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A review of integrated surface-subsurface numerical hydrological models

Lele SHU[1], Hao CHEN[1], Xianhong MENG[1*], Yan CHANG[1], Litang HU[2], Wenke WANG[3], Longcang SHU[4], Xuan YU[5], Christopher DUFFY[6], Yingying YAO[7] & Donghai ZHENG[8]

[1] *Key Laboratory of Cryospheric Science and Frozen Soil Engineering, Northwest Institute of Eco-Environment and Resources, Chinese Academy of Sciences, Lanzhou 730000, China;*
[2] *College of Water Sciences, Beijing Normal University, Beijing 100038, China;*
[3] *School of Water and Environment, Chang'an University, Xi'an 710064, China;*
[4] *College of Hydrology and Water Resources, Hohai University, Nanjing 210098, China;*
[5] *State Key Laboratory of Soil and Sustainable Agriculture, Institute of Soil Science, Chinese Academy of Sciences, Nanjing 210008, China;*
[6] *Department of Civil and Environmental Engineering, Pennsylvania State University, State College, PA 16801, USA;*
[7] *Department of Earth and Environmental Science, School of Human Settlements and Civil Engineering, Xi'an Jiaotong University, Xi'an 710049, China;*
[8] *Institute of Tibetan Plateau Research, Chinese Academy of Sciences, Beijing 100101, China*

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Abstract Hydrological modeling, leveraging mathematical formulations to represent the hydrological cycle, is a pivotal tool in representing the spatiotemporal dynamics and distribution patterns inherent in hydrology. These models serve a dual purpose: they validate theoretical robustness and applicability via observational data and project future trends, thereby bridging the understanding and prediction of natural processes. In rapid advancements in computational methodologies and the continuous evolution of observational and experimental techniques, the development of numerical hydrological models based on physically-based surface-subsurface process coupling have accelerated. Anchored in micro-scale conservation principles and physical equations, these models employ numerical techniques to integrate surface and subsurface hydrodynamics, thus replicating the macro-scale hydrological responses of watersheds. Numerical hydrological models have emerged as a leading and predominant trend in hydrological modeling due to their explicit representation of physical processes, heightened by their spatiotemporal resolution and reliance on interdisciplinary integration. This article focuses on the theoretical foundation of surface-subsurface numerical hydrological models. It includes a comparative and analytical discussion of leading numerical hydrological models, encompassing model architecture, numerical solution strategies, spatial representation, and coupling algorithms. Additionally, this paper contrasts these models with traditional hydrological models, thereby delineating the relative merits, drawbacks, and future directions of numerical hydrological modeling.

Keywords Numerical Hydrological Models, Surface-Subsurface Process Coupling, Numerical Methods, Hydrological Modeling

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* Corresponding author (email: mxh@lzb.ac.cn)

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1. Introduction

Scientific modeling is a mathematical method of calculating unknown variables through known variables based on understanding the laws of nature. Hydrological models represent state-of-art understanding of the hydrological processes and express the spatial and temporal laws of hydrological processes through mathematical formulas. Model combined with observational data can be used to validate the reliability and appropriateness of the theory as well as to predict future changes, thus understanding and predicting natural processes (Wagener et al., 2010; Ren et al., 2011; Vallis, 2016; Fatichi et al., 2016; Duffy, 2017; Peel and McMahon, 2020). Presently, as efficient and economical scientific experimental tools, hydrological models are indispensable in supporting decisions in agricultural production, water resource management, disaster prevention and mitigation, pollutant control, and socio-economic development (Ren et al., 1996; Xu, 2010; Zheng et al., 2010; Fatichi et al., 2016; Tang et al., 2019; Yu et al., 2020). It has also been used to validate water cycle theories and guide the layout of scientific observation networks, etc. (Beven, 2012; Li et al., 2018; Blöschl et al., 2019).

Hydrological models describe the fundamental processes of the hydrological cycle, typically encompassing precipitation, interception, infiltration, flow through porous media, evapotranspiration, and runoff. In cold regions, the phase change induced by glaciers, permafrost, and snow cover adds complexity, profoundly affecting the typical hillslope hydrological processes (Wang et al., 2014; Yang et al., 2018). Beyond natural hydrological processes, models must also account for the anthropological impact on the hydrological cycle. Figure 1 illustrates the entire process of watershed hydrology and its various elements, such as precipitation, evaporation, snow melting, runoff generation, routing, river runoff, infiltration, interflow, groundwater recharge, and baseflow. It also includes glacial, snow, permafrost, vegetation cover, land cover, lake, and other surface hydrological processes. At the micro-scale, hydrological processes exhibit high complexity and heterogeneity. At the macro-scale, due to the averaging of micro-scale features, the complexity of hydrological processes is actually reduced, and the description of streamflow in large-scale hydrological models becomes more conceptualized, with relatively less computational process and complexity (Wood et al., 1988; Grayson et al., 1992; Blöschl et al., 1995; Savenije, 2001; Sivapalan, 2003; Peel and McMahon, 2020).

Existing hydrological models have yet to fully meet the complex and various needs of water-related research and engineering applications. Peel and McMahon (2020) summarized and compared 279 rainfall-runoff models, citing a comment by Clark et al. (2011): "*The current overabundance of models is symptomatic of an insufficient scientific understanding of environmental dynamics at the catchment scale, which can be attributed to difficulties in measuring and representing the heterogeneity encountered in natural systems.*" Consequently, new hydrological models are continually emerging.

The development of hydrological models grapples with the contradiction between reducing model complexity and finely representing hydrological physical processes; therefore, that has led to two divergent model development approaches: top-down and bottom-up. These approaches focus on the physical parameterization of hydrological processes, data limitations, uncertainty, and computational resource constraints (Franchini and Pacciani, 1991; Ren et al., 1996; Sivapalan, 2003, 2018; Sivapalan et al., 2003; Wagener et al., 2004; Savenije, 2010; Semenova and Beven, 2015; Vallis, 2016; Clark et al., 2017; Novotny, 2018).

The top-down modeling approach takes the long-term and large-scale hydrological response of the watershed as a starting point and progressively refine and complicate the simulation of specific physical processes at small representative areas. Watershed/sub-watershed are conceptualized as imaginary storage spaces—the "bucket model", where driving factors on the computational units or watershed responses are expressed through simple empirical, linear/non-linear, or multivariate collinear fitting relationships. Hydrological models based on the bucket concept focus on how surface and subsurface processes form hydrographs at river outlets. They simplify the flow processes on slopes and river channels, and the bidirectional exchange between surface and groundwater; hence, their descriptions of runoff and baseflow processes are distinctly conceptualized. However, in natural watersheds, surface water and groundwater interactions are frequent, and the direction and intensity of fluxes at the interaction interface vary with the dynamic hydraulic gradient (Winter, 1999; Levine and Salvucci, 1999; Maxwell and Miller, 2005; Wang et al., 2007; Sulis et al., 2012; Krause et al., 2014; Maxwell and Condon, 2016; Mukherjee et al., 2018).

The bottom-up modeling approach starts from the micro-scale Hydrological Computation Unit (HCU) and fundamental physical equations, aggregating the hydrological processes of all HCUs to represent the long-term, macro-scale hydrological response of the entire watershed. This modeling type is also called a process-based or physics-based model. The HCUs are small areas in the watershed required to express spatial heterogeneity. Fundamental governing equations are constructed based on conservation principles (mass, energy, momentum). Micro-scale physical equations describe hydrological processes, calculating water and energy storage, movement, and phase-change in three-dimensional space at high spatiotemporal resolution. These models reflect watershed-scale hydrological responses by aggregating micro-scale physical processes. It is important to emphasize that the foundational principles of these hydrological models, such as mass/energy conservation principles and hydraulic laws (e.g., Darcy's Law), are universal. They exist independently of any single model, can be validated in laboratory and field experiments, and their parameters have definite physical meanings (Beven, 1989; Fatichi et al., 2016; Li et al., 2018; Ntona et al., 2022).

Figure 2, adapted from Hrachowitz and Clark (2017), showcases different watershed hydrological models' spatial and process characteristics. In the two-dimensional continuum of "spatial resolution–process complexity", the horizontal axis reflects the spatial resolution of hydrological models, i.e., the degree of detail in representing the spatial heterogeneity of watersheds. The vertical axis indicates the complexity of the physical processes. Traditional hydrological models, exemplified by SWAT and VIC, tend to be

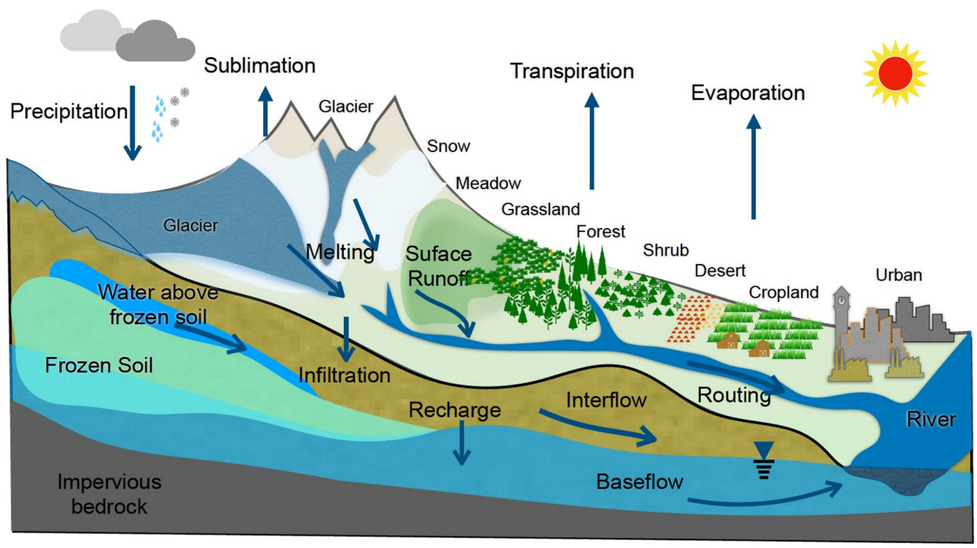

Figure 1 Schematic diagram of the hydrological cycle in the watershed.

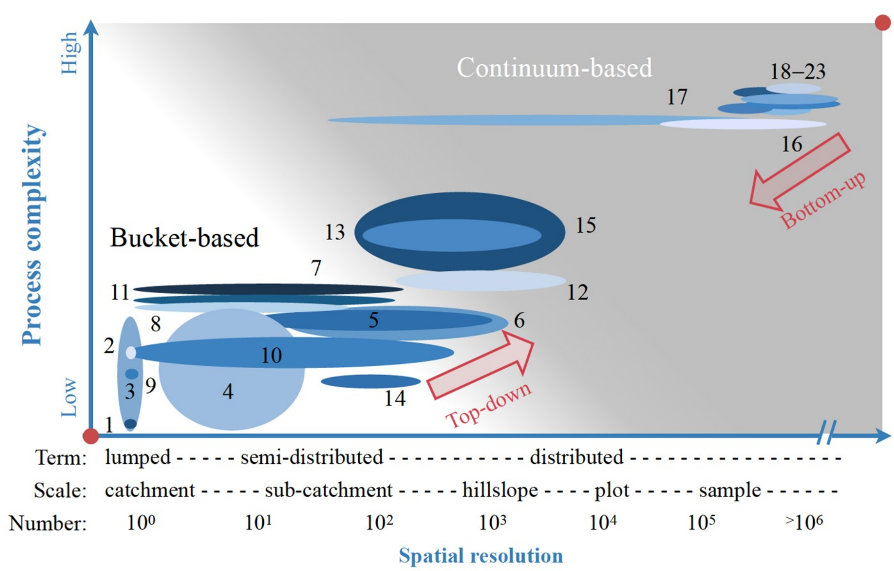

Figure 2 Schematic representation of hydrological models in the space of spatial resolution versus process complexity (adapted from Hrachowitz and Clark, 2017). The spatial resolution axis depicts the number and scale of HCUs in each model, while the process complexity axis represents the number of processes within a single HCU. The shading indicates the transition from bucket models (white) to spatiotemporally continuum-based models (gray), with red dots marking the two extremes of resolution and process complexity. The models in the figures are: 1, unit hydrograph (Sherman, 1932); 2, HBV (Bergström, 1992); 3, SUPERFLEX (Fenicia et al., 2011); 4, FLEX-Topo (Gharari et al., 2014); 5, mhM (Samaniego et al., 2010); 6, mhM-topo (Nijzink et al., 2016); 7, SWAT (Arnold et al., 1998); 8, NWS-Sacramento (Burnash and Singh, 1995); 9, GR4J (Perrin et al., 2003); 10, HYPE (Lindström et al., 2010); 11, VIC (Liang et al., 1994); 12, TOPMODEL (Beven and Kirkby, 1979); 13, CRHM (Pomeroy et al., 2007); 14, TACD (Uhlenbrook et al., 2004); 15, WASIM-ETH (Schulla and Jasper, 1998);16, DHSVM (Wigmosta et al., 1994); 17, MIKE-SHE (Refsgaard and Storm, 1996); 18, ParFlow (Kollet and Maxwell, 2008); 19, CATFLOW (Zehe et al., 2001); 20, HYDRUS-3D (Šimůnek et al., 2008); 21, CATHY (Camporese et al., 2010); 22, HydroGeoSphere (Jones et al., 2006); 23, PIHM/SHUD (Qu and Duffy, 2007; Shu et al., 2020).

positioned in the lower-left corner. These models, characterized by their lower spatial resolution and simplified hydrological processes, utilize sub-watersheds or hydrological response units as HCUs. Therefore, they are classified as the top-down category. In contrast, integrated surface-subsurface numerical hydrological models, represented by MIKE-SHE, ParFlow, and PIHM/SHUD, occupy the upper-right corner. These bottom-up models imply a higher spatial resolution and physical continuity, offering a more refined depiction and expression of physical processes.

Integrated Surface-Subsurface Numerical Hydrological Models (referred to simply as Numerical Hydrological Models) are based on a bottom-up modeling approach and form a unique category within distributed hydrological models (Figure 3). They mathematically couple surface and subsurface hydrological processes using numerical methods. They differ from numerical solution-based groundwater models like MODFLOW (McDonald and Harbaugh, 1984; Niswonger et al., 2011) and traditional hydrological models conceptualizing surface-subsurface processes. Groundwater models, often employing numerical methods, focus on spaces tens to hundreds of meters below the surface, encompassing processes like flow in low-permeability layers and fractures, extending beyond the "rainfall-runoff" scope of hydrological models. Groundwater models treat surface water processes as boundary conditions instead of directly coupled processes. In conceptual hydrological models, the groundwater module lacks a realistic depiction of depth, instead using conceptual bucket models to reflect groundwater recharge-storage-release processes with their release curves (Savenije, 2001), as seen in models like the Xin'anjiang model (Zhao and Wang, 1988), VIC (Liang et al., 1994), and the WRF-Hydro model (Gochis et al., 2018). Numerical hydrological models offer universal descriptions of physical processes, more accurately reflect human activities′ impacts, and provide a scientific basis for coupling with other physical processes (hydrothermal coupling, pollutant transport, vegetation dynamics), which has become an emerging and important direction in hydrological modeling in recent decades (Hu et al., 2007; Wang et al., 2008; Maxwell et al., 2014; Paniconi and Putti, 2015; Hrachowitz and Clark, 2017; Peel and McMahon, 2020; Shu L C et al., 2022;

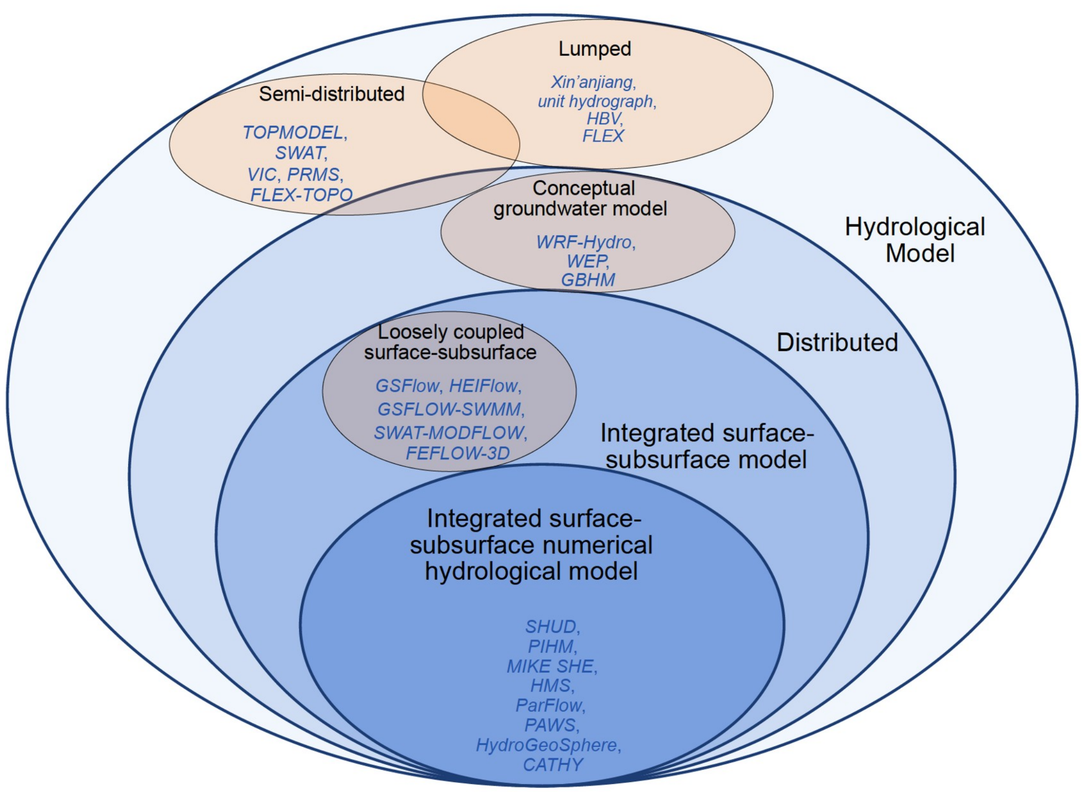

Figure 3 Schematic diagram of hydrological model classification (blue italicized text in the diagram represents representative models of each category. The models included are Xin'anjiang (Zhao and Wang, 1988), unit hydrograph (Sherman, 1932), HBV (Bergström, 1992), FLEX (Gharari et al., 2014), TOPMODEL (Beven and Kirkby, 1979), SWAT (Arnold et al., 1998), VIC (Liang et al., 1994), PRMS (Leavesley et al., 1983), WRF-Hydro (Gochis et al., 2018), WEP (Jia et al., 2001), GBHM (Yang et al., 1998), GSFlow (Markstrom et al., 2008), HEIFlow (Tian et al., 2018; Zheng et al., 2020; Han et al., 2021), GSFLOW-SWMM (Tian et al., 2015), SWAT-MODFLOW (Park et al., 2019), FEFLOW-3D (Hu et al., 2020), SHUD (Shu et al., 2020), PIHM (Qu and Duffy, 2007), MIKE-SHE (Refsgaard and Storm, 1996), HMS (Yu et al., 1999, 2006; Yu, 2000), ParFlow (Kollet and Maxwell, 2006), PAWS (Shen and Phanikumar, 2010), HydroGeoSphere (Aquanty, 2013), CATHY (Bixio et al., 2002; Camporese et al., 2010)).

Ntona et al., 2022). Mainly since 2000, global hydrologists have developed over 20 significant new numerical hydrological models, considerably propelling the field's advancement.

2. Brief discussion of numerical hydrological models

Numerical hydrological modeling originated in the 1970s. Freeze and Harlan (1969) proposed a modeling method based on hydrodynamic partial differential physical equations and a unified model blueprint for surface and subsurface hydrological processes (Freeze and Harlan, 1969; Cooley, 1971). However, due to the limitations of computational capacity at that time, it wasn't until the 1980s, with the emergence of the SHE model (Abbott et al., 1986), that numerical hydrological models began to gain prominence. Beven (2012, Figure 1.2) summarized the five fundamental steps of hydrological modeling: conceptual modeling, mathematical modeling, process modeling, model calibration, and model validation.

2.1 Governing equation

Numerical hydrological models use the mass conservation formula as their governing equation, explicitly describing the relationship between surface and groundwater storage and fluxes (eqs. (1) and (3)). Typically, the Saint-Venant equation (eq. (1)) and the Richards equation (eq. (4)) are used to calculate surface and subsurface flow processes (Freeze and Harlan, 1969; Maxwell and Miller, 2005; Farthing and Ogden, 2017; Singh, 2018; Haque et al., 2021). While the governing equations of these models are basically the same, their simplification and solution methods vary, applying different one-, two-, and three-dimensional simplifications for surface and subsurface processes.

$$\frac{\partial h}{\partial t} = \nabla \cdot (vh) - \frac{Q_e}{A} + \frac{Q_{su}}{A}, \tag{1}$$

$$v = n^{-1} R^{\frac{2}{3}} S_f^{\frac{1}{2}}, \tag{2}$$

$$S_w(h)\frac{\partial h}{\partial t} = \nabla \cdot q + \frac{Q_e}{V} + \frac{Q_{ss}}{V}, \tag{3}$$

$$q = -k_e(h)\,\nabla (h + z), \tag{4}$$

Eqs. (1) and (3) are the mass conservation governing equations for surface water and groundwater, respectively, while Eqs. (2) and (4) are the calculation formulas for their flow. In the formula, h is the groundwater hydraulic head, the water content of an unsaturated layer, or the height of surface water (L); t is the time (T); v is the horizontal mean flow rate of surface water ($L\ T^{-1}$); Q_e is the surface-subsurface interaction flow ($L^3\ T^{-1}$), with positive surface-to-subsurface flow; Q_{su} is the source-sink term or boundary condition for surface water ($L^3\ T^{-1}$), which may include precipitation, irrigation, and water supply; A is the vertical projected area of the control unit (L^2); n is the Manning's coefficient $\left(TL^{-\frac{1}{3}}\right)$; R is the hydraulic radius; S_f is the friction slope ($L\ L^{-1}$); $S_w(h)$ is the water storage coefficient ($L^3\ L^{-3}\ L^{-1}$), which is the water volume released per unit volume after unit head falls, and includes the storage coefficient of groundwater (L^{-1}) and the water content of the unsaturated soil layer ($L\ L^{-1}$); q is the groundwater flux ($L^3\ L^{-2}\ T^{-1}$), which is a function of head height or water content and is calculated using Darcy's law or Richards' equation (eq. (4)); Q_{ss} is the source/sink term for groundwater or soil water ($L^3\ T^{-1}$), including percolation, injection, extraction, and evapotranspiration rates per unit area in practical computation; V is the volume of the control unit (L^3); $K_e(h)$ is the effective hydraulic conductivity ($L\ T^{-1}$), a function of soil moisture content or matric potential; and z represents the vertical distance from a datum (L). The calculations of q and v are based on Manning's equation (eq. (2)) and the Richards equation (eq. (4)), respectively. The coupled computation of surface and subsurface processes at the watershed scale hinges on the continuity of the hydraulic head and the exchange of water volumes Q_e between them. Eq. (3) articulates the groundwater balance, positing the change in the control volume resulting from a unit change in water head on the left-hand side (LHS), while the right-hand side (RHS) encompasses the divergence of percolation flux, surface-subsurface interactions computed by Darcy's Law and the Richards equation, and source-sink terms.

Watershed hydrological models also require other surface processes, such as snowmelt and evapotranspiration, which are included as source-sink terms in the model. Glaciers, snowpack, and evapotranspiration are usually loosely coupled to surface and subsurface hydrological processes as modules, i.e., computed at different time steps or without iterative computation. Processes such as land cover, agricultural activities, etc., are modeled to affect hydrological and land surface processes through changes in plant phenology and hydraulic parameters.

2.2 Boundary condition

Boundary conditions (BCs) in hydrological modeling are typically categorized into Dirichlet and Neumann. The Dirichlet boundary condition (DBC) represents the first type of boundary condition for partial differential equations, also known as a prescribed boundary condition, which prescribes a constant value for the target variable at a specific location. For instance, in groundwater flow problems, the Dirichlet condition sets a fixed groundwater head. The Neumann boundary condition (NBC), also referred to as the second type of boundary condition for partial differential equations, specifies the first-order derivative of the target variable at a specific location. This might involve assigning a prescribed flux, such as the water injection or extraction rate. In three-dimensional numerical hydrological models, boundary conditions can be applied in any direction at any location. Numerical hydrological models incorporate common boundary conditions or assumptions, which include:

(1) Watershed's impervious bottom boundary. It is characterized as an NBC, assuming a zero flux, which is an assumption widely applicable in hydrological studies of many watersheds. When it is crucial to reflect the influence of deep groundwater on the simulation system, non-zero bottom boundary conditions can be adaptable to enable interaction with this deeper groundwater.

(2) Closed watershed boundaries. There is neither influx nor outflow of water from external sources or to the exterior in the horizontal direction at the hillslope units. Namely, the flow across the boundary for the HUCs is zero. This assumption is valid when the simulated boundary aligns with the actual watershed boundary and when the surface and groundwater boundaries coincide. If the simulation domain encompasses only a portion of the watershed (e.g., for riparian zone studies), specific DBCs or NBCs must be set to maintain the water balance. However, boundary conditions are often challenging to ascertain via observation in practical applications. Thus, an alternative approach is to expand the simulation domain to the zero-flux watershed boundaries. By employing fine grids in focal research areas and coarser grids from surrounding areas to the watershed boundary, the model ensures reasonable boundary conditions without the constraints of lacking boundary data.

(3) Top boundary. The upper boundary of a watershed is subject to precipitation and irrigation, which are applied as NBCs. Evapotranspiration is typically treated as an NBC affecting both the surface and subsurface. However, unlike precipitation or irrigation, evapotranspiration is not an external input but is computed based on meteorological data and soil temperature and moisture content.

(4) River outlet boundaries. The river outlet is the only horizontally oriented outlet of water from the watershed, so hydrologic models are consistent with the law of conservation of mass or the water balance equation: $\Delta S=P-\mathrm{ET}-Q$, the ΔS is the water storage in the watershed, and P is the amount of precipitation, and ET is evapotranspiration, and Q is the amount of runoff.

2.3 Numerical solution

It is evident from the governing equations (eqs. (1) and (3)) that the target variable h is a function of both time and space, necessitating the discretization of the subject matter in both temporal and spatial dimensions. Discretization of the watershed in three-dimensional space, both horizontally and vertically, is a critical step in numerical hydrological modeling. An efficient spatial discretization scheme must not only satisfy the simulation accuracy required for the study area and comply with boundary condition constraints but also optimize the number of discretization units to lessen the dependency on computational resources. Horizontal spatial discretization approaches are typically categorized into structured and unstructured schemes, which will be discussed in detail in the model comparison section. Vertically, the focus is primarily on partitioning soil layers from the surface down to the impervious bottom boundary. The vertical discretization scheme is flexible, and layering of isotropic, isoparametric, or arbitrary division exists. It can also be divided into saturated or unsaturated layers.

Numerical methods can also be categorized into explicit and implicit methods: an explicit method directly calculates the variables at the next time step from those of the previous step, while an implicit method derives the variables at the next time step through a series of formulas, matrices, or iterative algorithms. Under the same spatiotemporal resolution, explicit methods offer significantly faster computational performance than implicit methods. However, implicit methods ensure the computational stability of numerical solvers, allowing for larger time steps. In contrast, explicit methods must adhere to the Courant-Friedrichs-Lewy (CFL) condition, a necessary (but not sufficient) criterion for the convergence and stability of numerical methods (Courant et al., 1928). The CFL condition stipulates that the time step in numerical methods must be sufficiently small to guarantee computational accuracy, as larger time steps may result in non-convergence or instability in the outcomes.

Temporal discretization refers to the time step in a model. The time step and spatial resolution combination significantly influence the stability and convergence of numerical solutions constrained by the CFL condition. A higher spatial resolution necessitates a correspondingly higher temporal resolution to ensure stability in numerical methods. A direct proportional relationship exists between temporal resolution and spatial resolution, often expressed as a power (first or higher order) of the spatial resolution.

3. Comparison of numerical hydrological models

The following section compares major numerical hydrological models based on various criteria, including numerical methods, spatial grid structures, coupling mechanisms, variable transfer, river channel topology, and the availability of source codes (Table 1).

3.1 Numerical methods

The primary numerical techniques include Finite Difference

Table 1 Comparison of major numerical hydrological models regarding model structure, solution algorithms, spatial characteristics, etc

Model	Numerical method	Grid	River topology	Coupling	Variable passing	Source code	Literature	Country
SHUD	FV	Unstructured	Cross	Global implicit	Pressure continuity	Yes	Shu et al. (2020, 2024a, 2024b)	China/USA
PIHM	FV	Unstructured	Touch	Global implicit	Pressure continuity	Yes	Qu and Duffy (2007)	USA
CATHY	FE	Unstructured	No channel	Sequential iteration	BC switching	No	Bixio et al. (2002); Camporese et al. (2010)	Italy
HydroGeoSphere	FE	Unstructured	No channel	Global implicit	First-order exchange	No	Aquanty(2013)	Canada
OpenGeoSys	FE	Unstructured	Touch	Sequential iteration	First-order exchange	Yes	Delfs et al. (2009, 2012)	Germany
ParFlow	FD	Structured	Cross	Global implicit	Pressure continuity	Yes	Kollet and Maxwell (2006)	USA
PAWS	FD	Structured	Cross	Asynchronous linking	First-order exchange	No	Shen and Phanikumar (2010)	USA
tRIBS	FE	Unstructured	Touch	Asynchronous linking	First-order exchange	No	Ivanov et al. (2004)	USA
inHM	FE	Unstructured	No channel	Sequential Iteration	First-order exchange	No	VanderKwaak and Loague (2001)	USA
MIKE SHE	Structured	Structured	Cross	Asynchronous linking	BC switching	No	Abbott et al. (1986)	Denmark
GEOtop	FV	Structured	No channel	Global implicit	Pressure continuity	Yes	Rigon et al. (2006); Endrizzi et al. (2014)	Swiss/Italy

(FD), Finite Element (FE), and Finite Volume (FV) methods. The FD method, known for its simplicity, clear physical interpretation, and ease of programming, is the most widely used in hydrology and meteorology (Paniconi and Putti, 2015). The FE method ensures global mass balance but may not maintain local balance. The FV method addresses this limitation of the FE method, ensuring both global and local water balance. While there is no clear superiority among these three methods, their mathematical implications slightly differ: the FD method calculates approximated values at specific points in space, the FE method approximates fitting curves within an HCU, and the FV method, a particular case of the FE method, computes the mean value within the HCUs. Therefore, the interpretation of results from these three methods should differ slightly, although model users in practical applications often treat them as equivalent meanings.

3.2 Spatial decomposition

Horizontal grids in the spatial representation of hydrological models are primarily categorized into structured and unstructured types. HCUs with uniform geometric shapes and areas characterize structured grids. These grids offer several advantages: (1) The solution is intuitive and logical; (2) They are conducive to programming, offering simplicity and efficient parallel computing; (3) Data input and output can be expressed in matrix structures, facilitating efficiency and intuitiveness in data preprocessing, postprocessing, and visualization. Although rectangular structures are most common in structured grids, equilateral triangles, and hexagons are also viable options.

In contrast, unstructured grids (or irregular grids) exhibit the following distinct advantages: (1) They provide a more effective representation of complex three-dimensional terrain; (2) They offer higher adaptability to irregularly shaped research areas, and ensure that boundary conditions align closely with the theory of numerical simulations (Beven, 2012); (3) They allow for the dynamic adjustment of HCU size, enabling finer or coarser resolution in specific areas while maintaining overall boundary conditions. Therefore, the use of unstructured grids not only ensures high-resolution simulation in focal areas but also maintains stability in boundary conditions without significantly increasing the HCU numbers. This achieves a balance between simulation accuracy and computational expense.

Figure 4 demonstrates the watershed's spatial discretization using regular rectangular grids and irregular triangular grids (Figure 4a–4d). Under a roughly equivalent average HCU area, the number of units in the rectangular grid is close to that of the unstructured grids. However, the rectangular grid carries the burden of inactive units (blank cells outside

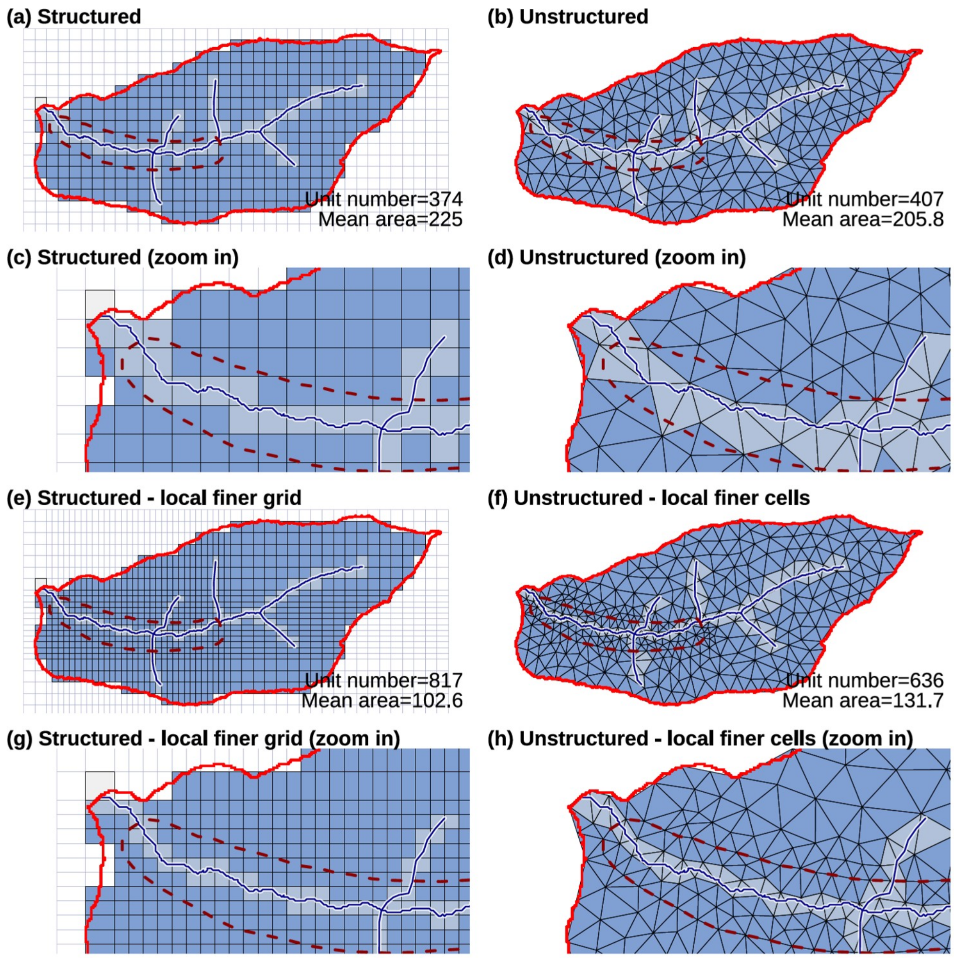

Figure 4 Differences in watershed, river (blue lines), watershed boundary (red solid line), and focal area (red dash line) as described by structured and unstructured grids (irregular triangles). Unstructured grids not only better represent the irregular boundaries of a watershed at the same resolution but also enable local densification of the watershed without a significant increase in the total number of hydrological computation units.

the watershed), and its boundary representation significantly deviates from the actual boundary (Figure 4c). When local refining of the watershed is required (area outlined in dark red dashed lines), the number of HCUs in the rectangular grid increases substantially, whereas the increase is much smaller in the unstructured grids (Figure 4e–4h). The main drawbacks of unstructured grids are: (1) The computation is relatively complex, compatible only with FE and FV methods; (2) Data interpretation and visualization are somewhat more complicated, necessitating specialized pre- and post-processing software.

3.3 Variable coupling

The coupling of surface and subsurface hydrological processes represents a significant technical difference among models and is one of the challenges in model development. Figure 5 illustrates three different coupling methods: The asynchronous linking method calculates the surface and subsurface hydrological processes separately with different time steps, then exchanges variables to form new boundary conditions in the following step. The sequential iteration method is similar to asynchronous linking, but after exchanging boundary conditions, it requires further iteration to find a convergent state for both surface and subsurface water. The global implicit method solves all variables within a unified set of nonlinear equations and time steps (Panday and Huyakorn, 2004; Furman, 2008; Maxwell et al., 2014). The computational difficulty and complexity increase with each method. Due to the significant difference in water movement rates between surface and subsurface processes and the iterative time step constrained by the CFL condition (often subjected by surface and river fluxes), the global implicit method is the least efficient under similar conditions. However, this method more accurately depicts the continuous movement of water in natural spaces and ensures global water balance.

Variable exchange refers to the transfer of key variables between different governing equations. A typical example of variable exchange is the infiltration rate, a crucial variable

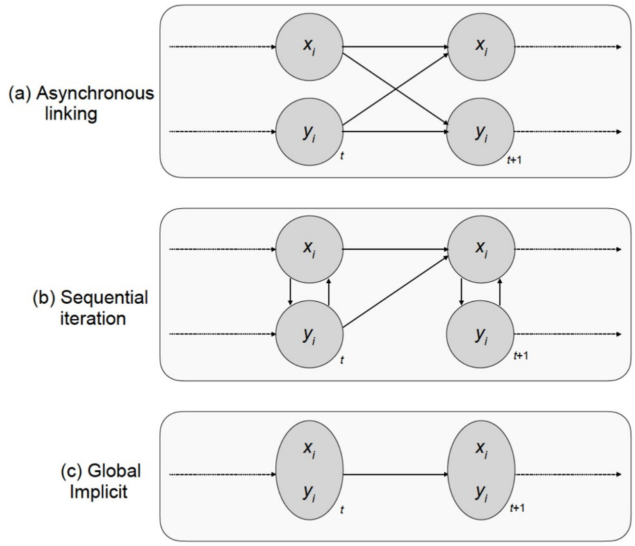

Figure 5 Conceptual structures of the three main methods for coupling and variable transfer among surface and subsurface processes. In the diagram, variables x and y represent the values of surface and subsurface variables at times t and t+1, respectively.

for the interaction between surface and subsurface water, which determines surface runoff and soil moisture content. In first-order variable exchange methods, the infiltration flux is computed in the surface process module and then passed on to the soil water calculation module. In the boundary condition exchange approach, the infiltration is treated as a boundary condition for the deeper soil layers. The method of variable exchange is closely related to the coupling strategy of surface and subsurface processes.

3.4 River channel coupling

River runoff is a crucial variable in watershed simulation. Numerical models employ various topological solutions to describe river channels, compute streamflow, and calculate the exchange relationships between river channels and hillslope units (Figure 6). Some models lack explicit river channel units, treating all HCUs as hillslope units. However, when water on the HCU surface exceeds a threshold, it is considered a river channel unit and calculated using the particular formula for river channels, as seen in models like inHM (VanderKwaak and Loague, 2001), CATHY (Bixio et al., 2002), and GEOtop (Rigon et al., 2006). Other models incorporate explicit river channel units, where the model solves for both hillslope and river channel units, each with distinct geometric shapes and calculation methods.

The spatial topological relationship between river channels and hillslope units can be crossed or touched in different models. For example, in the PIHM model, the hillslope units are triangular in plane view, while the river channels are rectangular (defined by the length and width of the channel), sharing one edge with adjacent hillslope triangles. Hence, in such a touch relationship, the river channel only exchanges water with the two units on either side. The advantages of touch are simplicity in spatial relationships and the ability to calculate water fluxes on either side of the river. However, its drawbacks include (1) numerically inefficient obtuse triangles along winding rivers; (2) a dependency between the detail of the river channel discretization and the size of the HCUs, requiring oversimplification of the river for computational efficiency; (3) potential formation of sink units at river start points, where excessive accumulation of water may lead to instability in a numerical solver. Cross relationship between river channels and hillslope units avoids these issues but requires predefined spatial topological relationships and circumspect vertical matching between river and hillslope topographies. The solution matrix formed from the cross relationship is no longer a regular diagonal or sparse matrix, which challenges the solver.

3.5 Open source code

Although the open source code is not a requirement of scientific models, its availability is significant for numerical hydrological models due to the models' high development complexity. Open-source code enables users to understand the internal formulas and solving processes. Additionally, open-source models facilitate user engagement in model enhancements and are advantageous for coupling studies with other related scientific models, thereby enhancing the reproducibility of scientific experiments (Yu et al., 2013, 2016). On the other hand, proprietary models often achieve commercial success, as seen with MIKE SHE and HydroGeoSphere. Currently, the development and application of numerical hydrological models in research and commercial spheres are predominantly led by developed countries in Europe and North America.

4. Characteristics of numerical hydrological models

The summary of the characteristics of numerical hydrological models is based on a comparison with other non-numerical hydrological models.

4.1 Advantages

Strong Physical Process Description: Numerical hydrological models use physical equations (such as the Darcy-Richards equation, Saint-Venant equation, Green-Ampt equation, etc.) to describe watershed hydrological processes. Their parameters are often based on measurable or derivable hydraulic properties like soil hydraulic conductivity, porosity, surface roughness, etc. These models utilize fundamental

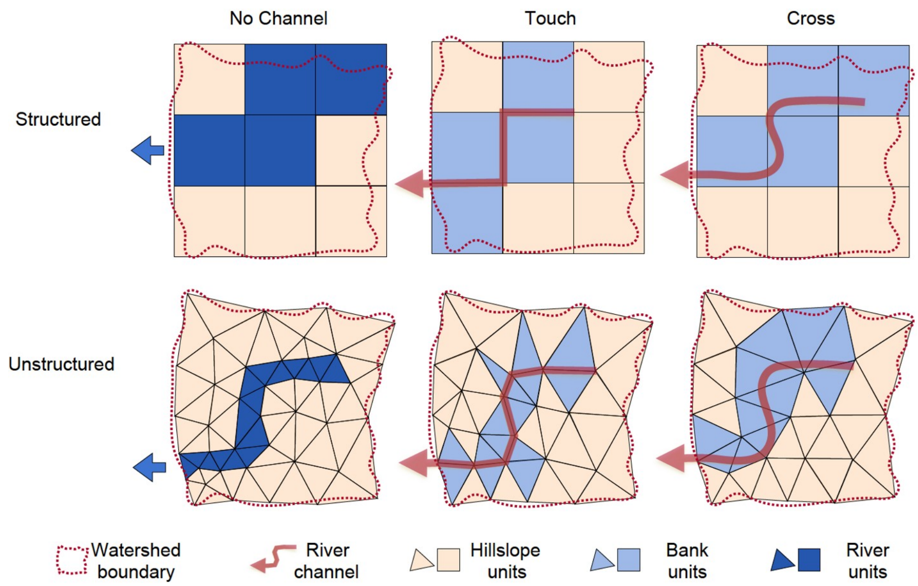

Figure 6 Various spatial topological relationships between river channels and hillslope units.

mass and energy conservation principles to solve for the overall watershed response, representing a bottom-up approach and a mathematical depiction of objective natural processes. Regarding physical process representation and spatial structure, physically-based numerical hydrological models surpass conceptual and lumped models. They are not only beneficial for breakthroughs in ungaged watersheds but also provide reliable physical insights for hydrological research under historical and climatic changing conditions (Abbott et al., 1986; Vertessy et al., 1993; Wagener et al., 2004; Held and Soden, 2006; Todini, 2007; Milly et al., 2008; Peel and McMahon, 2020). Lumped and semi-distributed models often use abstract parameters to represent hydrological, physical processes; for instance, the runoff process in SWAT is determined by the Curve Number (CN), which integrates multiple hydrological factors such as soil, land cover, agricultural management, and slope (Bartlett et al., 2016).

High Temporal Resolution: Due to the high resolution and constraints of the CFL condition, numerical hydrological models operate at a temporal resolution ranging from seconds to hours. This feature provides a significant advantage in describing rapid processes like flood, inundation, and hydrochemical processes. Some models feature adaptive time stepping—where the algorithm automatically adjusts the time step based on the rate of change and systematic convergence—thus significantly enhancing overall model efficiency while meeting the requirements for numerical convergence. In the comparative study of numerical hydrological models, many models operate with time steps ranging from 0.001 s to 30 min due to the smaller scale of simulation targets (Kollet et al., 2017).

High Spatial Resolution and Continuity: High spatial resolution means the model can better represent the natural heterogeneity of the watershed (McDonnell et al., 2007; Maxwell and Kollet, 2008; Mirus et al., 2011; Mascaro et al., 2015; Fatichi et al., 2016). Spatial continuity is manifested in the continuous process of hydrological variables within a discretized space of higher resolution, such as the tracking of water flow along the surface/subsurface paths from "ridge-midslope-slope bottom-river channel-river outlet" in numerical hydrological models. In contrast, SWAT computes runoff generation and routing based on Hydrological Response Units (HRUs) but cannot describe the process of water traveling from the furthest point of an HRU to a river, nor can it track the path of pollutant dispersion within an HRU.

Surface-Subsurface Process Coupling: Numerical hydrological models more accurately represent the interaction between surface and sub-surface processes, enhancing the model's applicability across various watersheds. For example, most conceptual models fix the direction of groundwater flow towards rivers from the hillslope to the river channel; they fail to uniformly represent processes such as river seepage replenishing groundwater in arid areas during dry seasons and groundwater feeding rivers in wet seasons. In the tightly coupled surface-subsurface approach of numerical hydrological models, the direction of interaction between groundwater and rivers is determined by real-time hydraulic gradients, allowing for bidirectional water flow. Traditional models divide the watershed into sub-watersheds, directly drain sub-watershed groundwater to local runoff, and then route to the outlet. This approach may not adequately reflect scenarios in mountainous areas where high-altitude groundwater contributes to downstream flow through deep groundwater pathways. In contrast, numerical models that couple surface and subsurface hydrological processes are well-suited for such complexities.

Hydraulic Representation of Climate Change and Human Activities: Physical models inherently can represent environmental dynamics, as they are based on the laws of conservation of mass and energy rather than relationships fitted to observations specific to a time and space (Fatichi et al., 2016). The primary impacts of human activities on the hydrological cycle of watersheds include (1) changes in land cover (e.g., deforestation); (2) hydraulic engineering (e.g., dams, levees); (3) water extraction and irrigation (Peters and Meybeck, 2000; Ntona et al., 2022). Numerical hydrological models reflect land cover through four aspects: evaporation, surface resistance for runoff, phenological patterns of vegetation, and changes in soil characteristics, effectively representing the hydraulic characteristics of land cover (Ewen and Parkin, 1996; Shu et al., 2020, 2024a). In contrast, in the SWAT model, the experiential CN represents land cover characteristics, which lack sufficient physical basis and are impossible to measure. The CN value encompasses soil permeability, roughness and impervious area, and struggles to represent phenological characteristics, leading to significant uncertainties in the model structure (Singh, 2018).

More Computable Spatial Variables: Numerical hydrological models discretize space in horizontal and vertical dimensions, resulting in numerous HCUs and three-dimensional computational outcomes. The data volume generated by these models is significantly larger than that of lumped and semi-distributed models. The high-resolution outputs of these models are advantageous for comparison with observations and provide valuable guidance for future observational system.

Tight Coupling with Disciplinary Models: Numerical hydrological models lay a solid theoretical foundation for coupling with other disciplinary models, thanks to their clear physical mechanisms, rich computable variables, adherence to mass and energy conservation constraints, and capability to track material transport in space (Ewen et al., 2000; Fatichi et al., 2016). The spatial continuity mentioned earlier is conducive to multidisciplinary coupling studies. For instance, the models′ detailed descriptions of water pathways from hillslopes facilitate integration with land surface processes (Shi et al., 2015; Kuffour et al., 2020), geochemistry (Shi et al., 2018), reaction transport (Bao et al., 2017; Li et al., 2017), agricultural economics (Cobourn et al., 2018), lake dynamics (Ladwig et al., 2021, Shu et al., 2024b), soil erosion and geomorphic changes (Zhang et al., 2016), coastal groundwater interactions (Yu et al., 2021), and coupling with cryospheric processes (Endrizzi et al., 2014). Examples of typical model couplings include CLM-PAWS (Shen et al., 2013), CLM-ParFlow (Kuffour et al., 2020), ATS (Painter et al., 2016), Flux-PIHM (Shi et al., 2013), LE-PIHM (Zhang et al., 2016), and tRIBS-VEGGIE (Ivanov et al., 2008).

4.2 Disadvantage

High Parameter Requirements: Numerical hydrological models face challenges due to the high number of parameters required, the need for reliable and physically-based parameters, and the difficulty in calibration (Maxwell and Miller, 2005; Ampadu et al., 2013). Lumped models need only 3–6 parameters to accurately simulate the "rainfall-runoff" process (Ye et al., 1997; Perrin et al., 2001; Wagener et al., 2004; Beven, 2010, 2012; Peel and McMahon, 2020), but numerical hydrological models, due to the number of governing equations and the complexity of watershed hydrological processes, require a larger number of parameters. Taking hydraulic conductivity (K) as an example, models like SWAT need only one representative K value for an HCU, but the SHUD model (Shu et al., 2020, 2024a) requires at least three K values for the surface vertical infiltration, subsurface vertical and horizontal directions; more Ks in three dimensions are needed for multi-layer groundwater processes. SWAT uses the CN value to express soil hydraulic characteristics, land cover, and agricultural management, but numerical hydrological models typically require more than 10 parameters to represent these features. The parameters in numerical hydrological models usually have specific physical meanings and are highly sensitive; thus, parameter reliability directly impacts simulation outcomes. The range of physical parameters is limited to specific reasonable intervals, and due to a large number of parameters, calibration is challenging (Vertessy et al., 1993; Anderman and Hill, 1999; Sivapalan, 2003; McDonnell et al., 2007; Keating et al., 2010; Fatichi et al., 2016). Additionally, the increase in the number of parameters leads to equifinality issues and parameter uncertainty (Savenije, 2001; Beven and Freer, 2001; Ebel and Loague, 2006; Li, 2013).

Computational Efficiency: The advantage of high spatiotemporal resolution in numerical hydrological models comes at the cost of limited computational efficiency. The efficiency of a minute-scale model with high spatial resolution is significantly lower than daily-scale models with coarser resolution for the "rain-runoff" process. The primary reasons for this low efficiency are (1) a large number of HCUs with high resolution, (2) small computational time steps, and (3) complex solution methods that require iteration for convergent time steps. This efficiency constraint limits the applicability of the models, with typical applications ranging from 10^{-6} to 10^{6} km^2 (Maxwell et al., 2014; Paniconi and Putti, 2015; Kollet et al., 2017). When applying these models, enhancing solution efficiency through parallel computing is a significant challenge. While numerical hydrological models have parallelization strategies, their computational efficiency is still insufficient for extensive, long-term simulations. The crux of parallelizing these models lies in the direct spatial interdependence of HCUs, rendering HCU grouping the foremost challenge. Furthermore, the inter-group computational dependencies within each time step, often necessitating iterative exchanges, imply that synchronization of inter-group data at each time step is essential, with a significant computation resources being dedicated to data synchronization. Therefore, extending the data synchronization interval emerges as a pivotal technical strategy in advancing parallel computation.

Complex Model Deployment: The complexity of the model deployment in numerical hydrological models is manifested in several aspects: (1) Complex horizontal spatial decomposition, where horizontal space division is commonly structured (rectangles, triangles, hexagons) or unstructured (irregular triangles, quadrilaterals, or a hybrid); (2) Complex vertical spatial discretization, which includes fixed-depth layering, hydrologically characterized layering, or dynamic layering; (3) Intricate spatial topological relationships, primarily concerning the coupling relationships between different HCUs. This includes the interaction between land and hydrological processes, as well as the interplay between explicit river channels and hillslope units. Such complexities require a nuanced understanding of spatial interdependencies and precision in modeling physical interactions across the watershed.

Substantial Development Challenges: The development of numerical hydrological models poses significant challenges due to the multitude of physical processes involved, the complexity of mathematical solutions, the abundance of parameters, high computational resource demands, and intricate model debugging. Most existing numerical hydrological models culminate years of collaborative effort by large research teams. For instance, despite building on 17 years of research accumulated from PIHM since 2004, the SHUD model still underwent a 6-year development journey (see https://github.com/shud-system/shud). Analysis of the development history of ParFlow from its GitHub repository (https://github.com/parflow/parflow) reveals that it took a team of three scientists six years to release the first version of ParFlow. Subsequent versions have been released over time, with collaboration from renowned institutions such as Princeton University, Colorado School of Mines, Washington State University, Syracuse University, Lawrence Livermore National Laboratory in the U.S., University of Bonn, Jülich Research Center, and the Centre for High-Performance Scientific Computing in Terrestrial Systems in Germany, and the French Institute of Environmental Geosciences. These collaborations highlight the significance and complexity of the research involved in developing such models (see https://parflow.org/#team).

4.3 Spatial-temporal scale issue

The scale issues in hydrological modeling remain a crucial and unresolved challenge. Blöschl et al. (2019) listed 23 unsolved problems in hydrology, many of which pertain to the scale issues of hydrological laws and models, including spatial parameters and the spatial heterogeneity of hydrological responses. While the study scale of natural water cycles spans from molecular to planetary scales (10^{-2}–10^{7} m) (Dooge, 1988), practical hydrological research, particularly in modeling, primarily focuses on the range of 10^{-2}–10^{7} m.

The scale of hydrological models is interpreted in two ways. (1) Granularity or spatial resolution, refers to the observation, summarization, or calculation of hydrological laws or parameters for a specific spatial area. For example, Figure 2 describes the basic computational units and coverage areas of hydrological models (Blöschl, 1999; Hrachowitz and Clark, 2017), focusing primarily on granularity. (2) Extent pertains to the spatial extension of the study object, namely, a large-scale or small-scale research area (Becker, 1992; Su, 2001; Gao and Zhao, 2020; Gou et al., 2022). This classification often involves various scales such as slopes, watersheds, continents, etc., but there is a significant difference in HCU areas across these scales.

Granularity inevitably leads to issues like internal spatial heterogeneity within units, optimal unit resolution, and representativeness of parameters. In fact, there is no perfect unit (Blöschl, 1999). For instance, the HCUs in numerical hydrological models are often smaller units, primarily because the formulas they rely on (like the Darcy-Richards equation and Saint-Venant equation) originate from laboratory observations and theoretical studies on ideal slopes. As the area of an HCU increases, its connection to these physical formulas becomes more tenuous, trending more towards a conceptual or statistical fitting framework. By integrating these small-scale physical formulas, numerical hydrological models attempt to simulate the hydrological cycle across watersheds and even at planetary scales. Within their basic HCUs, the models use a single set of hydrological parameters, so the spatial heterogeneity of a watershed is expressed by the variation of HCUs' parameters. For example, each HCU might have a unique value for soil hydraulic conductivity (K), and a watershed with n HCUs would have n different K values. Ideally, the K value for each HCU should represent the actual soil hydraulic conductivity for that specific unit. However, since the area of an HCU is much larger than that of a sampling point, the derived K value may not be consistent with K values measured at different locations within the HCU. Nevertheless, the spatial trends exhibited by models in practice can largely be represented by this simplified approach, such as the distribution of K values across multiple HCUs from upstream to downstream, generally aligning with the actual distribution in soil hydraulic conductivity (Yu et al., 2014). Parameter optimization is still indispensable for numerical hydrological models, while preserving the spatial heterogeneity of parameters.

Although field hydrological observations are often based on specific locations, the observational data reflect the hydrological response characteristics of a much larger area. For instance, observations at the outlet of a watershed—an area of only a few square meters, represent the cumulative effect of numerous surface and subsurface hydrological processes from various upstream contributing areas. Such measurements, like water level, flow rate, and sediment content, provide insights into the broader watershed dynamics. In contrast, small-scale measurements typically focus on completely enclosed and controllable hydrological processes. These include laboratory experiments like Darcy's on saturated soil and Vauclin's experiments (Vauclin et al., 1979) on water movement in saturated and unsaturated soils under fixed boundary conditions. The relationships between precipitation and runoff observed at larger scales, such as infiltration-excess and saturation-excess conceptualization, are often fitted using conceptual formulas or experimental curves. In contrast, the description of small-scale hydrological processes tends to utilize more physically reliable formulas. These include physical equations such as the Saint-Venant equation, Manning's formula, Darcy-Richards equation, and the Green-Ampt equation, which provide a more detailed and physically accurate representation of water movement at these finer scales.

Numerical hydrological models are applied across a broad range of areas. When testing and releasing these models, they are often simulated in the V-Catchment, Vauclin experiments, and impervious slab test cases (with areas ranging from 10^0 to 10^3 m^2) to verify their algorithms. Subsequently, these models are validated in smaller watersheds (approximately 10^4–10^8 m^2). The application scope of these models extends from individual watersheds to national and continental extents (Kollet and Maxwell, 2006; Shen and Phanikumar, 2010; Paniconi and Putti, 2015; Shu et al., 2020; Chen et al., 2023). Theoretically, numerical hydrological models based on physical principles should not be limited by geographical extent. However, in practical applications, limitations mainly arise from data availability and computational resources. With the growth of global baseline geographic data, data limitations have significantly decreased (Shu et al., 2024a), positioning computational resources and the efficiency of model algorithms as the primary challenges for numerical hydrological models.

Temporal resolution and period are also critical factors when applying hydrological models. The time resolution or time step of numerical hydrological models is constrained by the CFL condition and is determined based on the spatial resolution and flow velocity. As a result, most numerical hydrological models do not have a fixed computational time step. Instead, they dynamically adjust it based on whether specific variables satisfy the CFL condition or whether the error converges within a given time step. Typically, the finer the spatial resolution and the higher the rate of change of variables, the smaller the actual time step requires. Numerical hydrological models are versatile, enabling not only short-term simulations for hydrological events but also extensive applications in long-term water resource management and climate change research. This flexibility allows them to adapt to various research and practical applications, from immediate hydrological responses to long-term environmental impacts.

Numerical hydrological models are sensitive to the temporal resolution of forcing data. In these models, the runoff generation is governed by the Saint-Venant equation, and the infiltration process is governed by Darcy's Law. The intensity of rainfall significantly affects the water partitioning between surface runoff and infiltration. For instance, it is impossible to unevenly redistribute a daily rainfall of 24 mm d^{-1} over 24-hour intervals. Therefore, it is typically averaged to 1 mm h^{-1} (24 mm/24 h) or 0.167 mm min^{-1}. Redistributing daily rainfall intensity evenly over hourly or minute intervals significantly reduces the intensity at higher temporal resolutions, directly impacting runoff generation. Similar resolution requirements apply to other meteorological elements like radiation, temperature, and wind speed. Consequently, numerical hydrological models typically demand meteorological data with a resolution finer than daily (e.g., hourly or sub-hourly) to meet their theoretical and practical requirements. This necessity arises from the models′ intrinsic design to capture fine-scale hydrological dynamics, which are strongly influenced by the temporal variability of meteorological conditions.

4.4 Uncertainty and parameter calibration

Uncertainty is a persistent and significant issue in hydrological research, directly impacting the applicability and credibility of model results, yet remains without definitive resolution (Beven and Binley, 1992; Georgakakos et al., 2004; Beven, 2006; Montanari, 2007; Pechlivanidis et al., 2011). The uncertainties in hydrological models manifest in data, model structure, parameters, and initial conditions (Refsgaard et al., 2006; Clark et al., 2016). Reliance on data such as precipitation, temperature, soil moisture, and runoff, introduces uncertainties due to measurement errors, data processing errors, and spatiotemporal variability. Structural uncertainties in models arise from simplifications and assumptions; no model can fully capture the complexity of natural systems, leading to inherent structural uncertainties. For instance, simplifying or omitting cryospheric processes (glaciers, snow, and permafrost) in models hinders the accurate representation of hydrological processes in cold regions. Uncertainties introduced by initial conditions generally dissipate after a certain simulation period, which is defined as the warm-up period. Reliable algorithms for estimating the length of the warm-up period are lacking; current research relies on personal experience or identifies a period when a variable stabilizes (Bernsen et al., 2008; Rahman and Lu, 2015; Seck et al., 2015; Kim et al., 2018).

Parameter uncertainty in hydrological models manifests as the equifinality phenomenon, which refers to multiple different parameter sets producing similar simulation results within an acceptable accuracy threshold. However, not every parameter set accurately reflects the actual hydrological process (Beven and Freer, 2001; Savenije, 2001; Todini, 2007; McDonnell et al., 2007; Zehe et al., 2014). The parameter uncertainty issue is significant in numerical hydrological models, primarily due to the large number and high dimensionality of parameters (Orth et al., 2015). Through parameter optimization methods, the results from different parameter combinations can always approximate the observed data. Parameter optimization often targets a single variable (e.g., outlet streamflow). Using multiple observational variables with high spatiotemporal resolution as optimization targets can reduce parameter uncertainty (Aubert et al., 2003; Camporese et al., 2009; Shi et al., 2013). Numerical hydrological models can simulate more variables with higher temporal and spatial resolutions than traditional hydrological models, making multi-variable parameter optimization feasible (Maxwell et al., 2015; Hrachowitz and Clark, 2017).

During the model parameter calibration/optimization process, the selection of sensitive parameters, calibration methods, and objective functions directly influences the results, leading to varying degrees of error and uncertainty (Madsen et al., 2002; Cuntz et al., 2015; Flipo et al., 2023). Numerical hydrological models feature a multitude of adjustable parameters, which often have non-linear relationships with the objective functions used for model evaluation. This complexity makes manual parameter adjustment impractical for calibration, rendering automated parameter optimization almost the only viable approach. Given the uneven distribution of effective parameters in parameter space, their complex non-linear interrelationships, and the low computational efficiency of numerical hydrological models, enumeration and Monte Carlo sampling methods are inefficient or are trapped in local optima. Consequently, evolutionary optimization algorithms are commonly used in practice (Vrugt et al., 2003; Tolson and Shoemaker, 2007; Shen and Phanikumar, 2010; Razavi and Tolson, 2013; Shi et al., 2014; Yu et al., 2014; Hansen, 2016).

5. Prospects

5.1 Universal datasets

Where complex models and their higher attention to spatial and temporal details are required, the data resource requirements also are increased. For numerical hydrological models to demonstrate their adaptability across diverse watersheds, climatic conditions, and human activities and to highlight the advantages of their physical structure, extensive testing in various watersheds is necessary. However, preparing model data is a bottleneck in the model application. Therefore, establishing universal model datasets and data preparation tools is of practical value for developing and applying these models (Leonard and Duffy, 2013; Li et al., 2021; Ntona et al., 2022). Before preparing a universal dataset, it is necessary to identify the essential data required for constructing hydrological models. The three groups of essential data needed for hydrological simulation are (1) Watershed geographic characteristics, including watershed boundaries, elevation, slope, river networks, etc.; (2) Soil, geology, and land use data, along with their physical parameters such as soil hydraulic properties, impervious area, roughness, etc.; (3) Meteorological data, including precipitation, and data forcing energy transfer and evapotranspiration processes such as temperature, wind speed, humidity, air pressure, and radiation (Leonard and Duffy, 2013; Peckham et al., 2017; Ntona et al., 2022).

Establishing a public platform that provides these three groups of key data would not only lower the barriers to learning, researching, and disseminating hydrological models but also facilitate scientists to conduct extensive, reproducible, and comparative experiments. The Model Integration (MINT) project (http://mint-project.info), funded by the Defense Advanced Research Projects Agency of the United States, has established a global dataset on a private server, enabling rapid and reproducible model deployment for any watershed globally. However, its services are not yet public (Garijo et al., 2019; Gil et al., 2021). HydroTerre (https://hydroterre.psu.edu) is a universal data platform for hydrological models, but currently, it only supports data sharing services for HUC12 (Hydrological Unit Code level 12) level within the United States, which averages about 100 km^2 in area (Leonard and Duffy, 2013). The Global Hydrologic Data Cloud (https://ghdc.ac.cn/) can provide essential terrestrial data for model deployment in most global watersheds and prepare input files for specified models (Shu et al., 2024a).

Beyond the challenges of planning and constructing data platforms, data availability poses a significant obstacle to developing public data platforms. Data availability encompasses two aspects: (1) The existence of data or whether its quality meets the required standards; (2) Open access to data or permission for redistribution. Global watershed boundary classification and river network data face the former issue, characterized by scarcity or inferior quality. Even comprehensive global datasets like HydroSheds and MeritHydro are insufficient to meet the quality demands for rapid model deployment. Some global datasets (e.g., ASTER GDEM, USGS Global Land Cover, SoilGrids, GLDAS, FLDAS) utilize public domain protocols, allowing for data reorganization and redistribution on any platform. However, certain datasets remain under private protocols, limiting data sharing beyond their original platforms. For instance, numerous datasets from the China Meteorological Data Service Centre (http://data.cma.cn) and the Resource and Environment Science and Data Center of the Chinese Academy of Sciences (https://www.resdc.cn) explicitly prohibit data sharing or redistribution outside of their websites.

5.2 Multi-process coupling

The primary focus of numerical hydrological models remains on the "rainfall-runoff" process, with a generally loose coupling approach for processes that directly influence water movement, such as evapotranspiration, vegetation dynamics, spatiotemporal distribution of temperature/energy, and cryospheric elements like glaciers, snowpack, and permafrost. The computation of potential evapotranspiration often employs the Penman-Monteith equation, which is then multiplied by a moisture stress coefficient derived from soil moisture content to estimate actual evapotranspiration. Vegetation phenology influences hydrological processes unidirectionally through a time series of parameters such as leaf area index, stomatal conductance, and root depth, while soil moisture fluctuation does not feedback into plant dynamics. Glacial and snow processes are primarily modeled using degree-day models, with ice and snowmelt treated as additional surface boundary conditions or precipitation in the models. Due to the lack of coupled temperature and energy calculations, these models fail to represent the impact of soil freezing and thawing in permafrost regions on hydrological processes (Wang et al., 2014; Sun et al., 2019, 2023). Current land surface models provide a more detailed depiction of these processes. Hence, coupling numerical hydrological models with land surface models could enhance the representation of energy, phase change in water, and vegetation dynamics.

5.3 Multidisciplinary coupling

Matter and energy have no boundaries, and models from different disciplines address different processes but intersect. The isolation of models is a byproduct of disciplinary divisions and scientific questions. Facing rapid human activities and climate change challenges, a systematic representation of the synergistic effects of human activities and natural processes requires coupling between multidisciplinary models. This approach aims for a rational, comprehensive, and systematic mathematical description of the laws governing the movement of matter and energy (Wagener et al., 2010; Clark et al., 2015). The Heihe Watershed Allied Telemetry Experimental Research (HiWATER) illustrates that the watershed hydrological cycle is a complex megasystem encompassing hydrology, meteorology, cryosphere, geomorphology, ecology, and human activities, characterized as "intricate, overlapping, intertwined, and endless" (Cheng and Li, 2015; Li et al., 2023).

Rapid development in coupling research across meteorology, land surface processes, the cryosphere, agriculture, ecology, environment, geomorphology, and oceanography models is evident. For instance, significant progress has been made in coupling numerical hydrological models with landslides (Simoni et al., 2008), vegetation ecology (Bertoldi et al., 2010; Chiesa et al., 2014), seawater intrusion (Mazzia and Putti, 2005; Povich et al., 2013; Yu et al., 2021), and cryospheric processes (Dall'Amico, 2010; Dall'Amico et al., 2011; Endrizzi et al., 2014; Painter et al., 2013, 2016). Maxwell and Condon (2016) revealed the strong influence of lateral groundwater flow on large-scale evapotranspiration by coupling the ParFlow and CLM models. The MINT program has established an automated model coupling framework, integrating hydrological (SHUD and TopoFlow (Peckham et al., 2017)), agricultural, and economic models to address natural and socio-economic risks triggered by climate change, providing rapid response and support for governmental decision-making (Garijo et al., 2019; Gil et al., 2021). The WRF-Hydro system (Gochis et al., 2018) successfully coupled meteorological (WRF), land surface (NOAH), and hydrological (Hydro) models, simulating energy and water in the earth system, though its hydrological model component still has room for improvement. The HEIFLOW, GBEHM, and other models focus on the "water-soil-air-bio-human" coupling (Li et al., 2010; Yang et al., 2015; Tian et al., 2015, 2018; Li et al., 2018) but also developed high-resolution ecohydrological products like precipitation, snow, evapotranspiration, soil moisture, and net primary productivity. These developments are extensively applied in critical process research, model development, and validation in watershed ecohydrology, revealing the complex hydrological cycle in the Heihe River Basin (Li et al., 2012, 2023).

5.4 Model testing and comparison

Numerical hydrological models have begun to take shape. Each model differs in its foundational design, mathematical methods, and solution algorithms, yet there is a notable lack of targeted and systematic inter-model comparisons. This paper provides a technical comparison of typical numerical hydrological models in terms of design and structure, but this is still insufficient compared to the inter-model comparisons within traditional hydrological models (Maxwell et al., 2014; Paniconi and Putti, 2015; Kollet et al., 2017; Newman et al., 2017; Haque et al., 2021).

Benchmarking is a starting point for model comparisons and has garnered attention recently (Woods et al., 2003; Smith et al., 2004; Sebben et al., 2013; Nearing and Gupta, 2015; Newman et al., 2017). Descriptive articles of several numerical hydrological models (e.g., SHUD, Parflow, PAWS) often include idealized experiments such as V-catchments, Vauclin et al. (1979) experiments, and low-permeability surface tests (Kollet and Maxwell, 2006; Paniconi and Putti, 2015). The model descriptive articles (e.g., Kumar et al., 2009; Shen and Phanikumar, 2010; Shu et al., 2020) compare different models against analytical solutions and laboratory observations of surface water and groundwater processes, effectively demonstrating the capabilities of the models.

Comparisons among several numerical hydrological models reveal that all tested models can complete the designed tasks. In simple tasks, the differences between models are less than 5%. However, for more complex hydrological processes (such as intense surface-subsurface interactions, strong spatial heterogeneity, rapid changes in groundwater, etc.), significant discrepancies are observed among the models′ results (Maxwell et al., 2014; Kollet et al., 2017; Tijerina-Kreuzer et al., 2021). Preliminary comparisons suggest that no single model is significantly superior or inferior. These studies, focusing primarily on theoretical and idealized experiments, lack comparative research on the simulation effects in real watersheds.

Moreover, the comparisons are limited to surface and groundwater hydrological variables without addressing other hydrological processes like evapotranspiration or baseflow partitioning. Comparisons using real watershed data should include runoff observations and simulation results, spatial soil moisture, groundwater, and evapotranspiration. Numerical hydrological models provide high spatiotemporal resolution hydrological variables, making the comparison of model results with observations complex and varied, involving data comparisons at different spatial and temporal scales. Reliable comparisons between models necessitate support from universal datasets.

6. Conclusion

This paper summarizes the theoretical foundations of numerical hydrological models and systematically compares different numerical hydrological models′ computational methods and surface-subsurface coupling techniques. It critically reviews the characteristics of numerical hydrological models and clarifies their advantages and disadvantages, to provide insights and methodological references for the future development of these models.

Numerical hydrological models, grounded in the principles of micro-scale conservation and physical equations, use numerical methods to couple surface and subsurface water flows, thus simulating watershed-scale hydrological response. Their main advantages include strong physical process description, high temporal and spatial resolution with spatial continuity, coupling of surface-subsurface processes, realistic representation of human activities in hydraulics, a wealth of computational variables, and facilitating multidisciplinary model integration. Current developmental limitations include high parameter demands, uncertainty, low computational efficiency, complex modeling processes, and significant development challenges. Future research in numerical hydrological models should focus on constructing universal datasets, multi-process coupling, interdisciplinary coupling, and further enhancement of computational performance to expand their application scope.

The integrated surface-subsurface numerical hydrological model research represents one of the cutting-edge and mainstream directions in hydrological model development and is seen as "*an opportunity not to be missed*" (O'Connell and Todini, 1996; Peel and McMahon, 2020). However, due to constraints related to the openness of source code, data preparation, and adaptability verification, the development of the numerical hydrological model in China has yet to manifest significant scientific influence. The scientific community should support the development of new models while also strengthening the global validation, promotion, and improvement of existing numerical hydrological models. This approach provides practical support for scientific research and engineering applications and enhances understanding of the natural hydrological cycle (Shu L L et al., 2022).

It is important to recognize that individual models, whether complex or simple, are developed to support particular physical predictions with limitations and strengths that must be recognized when implemented. This paper focuses on watershed-scale models centered on the core scientific issue of "rainfall-runoff". It does not delve into related aspects of watershed hydrology, such as geomorphic evolution, soil erosion, sediment transport, solute transport/reaction, water-heat transfer/phase change, or climate change. Addressing these topics requires a broader and more integrated approach, recognizing the interconnectedness of these processes within the watershed hydrological cycle.

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