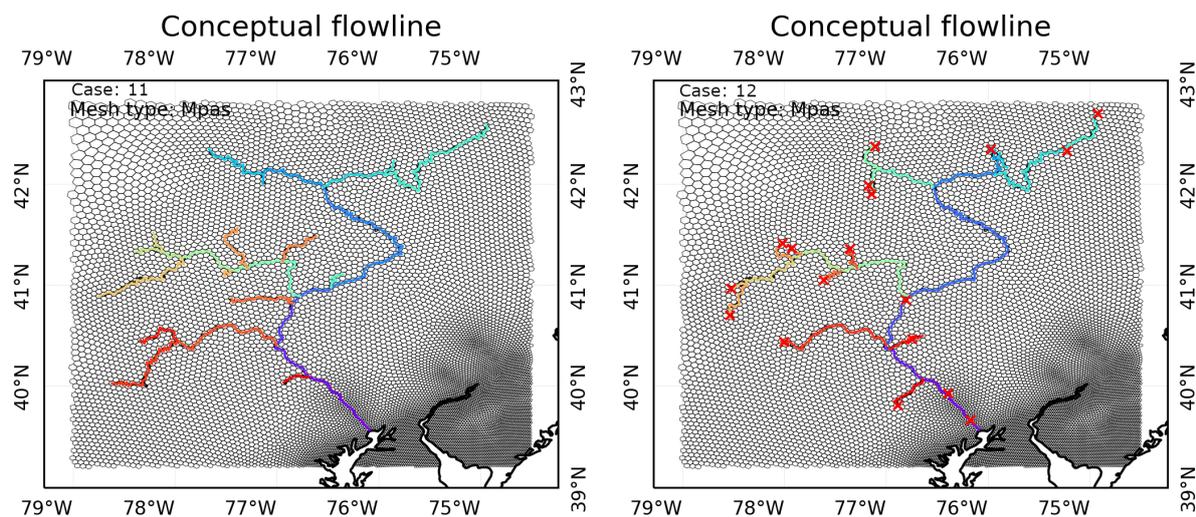


Figure S11. Modeled flowline-guided MPAS mesh (clipped to the study domain) and conceptual flowlines in the SRB from Cases 11 and 12 (Table 1). Black line features are the simplified flowlines. Colored line features are the modeled conceptual flowlines. (a) is modeled conceptual flowlines with a stream order 6 threshold. (b) is modeled conceptual flowlines with a stream order 7 with dam burnt in. Red crosses are dam locations. All the flowlines downstream of each dam are included.

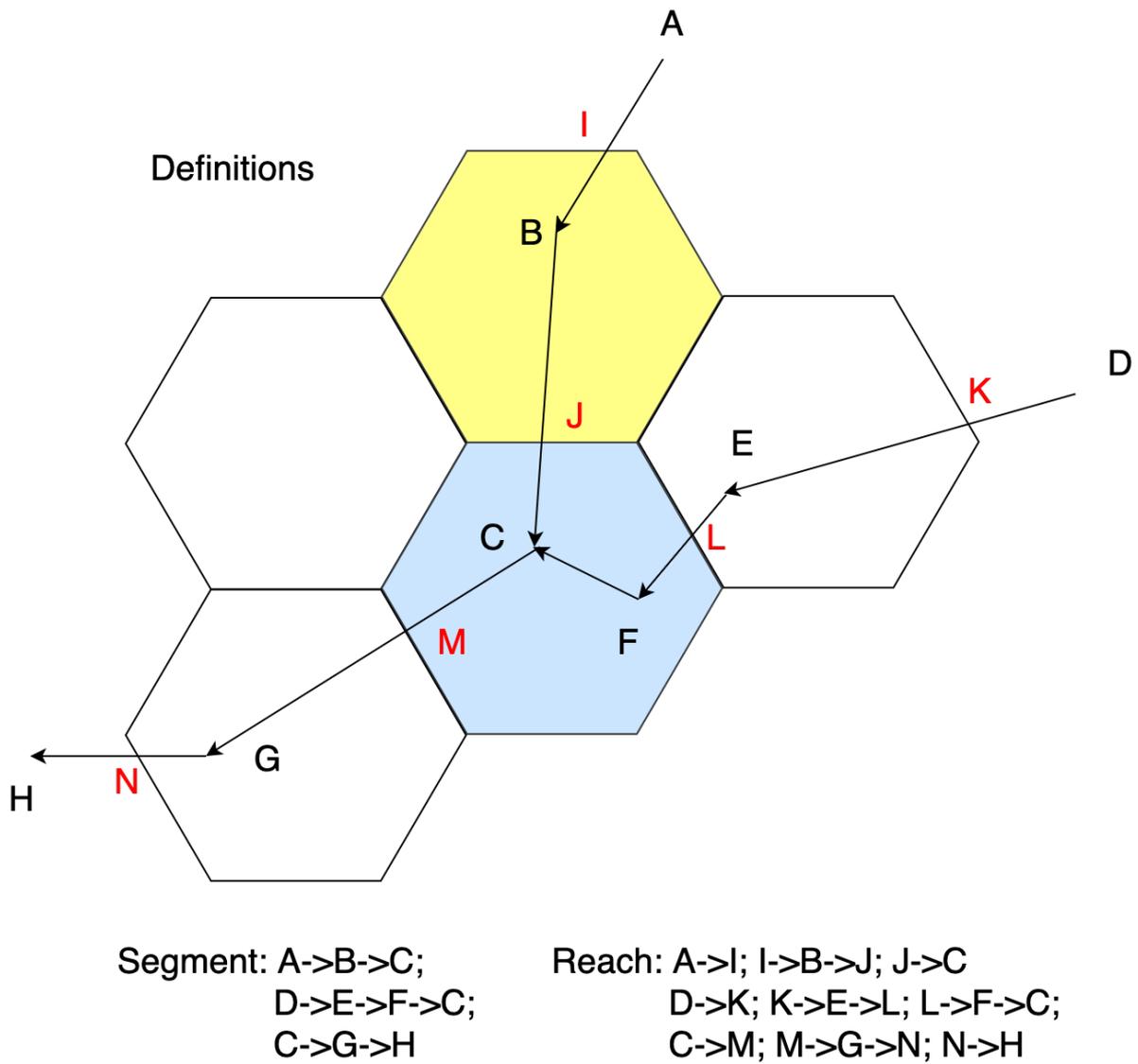


Figure S12. Definitions of stream segment and reach with an intersection in a hexagon mesh. Initially, there are 3 stream segments (A->B->C, D->E->F->C, and C->G->H). After the intersection, each segment is broken into several reaches. For example, segment A->B->C is broken into reach A->I, I->B->J, and J->C. The yellow cell has only one reach and the light blue cell has 3 reaches.

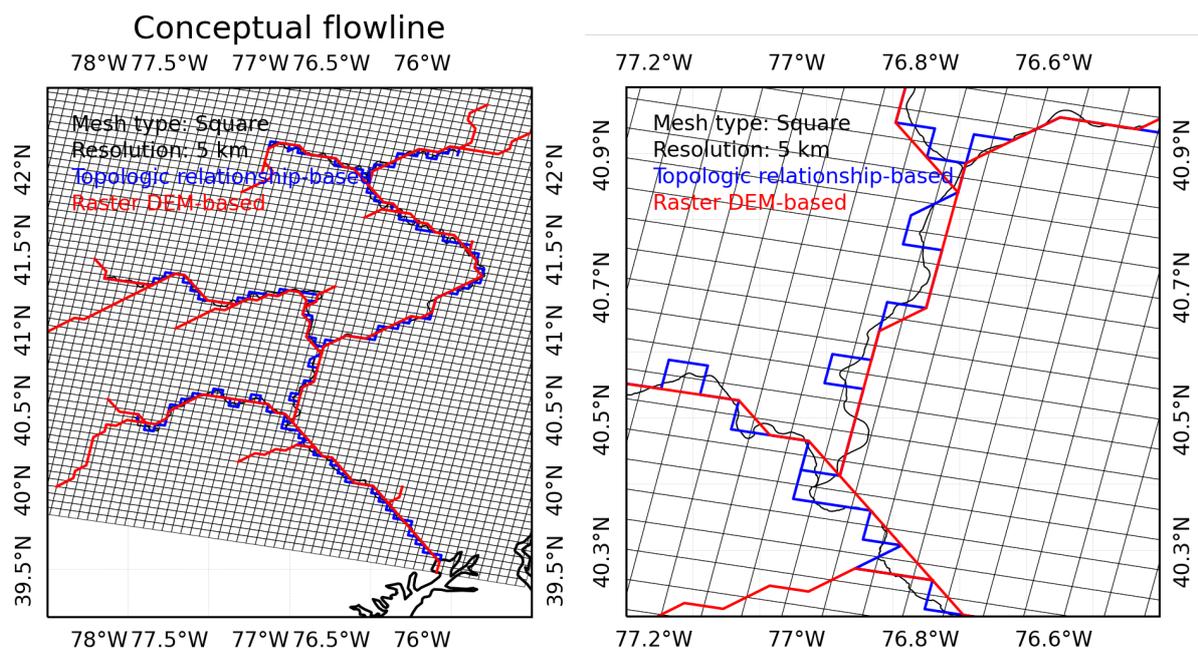


Figure S13. Comparisons of modeled flowlines from our model and the raster DEM-based method at a 5 km spatial resolution. The black, blue, and red lines are the simplified, square mesh topological relationship-based, and raster DEM-based flowlines, respectively. (b) is a zoomed-in view of (a) near the confluence.

Table S2. Major model configurations.

Parameter	Usage	Default
<i>iFlag_remove_smallriver</i>	Option to remove small river	1
<i>iFlag_shortcut</i>	Option to enable shortcut simplification	1
<i>dLongitude_outlet_degree</i>	Longitude of outlet in degree	0.0
<i>dLatitude_outlet_degree</i>	Latitude of outlet in degree	0.0
<i>dResolution_meter</i>	Mesh resolution	10000 m
<i>dThreshold_smallriver</i>	The threshold to remove small river	Same as resolution
<i>dThreshold_shortcut</i>	The threshold to ignore cell index	5000 m
<i>sMesh_type</i>	Mesh type	hexagon

References

- Engwirda, D. (2017). JIGSAW-GEO (1.0): locally orthogonal staggered unstructured grid generation for general circulation modelling on the sphere. *Geoscientific Model Development*, *10*(6), 2117–2140.
- Liao, C., Tesfa, T., Duan, Z., & Leung, L. R. (2020). Watershed delineation on a hexagonal mesh grid. *Environmental Modelling & Software*, *128*, 104702. Retrieved from <http://www.sciencedirect.com/science/article/pii/S1364815219308278> doi: 10.1016/j.envsoft.2020.104702
- Liao, C., Zhou, T., Xu, D., Barnes, R., Bisht, G., Li, H.-Y., ... Engwirda, D. (2022). Advances in hexagon mesh-based flow direction modeling. *Advances in Water Resources*, 104099. doi: 10.1016/j.advwatres.2021.104099
- Ringler, T., Petersen, M., Higdon, R. L., Jacobsen, D., Jones, P. W., & Maltrud, M. (2013). A multi-resolution approach to global ocean modeling. *Ocean Modelling*, *69*, 211–232. doi: 10.1016/j.ocemod.2013.04.010
- USGS. (2013). *National Hydrography Geodatabase: The National Map viewer available on the World Wide Web, accessed [June 02, 2015], at url [http://viewer.nationalmap.gov/viewer/nhd.html?p=nhd]. Retrieved from http://viewer.nationalmap.gov/viewer/nhd.html?p=nhd*
- Winchell, M., Srinivasan, R., Di Luzio, M., & Arnold, J. (2007). ArcSWAT interface for SWAT 2005. *User's Guide, Blackland Research Center, Texas Agricultural Experiment Station, Temple.*
- Wu, H., Kimball, J. S., Li, H., Huang, M., Leung, L. R., & Adler, R. F. (2012). A new global river network database for macroscale hydrologic modeling. *Water resources research*, *48*(9).

doi: 10.1029/2012WR012313