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Residual-based hybrid modeling combining GR4J and machine learning for streamflow prediction in data-scarce catchment: case of the Ouémé catchment at Bonou (Benin, West Africa)

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Abstract. Accurate streamflow forecasting is essential for water resource management, yet remains challenging in data-scarce regions. This study develops and evaluates a hybrid modeling framework for the Ouémé River basin (Benin) that combines the conceptual GR4J hydrological model with machine learning (ML) via a residual-correction strategy. The approach integrates GR4J with three ML techniques Random Forest (RF), Extreme Gradient Boosting (XGBoost), and Long Short-Term Memory (LSTM) networks to correct systematic errors in simulated streamflow. Models were trained on daily data from 1996–2012 and validated on an independent period (2013–2020) using performance metrics including Kling–Gupta efficiency (KGE), Nash–Sutcliffe efficiency (NSE), and percent bias (PBIAS). Results show that all hybrid models (GR4J–RF, GR4J–XGB, and GR4J–LSTM) outperform the standalone GR4J model. The tree-based hybrids (GR4J–RF and GR4J–XGB) achieved the highest performance gains, with validation KGE values of 0.80 and 0.79, respectively, compared to 0.75 for GR4J alone. While the GR4J–LSTM hybrid also improved baseline results, it exhibited comparatively lower performance, attributed to the data-intensive nature of deep learning in a limited-data context. The study demonstrates that hybrid residual-correction frameworks, particularly those employing efficient tree-based ML, offer a robust and practical pathway for enhancing streamflow prediction in data-scarce catchments.

1 Introduction

With the intensification of global climate change and the increasing frequency of extreme weather events, the uncertainty of runoff processes continues to rise, posing severe challenges to global water resource security, ecosystem stability, and socio-economic development (Amoussou et al., 2020). However, reliable hydrological models for streamflow simulation are fundamental for water resources management such as; flood risk reduction, reservoir management, irrigation planning, and climate adaptation particularly in data-scarce regions exposed to hydro-climatic variability (Kumanlioglu et al., 2019; Li et al., 2022).

Process-based hydrological models (PBHM) such as, the TOPMODEL, the SWAT model and the GR4J model have been widely used for streamflow simulation (Affėwé et al., 2025; Janjić and Tadić, 2023; Perrin et al., 2003). These models are grounded in physical laws and empirical formulations, describing hydrological processes by means of discretized sets of ordinary differential equations or simplified sets of partial differential equations. In fact, PBHM models provide interpretability and physical consistency in hydrological science, their face challenges related to structural uncertainties, simplifying assumptions to represent complex physical processes, parameter calibration, and computational demands (Li et al., 2022) lead to systematic simulation errors. In parallel, machine learning (ML) methods have demonstrated strong predictive capability in hydrology. Tree-based ensemble techniques such as Random Forest (Breiman, 2001) and Extreme Gradient Boosting (Chen and Guestrin, 2016), as well as deep learning approaches such as Long Short-Term Memory networks (Hochreiter and Schmidhuber, 1997), are able to capture complex nonlinear relationships directly from data and widely used for streamflow simulation (Kumanlioglu et al., 2019; Nevo et al., 2022; Shen and Lawson, 2021; Zohou et al., 2023), but often lack interpretability regarding hydrological elements due to their "black-box" nature.

Whether we use ML model or a PBHM, the issue of accurate and interpretability of simulation arises, especially in regions where observed data are limited. If these challenges remain unaddressed, streamflow simulations may retain systematic biases and reduced reliability during extreme events. In data-scarce tropical basins, this can undermine the credibility of hydrological predictions used for flood preparedness, infrastructure planning, and climate change impact assessments. Improving predictive performance while maintaining physical coherence is therefore a critical challenge.

To overcome these limitations, recent research has explored hybrid modeling, integrating physically based models with ML techniques to benefit from the complementary strengths of physically based and data-driven models. Various integration strategies have been proposed, including model output fusion (Zhang et al., 2022), physics-guided ML where physical constraints are embedded into loss functions (Khandelwal et al., 2020), and feature augmentation using physically based models simulated variables as additional ML inputs (Kumanlioglu et al., 2019). Among these strategies, residual-based one of feature augmentation methods has been widely used for hybridization of PBHM and ML; assumes that a PBHM captures the dominant water balance dynamics, preserving physical consistency, while remaining systematic errors can be learned from data using machine learning model. In the Ouémé catchment, where this study is carried out, most existing work has focused on process-based hydrological models or a standalone machine learning (Affééwé et al., 2025; Biao et al., 2016; Obada et al., 2025; Zohou et al., 2023). To address these gaps, this study investigates a residual-based hybrid modeling framework combining the GR4J hydrological model with machine learning approaches. Specifically, the study addresses two research questions: (i) Does residual-based hybridization significantly improve the predictive performance of GR4J, and (ii) which machine learning family; tree-based models (Random Forest and XGBoost) or deep learning (LSTM) is most suitable for correcting GR4J residual errors and improving streamflow prediction in a tropical data-scarce catchment.

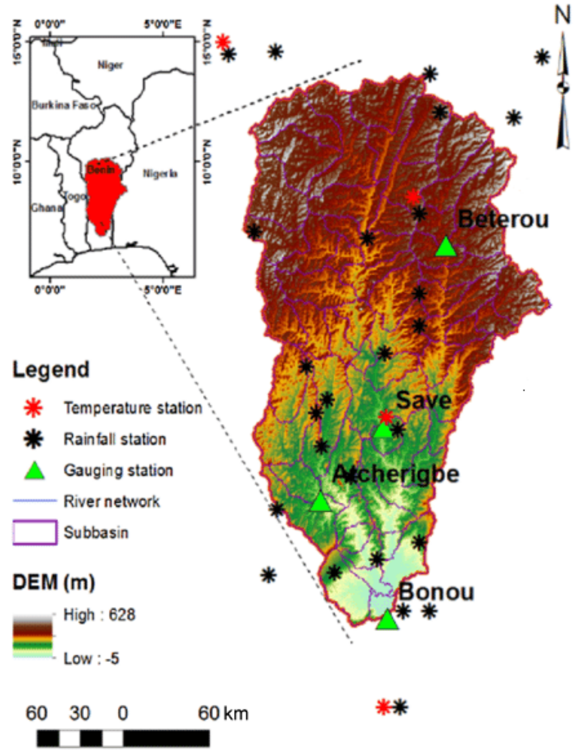

Figure 1. Study area.

2 Materials and methods

2.1 Study area

The study area is the Ouémé River basin in Benin, West Africa (Fig. 1). It spans from the source of the Ouémé River in the Tanéka mountains in northern Benin to the Nokoué and Porto-Novo lagoons through which the river flows into the Atlantic Ocean (Houngue, 2020). With a drainage area of almost 50 000 km^2, it covers 41.14% of Benin's total area (Japhet Kodja et al., 2018). The climate is equatorial in the south, with a long rainy season from May to July and a short rainy season from September to November, interspersed with dry seasons. Sudanian, in the north, has a rainy season from May to October and a dry season from November to April. The central area is a transition zone. The average annual rainfall in the region is 1000 to 1200 mm, the average temperature is around 28 °C and the relative humidity varies between 77 % and 93 % (Biao et al., 2016).

2.2 Input data

This study used multiple datasets to characterize the hydroclimatic settings of the Ouémé watershed from 1996 to 2020. Primary meteorological data, including daily precipitation, evapotranspiration and mean temperature from ERA5-LAND (Muñoz-Sabater et al., 2021) were used. Corresponding daily streamflow measurements were collected from

DGeau (Direction Générale de l'eau) at Bonou station for the same period.

2.3 Models *Description*

2.3.1 Conceptual Hydrological Model (GR4J)

The GR4J model is a lumped, daily conceptual rainfall–runoff model widely used for streamflow simulation. It represents catchment hydrological processes through four parameters controlling production, routing, groundwater exchange, and unit hydrograph dynamics (Perrin et al., 2003). GR4J requires precipitation and potential evapotranspiration as inputs and simulates streamflow through simplified representations of soil moisture accounting and flow routing. GR4J serves as the baseline physically based model and provides simulated streamflow used both for direct evaluation and as a reference for hybrid model development.

2.3.2 Random Forest (RF)

Random Forest is an ensemble machine learning method based on a collection of decision trees constructed using bootstrap sampling and random feature selection (Breiman, 2001). Each tree independently learns nonlinear relationships between inputs and outputs, and final predictions are obtained by averaging individual tree outputs. In this study, RF is used to correct the residual errors of streamflow simulated by the GR4J model.

2.3.3 Extreme Gradient Boosting (XGBoost)

Extreme Gradient Boosting (XGBoost) is a boosting-based ensemble learning algorithm that builds decision trees sequentially, with each tree correcting the errors of previous ones. It incorporates regularization techniques and gradient-based optimization, allowing efficient learning of complex nonlinear patterns while controlling overfitting (Chen and Guestrin, 2016). In this study, XGBoost also is used to correct the residual errors of streamflow simulated by the GR4J model.

2.3.4 Long Short-Term Memory (LSTM)

Long Short-Term Memory (LSTM) networks are a class of recurrent neural networks specifically designed to capture long-term dependencies in time series data (Hochreiter and Schmidhuber, 1997). Through gated memory cells, LSTM models can learn temporal patterns and delayed responses characteristic of hydrological processes. LSTM has been increasingly applied to streamflow modeling due to its ability to represent nonlinear and time-dependent relationships. In this study, we applied LSTM model to correct the residual errors of streamflow simulated by the GR4J model, enabling a hybrid framework that combines physical consistency with data-driven temporal learning.

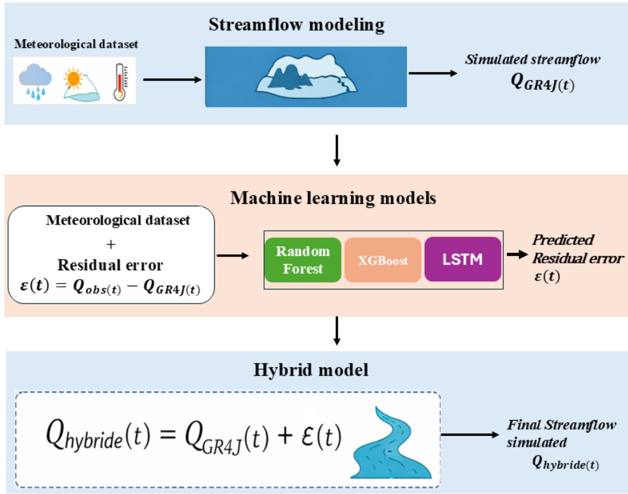

Figure 2. Schematic diagram of the GR4J–ML hybrid process.

2.3.5 The GR4J-ML hybrid approach

The study introduces a GR4J-ML hybrid approach that aims to improve streamflow prediction by integrating GR4J physical constraints. The hybrid framework follows a residual-correction strategy in which each machine learning (ML) model is trained to predict the systematic errors of the GR4J conceptual model. First, GR4J is calibrated and validated using precipitation and potential evapotranspiration to simulate daily discharge $Q_{\mathrm{GR4J}}(t)$. The residual error is then calculated as:

$$\varepsilon(t) = Q_{\mathrm{Obs}}(t) - Q_{\mathrm{GR4J}}(t) \tag{1}$$

where $Q_{\mathrm{Obs}}(t)$ and $Q_{\mathrm{GR4J}}(t)$ are respectively the observed discharge and simulated discharge at time t. The machine learning models are trained to predict the residual errors of the GR4J simulations using hydro-meteorological inputs. Specifically, precipitation, potential evapotranspiration and mean temperature have been used as predictors, while residual error is the target variable. This configuration allows the ML models to learn systematic discrepancies between observed and simulated streamflow. The final hybrid discharge is computed as:

$$Q_{\mathrm{Hybrid}}(t) = Q_{\mathrm{GR4J}}(t) + \hat{\varepsilon}(t) \tag{2}$$

where $\hat{\varepsilon}(t)$ is the simulated residual error by ML models. This approach assumes that GR4J captures the dominant water balance dynamics, while the residual error represents systematic and learnable deficiencies related to nonlinear runoff generation or routing simplifications. By correcting residual error rather than replacing the physical model, the framework preserves the hydrological structure of GR4J while improving predictive accuracy. Figure 2 illustrates the workflow of this approach.

2.3.6 Experimental designs

The study employed four models: GR4J, GR4J-LSTM, GR4J-RF and GR4J-XGB. Each GR4J model variant combined with MLs aimed to improve the accuracy of streamflow simulation. To ensure a consistent and comparison between models, the GR4J hydrological model was calibrated using daily data over the period 1996–2012 and subsequently validated over the independent period 2013–2020. Following the same experimental design, all hybrid models combining GR4J with machine learning techniques were trained on the 1996–2012 period and evaluated on the 2013–2020 period. The streamflow forecasts with various models were assessed utilizing four widely utilized measures for hydrological model evaluation: percent bias (PBIAS), Nash-Sutcliffe efficiency (NSE), Kling-Gupta Efficiency metric (KGE), and R^2.

2.3.7 Hyperparameters tuning

Hyperparameters are predefined parameters that cannot be learned during model training, yet they significantly influence an ML model's performance. In this study, the optimal hyperparameters were determined using a grid search procedure. For detailed information on the hyperparameters and optimal values, see Table 1.

3 Results and discussions

The Table 2 summarizes the performance of the GR4J model and the three hybrid approaches (GR4J–RF, GR4J–XGB, and GR4J–LSTM) over the training (1996–2012) and validation (2013–2020) periods using KGE, NSE, R^2, and PBIAS metrics.

The standalone GR4J model provides a reasonable baseline performance, with a KGE of 0.82 during training and 0.75 during validation. The corresponding NSE and R^2 values are 0.71 and 0.65 for the validation period, indicating a good ability to reproduce observed streamflow variability. The PBIAS values close to zero (−2.24 % for training and −0.86 % for validation) suggest a limited overall bias in simulated flows. All hybrid models outperform the standalone GR4J model across most performance metrics in both training and validation periods. The GR4J–RF model exhibits the highest performance among the tested approaches, achieving a KGE of 0.88 during training and 0.80 during validation. Similarly, NSE and R^2 values increase substantially compared to GR4J alone, reaching 0.85 (training) and 0.73 (validation). The PBIAS remains close to zero, indicating a good balance between overestimation and underestimation of streamflow.

The GR4J–XGB model also demonstrates strong performance, in validation period and achieve KGE, NSE, and R^2 values of 0.79, 0.73, and 0.73 respectively. Bias is minimal, with PBIAS values of 0.05 % during training and −0.36 % during validation, suggesting a stable correction of GR4J residuals across periods. The GR4J–LSTM model improves upon the standalone GR4J results but shows comparatively lower performance than the tree-based hybrid approaches. Validation KGE and NSE reach 0.78 and 0.69, respectively. The R^2 value of 0.74 during validation indicates a reasonable reproduction of flow variability, while PBIAS values of 3.57 % (training) and 1.47 % (validation) reveal a slight tendency toward overestimation.

Overall, the results indicate that hybridization with machine learning models leads to systematic improvements in model performance relative to the standalone GR4J model, with the most pronounced gains observed for the GR4J–RF and GR4J–XGB approaches. These results align with these of Kumanlioglu et al. (2019), Shen (2018), Li et al. (2022) and Immerzeel et al. (2015), who reported that ML model have the capacity to balance correlation, variability, and bias, making integrated models ideal for data scarce regions watershed, where accurate water management is critical. Then residual-based hybrid models outperform the standalone Process-based hydrological models for streamflow simulation. These improvements suggest that the hybrid modeling approach can provide more reliable streamflow information, which is essential for effective water resources planning, flood forecasting and early warning systems, reservoir operation, irrigation water allocation and hydrological analysis in data-scarce tropical catchments.

The graphical comparison between observed and simulated streamflow highlights clear differences in performance among the tested models (Fig. 3). Although the model generally matched observed outflow, it tended to overestimate during low water periods from November to April and the high-water period, due to the effect of rainfall totals amount in June, July, August, September and October over the study area. These findings are consistent with those Japhet Kodja et al. (2018) and Afféwé et al. (2025), who reported that GR4J model overestimate discharge during the low-water and high-period. The standalone GR4J model reproduces the general seasonal dynamics of the basin but exhibits limitations in capturing peak flows and short-term variability. The hybrid GR4J–RF and GR4J–XGB models substantially improve streamflow simulation, particularly during high-flow events, by effectively correcting systematic residuals while preserving the physically based structure of GR4J. These results are consistent with the findings of Yang et al. (2024), who reported that applying conceptual models with machine learning reduces residual errors in conceptual model simulation and improves the accuracy of runoff predictions, particularly during extreme events. These tree-based hybrid approaches show strong consistency across training and validation periods, indicating robust generalization. In contrast, the GR4J–LSTM hybrid model improves temporal coherence relative to GR4J alone but remains less effective in correcting extreme flows, suggesting sensitivity to data volume and model configuration.

Table 1. Optimal hyperparameters for RF, XGB, and LSTM.

Hyperparameters	Optimal values	description
Hyperparameters for RF		
Hyperparameters	Optimal values	description
n_estimator	300	number of trees
max_depth	5	maximum depth of trees
min_samples_split	2	minimum samples to split a node
min_samples_leaf	10	minimum samples at a leaf node
Hyperparameters for XGB		
n_estimator	110	Number of boosting rounds
max_depth	5	Maximum depth of trees
Learning_rate	0.05	Step size shrinkage
subsample	0.8	Fraction of sample per tree
colsample_bytree	0.6	Fraction of features per tree
Hyperparameters for LSTM		
num_layers	1	Number of LSTM layer
unit	256	Number of cells unit
dropout	0.4	Dropout rate
Learning_rate	0.0001	Learning_rate
Batch_size	128	Number of samples per gradient update
Sequence_length	365	Number of time steps in the LSTM input sequence
epochs	100	Number of training iterations

Table 2. The KGE, NSE, R2, and PBIAS metrics for different GR4J-ML model.

Model	GR4J		GR4J-RF		GR4J-XGB		GR4J-LSTM	
Dataset	train	test	train	test	train	test	train	test
KGE	0.82	0.75	0.88	0.80	0.86	0.79	0.85	0.78
NSE	0.71	0.65	0.85	0.73	0.82	0.73	0.74	0.69
R^2	0.71	0.65	0.85	0.73	0.82	0.73	0.69	0.74
PBIAS	−2.24	−0.86	−0.02	−3.13	0.05	−0.36	3.57	1.47

Overall, the figures demonstrate that residual-based hybrid modeling enhances streamflow prediction, with tree-based methods outperforming the deep learning approach in this application. The relatively lower performance of the GR4J–LSTM hybrid, compared to the tree-based methods (RF and XGBoost), can be attributed primarily to the data-intensive nature of deep learning models. LSTM networks, while powerful for capturing complex temporal dependencies, typically require large volumes of training data to generalize effectively and avoid overfitting (Shen, 2018). In data-scarce regions like the Ouémé catchment, the available daily record may be insufficient for the LSTM to fully learn the nuanced error patterns of the GR4J model (Zohou et al., 2023), especially given its substantial number of parameters and the need for careful hyperparameter tuning.

4 Conclusions

This study developed and evaluated a residual-based hybrid modeling framework that integrated the conceptual GR4J hydrological model with three machine learning techniques; Random Forest (RF), Extreme Gradient Boosting (XGBoost), and Long Short-Term Memory (LSTM) networks for daily streamflow simulation in the data-scarce Ouémé River basin. The key finding is that all hybrid models (GR4J–RF, GR4J–XGB, and GR4J–LSTM) outperformed the standalone GR4J model across multiple performance metrics (KGE, NSE, R^2, PBIAS), confirming the value of using machine learning to correct systematic errors in physically based simulations. The proposed hybrid modeling framework provides improved streamflow simulations compared with the standalone GR4J model and offers a promising tool for supporting water resources management. The GR4J–LSTM hybrid also provided improvement over the base model but to a lesser extent, a result largely attributable to

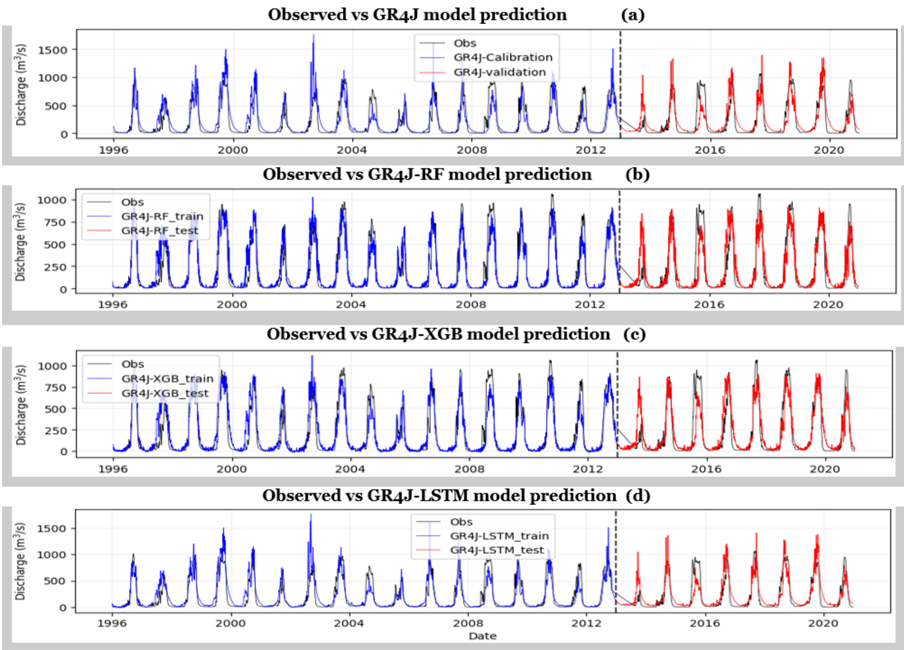

Figure 3. Time series observed and predicted streamflow during training and testing; **(a)** for GR4J standalone model, **(b)** for GR4J-RF integrated model, **(c)** for GR4J-XGB integrated model, and **(d)** for GR4J-LSTM integrated model.

the data-intensive nature of deep learning, which poses a significant constraint in regions with limited historical records.

Future research should test the performance of this approach across different sub-basins of the Ouémé River Basin to better understand the spatial variability of hydrological processes and model responses between basins. Further work should also focus on the use of large-scale, publicly available datasets such as Caravan a global hydrometeorological dataset could provide the extensive and diverse data needed to better train and validate deep learning models like LSTM, potentially unlocking their full potential within hybrid frameworks in data-scarce environments.

Code availability. All models developpement were performed using python (3.11). Custom scripts are available upon request from the respective author, as they contain site-specific data that cannot be made public.

Data availability. All data used in this study are available from the corresponding author upon request.

Author contributions. JEA developed the main idea, collect the data, ran the models, analysis and wrote the manuscript; AYB, and JH validate and supervise the manuscript.

Competing interests. At least one of the (co-)authors is a guest member of the editorial board of *Proceedings of the International Association of Hydrological Sciences* for the special issue ”Circular Economy and Technological Innovations for Resilient Water and Sanitation Systems in Africa II”. The peer-review process was guided by an independent editor, and the authors also have no other competing interests to declare.

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