Multiscale Learnable Physical Modeling and Data Assimilation Framework: Application to High-Resolution Regionalized Hydrological Simulation of Flash Floods

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Key Points:
• Multiscale spatially distributed Learnable Physical Modeling and learnable Parameter Regionalization with data assimilation framework
• Accurate and robust discharge performances at gauged and pseudo-ungauged flash flood-prone basins using multi-site spatialized learning
• Hybrid model space-time interpretability through conceptual parameters and internal states fields

Abstract
To advance the discovery of scale-relevant hydrological laws while better exploiting massive multi-source data, merging machine learning into process-based modeling is compelling, as recently demonstrated in lumped hydrological modeling. This article introduces MLPM-PR, a new and powerful framework standing for Multiscale spatially distributed Learnable Physical Modeling and learnable Parameter Regionalization with data assimilation. MLPM-PR crucially builds on a differentiable model that couples (i) two neural networks for processes learning and parameters regionalization, (ii) grid-based conceptual hydrological operators, and (iii) a simple kinematic wave routing. The approach is tested on a challenging flash flood-prone multi-catchment modeling setup at high spatio-temporal resolution (1km, 1h). Discharge prediction performances highlight the accuracy and robustness of MLPM-PR compared to classical approaches in both spatial and temporal validation. The physical interpretability of spatially distributed parameters and internal states shows the nuanced behavior of the hybrid model and its adaptability to diverse hydrological responses.

Plain Language Summary
Understanding and modeling flash flood-prone areas remains challenging due to limited observed data and limited scale-relevant hydrological theory. With the surge in artificial intelligence (AI), machine learning models have shown promising capabilities in addressing various challenges. However, effectively combining AI and process-based models causes difficulties. In this study, we present a new approach that incorporates machine learning into a high-resolution hydrological model, used to address the complex problem of transferring parameters between different watersheds. Our results highlight significant improvements in accurately predicting and understanding physical patterns, marking a crucial step towards developing our ability to build learnable and interpretable process-based models.

1 Introduction
Faced with the socio-economic challenges of floods and drought forecasting in a context of climate change, modeling approaches that make the most of the maximum amount of information available are needed to make accurate forecasts at high spatio-temporal resolution. Nevertheless, given the complexity and non-linearity of the coupled surface and subsurface physical processes involved, and their limited observability with respect to the number of parameters to estimate (“curse of dimensionality”), hydrological modeling remains a difficult task tinged with uncertainties (e.g., Liu and Gupta (2007)). Moreover, in the absence of directly exploitable first principles in hydrology (e.g., Dooge (1986)), as opposed to flow mechanistic
equations in continuous media such as river hydraulics, meteorology or oceanography, and given the high heterogeneities of continental hydrosystems compartments and the lack of "scale-relevant theories" (Beven, 1987), process-based hydrological models generally include a certain amount of empiricism, which represents an avenue for the fusion of data assimilation (DA) and uncertainty quantification (UQ) with machine learning (ML) and deep learning (DL, deeper neural networks, i.e., with more layers) techniques to better exploit the informative richness of multi-source data.

Pure ML applications in hydrology started decades ago (e.g., references in Maier and Dandy (2000) or Artigue et al. (2012) on flash floods). A recent explosion of DL applications, stemming from the rise of big data, computational power, and their capabilities to extract multi-level information from large datasets (LeCun et al., 2015), has led to a bloom of studies, in particular in hydrology (e.g., reviews by Nearing et al. (2021); Shen and Lawson (2021)) and water related disciplines (e.g., Tripathy and Mishra (2024)). The potential of using long short-term memory (LSTM) network (Hochreiter & Schmidhuber, 1997), a recurrent neural network adapted to long time series, for lumped continuous rainfall-runoff modeling, was introduced by Kratzert et al. (2018) and explored in hundreds of studies since (Shen & Lawson, 2021). In addition to the capability of LSTM to learn multi-frequent aspects, training those networks over large catchment samples using catchment physical descriptors within lumped models, in addition to meteorological forcings time series, leads to better performances in daily runoff prediction and in regionalization (Kratzert et al., 2018; Hashemi et al., 2022). A convolutional LSTM architecture, combining the strength of LSTM for capturing multiscale temporal dynamics and of convolutional layers for spatial patterns extraction, is found effective for spatio-temporal rainfall nowcasting (Shi et al., 2015) and for hydrological modeling (e.g., Xu et al. (2022); Chen et al. (2022)). Nevertheless, pure ML/DL algorithms are hardly interpretable and do not use the effective physical models, solvers as well as adjoint (differentiation) techniques developed over the past century. Hybrid approaches, that leverage ML/DL in sequential combination with process-based numerical models via their inputs/outputs, have been explored recently and enable to improve the accuracy of hydrologic predictions (e.g., Konapala et al. (2020), with DA in Roy et al. (2023) or with UQ in Tran et al. (2023)).

Merging process-based differential equations with ML can be very advantageous as recently shown with physics-informed neural networks (PINNs) (Raissi et al., 2019), where process-based model is used as weak constrain in the training cost function and is well adapted to assimilate observations (e.g., He et al. (2020)), or in universal differential equations that embed an universal approximator (Rackauckas et al., 2021). In hydrology, the combination of ML into process-based models looks promising as very recently shown for daily lumped models (Kumanlioglu & Fistikoglu, 2019; Jiang et al., 2020; H"oge et al., 2022; Feng et al., 2022). The routing part of a lumped GR model (Perrin et al., 2003) (algebraic model from temporally integrable ordinary differential equations (ODE)) has been replaced by an artificial neural networks (ANN) and leads to superior performances than GR or ANN alone on one basin in Kumanlioglu and Fistikoglu (2019). Including an ANN into a spatially lumped process-based hydrological ODE (H"oge et al., 2022), and adding an ANN-based regionalization pipeline (Feng et al., 2022), leads to learnable lumped model structures that reveal interesting in terms of performance and interpretability when trained.

A key technology to achieve is differential programming, in order to derive a numerical adjoint model enabling the computation of accurate cost function gradients with respect to high-dimensional parameters, as needed for their optimization and used in variational data assimilation (VDA) for fusing data with geophysical models (cf. Monnier (2021)). Regarding rivers networks, adjoint-based optimization has been applied to dynamic non-linear and highly parameterized spatially distributed models in 2D hydraulics (Honnorat et al., 2009), in spatially distributed hydrological VDA (Castaings et al., 2009; Jay-Allemand et al., 2020), and in ANN-based regionalization (Huynh, Garambois, Colleoni, Renard, et al., 2023). Nevertheless, incorporating neural networks into a differentiable spatialized hydrological model with a data assimilation framework, for learning physical processes parameterization from massive data, has never been performed and is a very challenging problem addressed here.

This article presents a novel framework for building Multiscale spatially distributed Learnable Physical Modeling (MLPM) with Learnable Parameter Regionalization (LPR). The approach builds on differentiable modeling and combines interpretable process-based modeling along with neural networks, including learnable regionalization of conceptual parameters with an ANN from Huynh, Garambois, Colleoni, Renard, et al. (2023), and another ANN introduced for process parameterization learning applied here to correct internal fluxes within a spatially distributed hydrological model. The MLPM-PR framework is illustrated with a parsimonious conceptual grid-based GR-like model (Perrin et al., 2003) with kinematic wave routing scheme, implemented in the open-source SMASH software (Spatially distributed Modelling and ASsignment for Hy-


drology) that enables multiscale modeling, numerical adjoint model derivation via automatic differentiation and VDA. The performances and interpretability of the proposed approach are studied over a very challenging flash flood-prone area, in a multi-basins modeling setup at a relatively high spatio-temporal resolution of 1 km and 1 h in regional calibration-validation.

2 Material and Methods

2.1 Forward Differentiable Model

The forward hybrid model $\mathcal{M}$ is obtained by partially composing a dynamic process-based, differentiable, and spatially distributed rainfall-runoff model $\mathcal{M}_{rr}$ with a learnable process parameterization-regionalization (LPR) operator $\phi$, resulting in Equation 1.

$$\mathcal{M} = \mathcal{M}_{rr}(\ldots, \phi(\ldots))$$

Let $\Omega \subset \mathbb{R}^2$ denote a 2D spatial domain with $x \in \Omega$ the spatial coordinate and $t \in [0, T]$ the physical time, $D_{\Omega}$ a D8 drainage plan. The spatially distributed rainfall-runoff model $\mathcal{M}_{rr}$ is a dynamic operator projecting the input fields of atmospheric forcings $\mathcal{F}$ onto the fields of surface discharge $Q$, internal states $h$, and internal fluxes $q$, as expressed in Equation 2.

$$U(x,t) = [Q,h,q](x,t) = \mathcal{M}_{rr}(D_{\Omega};\mathcal{F}(x,t); [f_q,h_0](x,t),\theta(x))$$

with $U(x,t)$ the modeled state-flux variables, $f_q$ the vector of spatially distributed corrections of $q$ the internal fluxes (which will be explained later), $\theta$ and $h_0$ the spatially distributed parameters and initial states of the hydrological model. In this study, the grid-based rainfall-runoff model $\mathcal{M}_{rr}$ consists in algebraic GR-like conceptual operators (Perrin et al., 2003; Ficchì et al., 2019) (temporally integrable ODEs) for runoff production at pixel scale with a kinematic wave-based routing model (Te Chow et al., 1988) (refer to Supporting Information (SI), Text S3 for mathematical details).

The learnable operator $\phi$, embedded within the gridded rainfall-runoff operator $\mathcal{M}_{rr}$ to form the complete model $\mathcal{M}$, is a pair of neural networks with the capability to ingest (i) neutralized atmospheric inputs $\mathcal{I}_n = (P_n, E_n)$ (using the wording from Santos et al. (2018)), along with the model states at previous time step $h(x,t-1)$, for correcting the internal fluxes $q$ (process parameterization pipeline) and (ii) physical descriptors $D$ (refer to SI, Figure S2 for information on the studied descriptors) for estimating the model parameters $\theta$ (regionalization pipeline), as shown in Equation 3.

$$\phi : \begin{cases} f_q(x,t) = \phi_1(\mathcal{I}_n(x,t),h(x,t-1);\rho_1) \\ \theta(x) = \phi_2(D(x);\rho_2) \end{cases}$$

with $\rho = (\rho_1, \rho_2)$ the vector of trainable parameters, invariant to the spatial coordinate $x$ over $\Omega$, of the pair of neural networks. In this study, we use two multilayer perceptrons, the first one $\phi_1$ for spatio-temporal corrections of the model internal fluxes $f_q$, and the second $\phi_2$ for spatialized parameters $\theta$ (regionalization as used in Huynh, Garambois, Colleoni, Renard, et al. (2023) (refer to SI, Text S2 for further details). Here, the fluxes correction $f_q$ is $\left(f_{q,i=1\ldots N_q}\right)^T$ predicted by $\phi_1$, are applied as multiplicative factors, for each pixel $x$ and time $t$, to the $N_q = 4$ internal fluxes of the GR hydrological operators to correct simultaneously the actual evapotranspiration and infiltration into the production reservoir, the net rainfall partitioning with a non-conservative exchange effect, and the non-conservative exchange flux. The vector of conceptual spatialized parameters, mapped by the ANN $\phi_2$, is $\theta = (c_p, c_t, k_{exe}, a_{kw}, b_{kw})^T$ composed of production and transfer reservoir capacities $c_p$ and $c_t$, exchange coefficient $k_{exe}$, kinematic wave parameters $a_{kw}$ and $b_{kw}$.

By construction, the complete forward model $\mathcal{M}$ is learnable, through the ANN-based mapping $\phi$ embedded into the spatially distributed rainfall-runoff operator $\mathcal{M}_{rr}$, while remaining differentiable.

2.2 Inverse Problem

Given observed and simulated discharge times series $Q^* = (Q_{g=1\ldots N_g})^T$ and $Q = (Q_{g=1\ldots N_g})^T$ with $N_G$ the number of gauges over the study domain $\Omega$, the model misfit to multi-site observations is measured through a cost function $J$, as shown in Equation 4.

$$J(Q^*, Q) = \sum_{g=1}^{N_G} w_g J_g(Q_g^*(t), Q_g(t))$$

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where $\sum_{g=1}^{N_G} w_g = 1$, here $w_g = 1/N_G$ and $j_g(Q^*_g, Q_g) = 1 - NSE(Q^*_g, Q)$ at each gauge with NSE as the quadratic Nash-Sutcliffe efficiency. Thus, $J$ is a convex and differentiable function, involving the response of the forward model $M$ through its output $Q$, and consequently depending on the model parameters $\theta$ and the fluxes corrector $f_q$, hence on the ANNs parameter $\rho$ (cf. Equation 3). Consequently the VDA optimization problem formulates as in Equation 5.

$$\hat{\rho} = \arg \min_{\rho} J(Q^*, M_{r\tau}(., \phi(., \rho)))$$

This high-dimensional inverse problem can be tackled through gradient-based optimization algorithms. A limited-memory quasi-Newton approach, such as L-BFGS-B (Zhu et al., 1997), is suitable for smooth objective functions, while an adaptive learning rate approach, exemplified by Adam (Kingma & Ba, 2014), is effective for non-smooth objective functions. These approaches necessitate obtaining the gradient $\nabla_\rho J$ of the cost function, achieved through automatic differentiation using the Tapenade engine (Hascoet & Pascual, 2013). The complete forward model and calibration process are illustrated in Figure 1.

![Figure 1](image)

**Figure 1.** MLPM-PR framework: Multiscale spatially distributed Learnable Physical Modeling (MLPM) and Learnable Parameter Regionalization (LPR) with data assimilation, for a differentiable grid-based hydrological model involving a pair of parameterization-regionalization neural networks and gridded hydrological operators. The pair of neural networks is used to (i) correct internal fluxes (using neutralized atmospheric data) and (ii) estimate the model parameters (using physical descriptors), with their weights optimized through high-dimensional optimization algorithms using an adjoint model to obtain accurate spatial gradients of the cost function.

### 2.3 MLPM-PR Framework Analysis and Experimental Design

After optimization with the proposed approach, enabling to jointly learn physical processes parameterization and regionalization, a hybrid process-based spatially distributed calibrated hydrological model $M_{r\tau}$ is obtained and is therefore reusable for space-time extrapolation. Contrarily to PINNs where the physical model residual serves as a weak constrain in optimization, in our proposed conceptualization, the physics
is used as a strong constrain. In this sense, the approach can be seen as a learnable spatialized physical model. Moreover, contrarily to PINNs and LSTM, which are composed of neural networks only, our hybrid model is physically interpretable through its conceptual parameters $\theta(x)$, internal states $h(x,t)$ and fluxes $q(x,t)$. Moreover, the ANNs $\phi_1$ and $\phi_2$ coupled with the conceptual model $M_{rr}$, may confer their capability to capture non-linear and multi-resolution effects. The conceptualization, where the physics is used as a strong constrain in the forward model, enables to use other differentiable hydrological and hydraulic models for example, on structured or unstructured meshes. Such an approach enables to integrate data that are not directly usable nor explicitly represented in the model such as the physical descriptors for regionalization of conceptual parameters here.

The study zone is located in the Eastern Mediterranean region of France, encompassing multiple gauges downstream of both nested and independent catchments (see SI, Figure S1). The SMASH model is run on a $dx = 1$ km spatial grid at $dt = 1$ h time step that is the resolution of the radar-raingauge rainfall product (refer to SI, Text S4 for details on the model setup). Calibration methods are performed for the evaluation of (i) the SMASH hybrid process parameterization pipeline (S-GRNN) versus the classical SMASH GR-based model (S-GR), and (ii) the hybrid regionalization pipeline (reg.NN) versus the lumped (spatially uniform parameters) regionalization approach (reg.U). Local calibration methods with lumped parameters (loc.U) are also conducted and referred to as reference performances when comparing regionalization methods. The calibration period, denoted as P1, spans four years from August 2009 to July 2013, while the validation period, denoted as P2, covers a three-year period from August 2013 to July 2016. The classical NSE is selected as the calibration metric, computed using data from gauged catchments in the case of regionalization (multi-site regionalization).

3 Results and Discussion

3.1 Regional Learning Performance

Figure 2a shows a global comparison of the performances, in terms of Nash–Sutcliffe efficiency (NSE) over the modeled time periods, of (i) the two model structures (S-GRNN versus S-GR) and (ii) the two regional mappings (reg.NN versus reg.U) used in calibration. The results in calibration and validation indicate that hybrid process parameterization pipelines (in darker colors), incorporating ANN into the forward structure (S-GRNN) consistently yield superior NSE scores and simulated discharges (as shown in Figure 2b) when compared to the classical models (S-GR in lighter colors). In addition, the hybrid regionalization pipelines (pink boxes) exhibit median NSE scores exceeding 0.8 in calibration, surpassing the two reference models (green boxes). In validation, the hybrid regionalization methods also demonstrate the capability to outperform the lumped regionalization approaches (blue boxes), achieving median NSE scores around 0.6 and 0.8 for spatial (regionalization) and temporal validation, respectively. Especially, the LPR framework, using a pair of neural networks (S-GRNN.reg.NN), attains in spatial validation a median NSE score of 0.65 and a lower quartile of 0.6. This outperforms the lower quartile score of 0.3 obtained by the reference model, S-GR.loc.U, and demonstrates comparable performance to the reference model S-GRNN.loc.U. Despite observing a slight decline in the lower quartile score during temporal validation in comparison to S-GR.reg.NN, the pair of neural networks framework consistently achieves a median and an upper quartile exceeding 0.84 which is the highest score in temporal validation (see also SI, Figure S3 for similar results obtained in terms of continuous Kling–Gupta efficiency (KGE)). This highlights the robustness of the hybrid methods, both spatially and temporally, along with their performance.

Moreover, Table 1 describes the capability of the models to reproduce the peak flow of selected flood events. Figures S4 to S6 in SI show the distribution of relative errors for additional flood signatures using the segmentation and signature algorithm of Huynh, Garambois, Colleoni, and Javelle (2023). The use of neural networks for regionalization ($\phi_1$) or process parameterization ($\phi_2$) leads to similar or improved median representation of those flood signatures compared to baseline model and uniform calibration (S-GR.regU) over the calibration period at pseudo-ungauged locations. Interestingly, the learnable approach S-GRNN.reg.NN that uses both $\phi_1$ and $\phi_2$, results in systematically improved representation, in median and average, of all flood signatures in calibration, spatial validation and temporal validation. This highlights the strength of the proposed framework, and in particular its pertinence for flood modeling with spatio-temporal extrapolation capabilities.
Figure 2. Performance in simulating discharges of different methods, hybrid models with process parameterization pipeline $\phi_1$ in darker colors (S-GRNN), with regionalization pipeline $\phi_2$ in different shades of pink (reg.NN). (a) Boxplot of NSE scores computed over the full time series across gauged and pseudo-ungauged catchments in calibration (number of catchments in parenthesis), spatial validation, and temporal validation for four regionalization methods (reg), alongside a reference obtained from two locally calibrated methods (loc). (b) Simulated and observed discharges from four regionalization methods at a pseudo-ungauged station (i.e., in spatial validation).

Table 1. Median (and average) relative error of peak flow over numerous selected flood events for calibration, spatial validation, and temporal validation.

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<tbody>
<tr>
<td>Calibration</td>
<td>0.65 (0.61)</td>
<td>0.31 (0.34)</td>
<td>0.64 (0.58)</td>
<td>0.26 (0.28)</td>
</tr>
<tr>
<td>Spatial Validation</td>
<td>0.62 (0.61)</td>
<td>0.61 (0.58)</td>
<td>0.52 (0.57)</td>
<td>0.41 (0.39)</td>
</tr>
<tr>
<td>Temporal Validation</td>
<td>0.64 (0.62)</td>
<td>0.32 (0.36)</td>
<td>0.37 (0.4)</td>
<td>0.31 (0.39)</td>
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3.2 Towards Learning Hydrological Behaviors

In this sub-section, we aim to analyze the hydrological behaviors learned by the hybrid models with ANNs. Physically interpretable properties of the learnable modeling approach can be explored by analyzing the behavior of internal states and conceptual hydrological parameters, as represented in Figures 3 and 4.

Figure 3a suggests that the spatially averaged states $h_p$ and $h_t$ reveal two distinct behaviors between lumped regionalization reg.U models (blue lines) and hybrid regionalization reg.NN models (pink lines). For production reservoir state, reg.NN models show relatively low and smooth saturation responses to rainfall events, in contrast to reg.U models that produce higher and sharper responses, while an inverted hydrological behavior is observed in the transfer reservoir. This somehow results in equivalent effective behaviors at the end of the transfer branch $Q_{ft}(x, t)$. These behaviors can be explained by the functioning point, in terms of conceptual parameters values reached through training process, as shown in Figure 3b. The spatially averaged production reservoir capacity $c_p$ of S-GRNN.reg.NN (respectively S-GR.reg.NN) is 514.9 mm (respectively
1264.7 mm), whereas lower production reservoir capacities of 115.1 mm and 39.9 mm are observed in the lumped regionalization methods S-GR.reg.U and S-GRNN.reg.U, respectively. Notably, it is unsurprising that the transfer reservoir capacity $c_t$ of reg.U models is relatively higher than that of reg.NN models. This discrepancy can be attributed to the minimal damping effect of local rain signal in reg.U models, a consequence of their lower production capacity. Interestingly, the reg.NN models yield kinematic wave routing parameters that are comparable between both models (e.g., with spatial averages of 6.4 versus 5.6 for $a_{kw}$). In contrast, reg.U models reach distinct optimized values for these parameters. Finally, the learning process enables to modify the production and transfer dynamics, with interpretable conceptual parameters and fluxes, of this hourly hydrological model applied to flash floods.

Figure 3. Interpretation of the calibrated model states and parameters for different methods. (a) Temporal variation of spatially averaged normalized production ($\bar{h}_p/c_p(x,t)$) and transfer ($\bar{h}_t/c_t(x,t)$) reservoir states. (b) Estimated conceptual parameter maps $\theta(x) = (c_p(x), c_t(x), k_{exc}(x), a_{kw}(x), b_{kw}(x))^T$, each calibrated parameter is denoted $\theta$, with $\mu$ and $\sigma$ its spatial average and standard deviation, $\theta_0$ the initial value before optimization.

Figure 4 depicts the versatile nature of the learnable hybrid models (S-GRNN) in comparison to the classical conceptual models (S-GR) for correcting internal fluxes and vividly illustrates the learned non-linear relationship between internal fluxes and states. The model response surface obtained with the learned flux corrector neural network $\phi_1$ is depicted for the production reservoir. Interestingly, this learned flux correction $f_{q,1}$, regardless of the level of production state (i.e., $h_p = 0.02, 0.2$, and $0.6$), is non-linear and decreasing as a function of increasing intensity of neutralized rainfall $P_n$ (Figure 4a). Compared to the uncorrected infiltrating rainfall $P_s$ that would be used with the classical GR operator (second row of Figure 4a), the corrected flux $f_{q,1} \times P_s$ with the hybrid S-GRNN structure shows a non-monotonic behavior with respect to neutralized rainfall $P_n$. This behavior leads to favoring the transfer of water through the direct runoff flux $P_n - f_{q,1} \times P_s$ rather than through the production store when $P_n$ increases (see GR schematics in Figure 1 and equations in SI). This somehow corresponds to an hortonian or infiltration flux capacity exceedance mechanism that can occur during flash floods triggered by high intensity rainfall (cf. Douinot et al. (2018)), but which is not well represented by the classical GR model, especially in dry conditions (cf. Astagneau et al. (2021)), i.e., with a low level of $h_p$. Therefore, these interpretations illustrate the physical learning capability of the MLPM-PR framework and provide valuable insights into the adaptability and nuanced behavior of the hybrid model, particularly when subjected to diverse spatial and temporal validation scenarios.

Following the proposed spatially distributed MLPM-PR framework, further research could study the modeling-learning of net rainfall production and repartition between rapid and slow lateral flow components (e.g., Douinot et al. (2018); Astagneau et al. (2022) and references therein), along with improving the representation of soil moisture, actual evaporation and groundwater exchanges.
Figure 4. Hydrological interpretation of the non-linear response surface obtained with the learned flux corrector neural network for the production reservoir, plotted here with $c_p = 50$ mm and $E_n = 0.5$ mm. (a) Correction $f_{q,1}$ of the internal flux of the original infiltrating rainfall $P_s$ into the production reservoir, uncorrected flux $P_s$ and corrected flux $f_{q,1}P_s$, as a function of neutralized rainfall $P_n$. (b) Response surface of infiltrating rainfall $P_s$ and corrected one $f_{q,1}P_s$ as a function of production state $h_p$ and neutralized rainfall $P_n$.

4 Conclusions and Perspectives

This article introduced a novel Multiscale Learnable Physical Modeling and Parameter Regionalization (MLPM-PR) framework, that incorporates a pair of neural networks to infer internal fluxes and conceptual parameters into a differentiable and gridded hydrological model, all encapsulated within a VDA algorithm. The numerical results over a complex flash flood-prone regionalization, highlight the superiority of the hybrid models, not only in terms of performance scores in both calibration and validation at gauged and pseudo-ungauged stations, but also in producing physically interpretable results of potentially improved simulated hydrological behavior.

The proposed approach, relying on process-based equations hybridized with ANNs, enables to obtain interpretable spatially distributed hydrological models, contrarily to pure machine learning approaches, while taking advantage of non-linear and multi-resolution effects of neural networks. Accordingly, MLPM-PR is applicable to any other differentiable hydrological, hydraulic or geophysical model, on structured or unstructured meshes.

Future work aims to enhance the MLPM-PR framework by incorporating (i) LSTM networks to learn multi-frequent temporal dependencies from various physical data and better inform model components, (ii) the mathematical properties and response of universal differential equations sets for flexible hydrological modeling in time and space, and (iii) coupling with differentiable river network hydraulic modeling to perform information feedback by assimilation of hydraulic observables (Pujol et al., 2022), such as the unprecedented hydraulic visibility (Garambois et al., 2017) brought by SWOT (Surface Water and Ocean Topography) and multi-satellite data (e.g., with VDA in Pujol et al. (2020); Malou et al. (2021)), enabling the efficient fusion of machine learning with process-based modeling to advance the discovery of scale-relevant hydrological laws.
Open Research

Data Availability Statement. The dataset, Version 0.1.0, that supports this study comprise preprocessed data sourced from SCHAPI-DGPR and Météo-France, and available at https://doi.org/10.5281/zenodo.8219627 (Huynh, Colleoni, & Demargne, 2023).

Software Availability Statement. The proposed algorithms in the study were implemented into the SMASH source code, Version 1.1.0-beta, which is preserved at https://doi.org/10.5281/zenodo.10469390 (Colleoni & Huynh, 2024), available via GNU-3 license and developed openly at https://github.com/DassHydro/smash.

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Pierre-André Garambois greatly acknowledges Pierre Brasseur from CNRS-IGE Grenoble for a fruitful discussion and a remark on “no directly exploitable first principles in hydrology and avenue for data assimilation and machine learning”. This work was supported by funding from SCHAPI-DGPR, ANR grant ANR-21-CE04-0021-01 (MUFFINS project, “Multiscale Flood Forecasting with INnovating Solutions”, https://muffins-anr-project.hub.inrae.fr), and NEPTUNE European project DG-ECO.

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Supporting Information for "Multiscale Learnable Physical Modeling and Data Assimilation Framework: Application to High-Resolution Regionalized Hydrological Simulation of Flash Floods"

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2. Figures S1 to S6

Introduction

The supporting information includes mathematical details concerning the complete forward model $\mathcal{M} = \mathcal{M}_{rr}(\cdot, \phi(\cdot))$ presented in the main article (Text S1 to S3), information regarding the model setup and watershed study (Text S4, Figures S1 and S2), and supplementary results on the learning performance (Figures S3 to S6).
Text S1. Notations

- Surface discharge: $Q(x, t) \in \mathbb{R}^N$, where $N = N_x \times N_t$ with $N_x$ the number of cells in the 2D spatial domain $\Omega \in \mathbb{R}^2$ and $N_t$ the number of simulation time steps in $[0, T]$;

- Internal states: $h = (h_1(x, t), ..., h_{N_h}(x, t)) \in \mathbb{R}^{N_x \times N_h}$ with $N_h$ the number of distinct state variables;

- Internal fluxes: $q = (q_1(x, t), ..., q_{N_q}(x, t)) \in \mathbb{R}^{N_x \times N_q}$ with $N_q$ the number of distinct flux variables;

- Atmospheric forcings: $I = (I_1(x, t), ..., I_{N_I}(x, t)) \in \mathbb{R}^{N_x \times N_I}$ with $N_I$ the number of distinct forcings;

- Physical descriptors: $D = (D_1(x), ..., D_{N_D}(x)) \in \mathbb{R}^{N_x \times N_D}$ with $N_D$ the number of distinct descriptors;

- Model parameters: $\theta = (\theta_1(x), ..., \theta_{N_\theta}(x)) \in \mathbb{R}^{N_x \times N_\theta}$ with $N_\theta$ the number of distinct model parameters;

- Model initial states: $h_0 = h(x, t = 0)$.

In this study, we investigate a hydrological model structure comprising the following model parameters and internal states:

- $c_i$: capacity of interception reservoir [mm];

- $c_p$: capacity of production reservoir [mm];

- $c_t$: capacity of transfer reservoir [mm];

- $k_{exc}$: non-conservative water exchange flux [mm/h];

- $a_{kw}$: first kinematic wave routing parameter;

- $b_{kw}$: second kinematic wave routing parameter;
• $h_i$: interception reservoir state [mm];
• $h_p$: production reservoir state [mm];
• $h_t$: transfer reservoir state [mm].

Text S2. Learnable Parameterization-Regionalization operator $\phi$

The LPR operator $\phi$ is composed of two neural networks, which are the parameterization network $\phi_1$ and regionalization network $\phi_2$.

The first one seeks to determine a spatio-temporal correction $f_q$ for the internal fluxes $q$ using neutralized rainfall and evapotranspiration $\mathbf{I}_n = (P_n, E_n)$, along with production and transfer states at previous time step $\mathbf{h} = (h_p, h_t)$:

$$f_q(x, t) = \phi_1([P_n, E_n](x, t), [h_p, h_t](x, t - 1); \rho_1)$$

where $\rho_1$ is the parameter vector to be optimized for $\phi_1$.

The output $f_q(x, t) = (f_{q,1}(x, t), f_{q,2}(x, t), f_{q,3}(x, t), f_{q,4}(x, t))^T$ will be applied as multiplicative factors to the GR operators internal fluxes as detailed in S3.

Here, the neural network $\phi_1$ is configured as a multilayer perceptron with two hidden layers (consisting of 32 and 16 neurons, respectively), a Leaky ReLU activation function between hidden layers, and a modified Softmax function in the output layer that is bounded from 0 to 2. The modified Softmax function is used to constrain the fluxes corrector. The total number of trainable parameters of $\phi_1$ is $N_{\rho_1} = 756$.

The second estimates the spatially distributed model parameters $\theta$ from physical descriptors $\mathbf{D} = (d_{i,i=1,7})^T$ (refer to Figure S2 for information on input descriptors):

$$\theta(x) = \phi_2([d_1, ..., d_7](x); \rho_2)$$

where $\rho_2$ is the parameter vector to be optimized for $\phi_2$. 
The output $\theta(x) = (c_p(x), c_i(x), k_{exc}(x), a_{kw}(x), b_{kw}(x))^T$ is composed of conceptual model parameters as detailed in S3.

Here, the neural network $\phi_2$ is a multilayer perceptron with three hidden layers consisting of 96, 48 and 16 neurons, respectively. ReLU activation functions are used between hidden layers, while the Sigmoid function is applied in the output layer and followed by a scaling function to constrain the model parameters in accordance with their boundary conditions.

The total number of trainable parameters of $\phi_2$ is $N_{\rho_2} = 6276$.

**Text S3. Differentiable, gridded rainfall-runoff operator $\mathcal{M}_{rr}$**

For a given cell $x \in \Omega$ and time step $t > 0$, $P(t)$ and $E(t)$ represent the local precipitation and potential evapotranspiration, respectively. The fluxes and states are computed as follows.

**Interception** (from Ficchi, Perrin, and Andréassian (2019)):

- Evapotranspiration from the interception reservoir: $E_i(t) = \min[E(t), P(t) + h_i(t - 1)]$;
- Remaining rainfall: $P_n(t) = \max[0, P(t) + h_i(t - 1) - c_i - E_i(t)]$;
- Remaining evapotranspiration: $E_n(t) = E(t) - E_i(t)$;
- Update of interception reservoir state: $h_i(t) = h_i(t - 1) + P(t) - E_i(t) - P_n(t)$.

**Production** (refined from Perrin, Michel, and Andréassian (2003) with neural network flux correction). The first order ordinary differential equation (ODE) describing the GR production store without percolation is:

$$\frac{dh_p}{dt} = \left(1 - \left(\frac{h_p}{c_p}\right)^2\right) p_n - \frac{h_p}{c_p} \left(2 - \frac{h_p}{c_p}\right) e_n$$
Assuming that instantaneous rainfall $p_n$ and evaporation $e_n$ are constant over a constant integration time step, one can obtain an analytical solution of infiltrating rainfall and actual evapotranspiration fluxes as follows.

- **Infiltrating rainfall flux:** $P_s(t) = c_p \left( 1 - \left( \frac{h_p(t-1)}{c_p} \right)^2 \right) \frac{\tanh \left( \frac{p_n(t)}{cp} \right)}{1 + \left( \frac{h_p(t-1)}{c_p} \right) \tanh \left( \frac{p_n(t)}{cp} \right)}$ (analytical solution from stepwise approximation of $P_n$);

- **Actual evapotranspiration flux:** $E_s(t) = h_p(t-1) \left( 2 - \frac{h_p(t-1)}{c_p} \right) \frac{\tanh \left( \frac{e_n(t)}{cp} \right)}{1 + \left( 1 - \frac{h_p(t-1)}{c_p} \right) \tanh \left( \frac{e_n(t)}{cp} \right)}$ (analytical solution from stepwise approximation of $E_n$);

- **Direct runoff flux:** $P_r(t) = P_n(t) - f_{q,1} \times P_s(t)$;

- **Update of production reservoir state:** $h_p(t) = h_p(t-1) + f_{q,1} \times P_s(t) - f_{q,2} \times E_s(t)$.

**Transfer** (adapted and refined from Perrin et al. (2003) with neural network flux correction).

- **Non-conservative exchange flux:** $F(t) = k_{exc} \times \left( \frac{h_t(t-1)}{c_t} \right)^{7/2}$;

- **Initial transfer reservoir state:** $h_t(t^*) = \max [\epsilon, h_t(t-1) + 0.9 f_{q,3} \times P_r(t) + f_{q,4} \times F(t)]$ with $\epsilon > 0$, a fixed small constant;

The transfer reservoir is described with a first order ODE with a power law leakage source term:

$$\frac{dh_t}{dt} + c_t h_t^5 = \left( \frac{h_p}{c_p} \right)^2 p_n$$

Again, assuming that instantaneous rainfall $p_n$ is constant over a constant integration time step, one can obtain an analytical solution of outflow flux from this transfer reservoir.

- **Outflow flux from transfer reservoir:** $Q_{ft}(t) = h_t(t^*) - \left( h_t(t^*)^{-4} + c_t^{-4} \right)^{-1/4}$;

- **Update of transfer reservoir state:** $h_t(t) = h_t(t^*) - Q_{ft}(t)$;

- **Outflow from direct runoff:** $Q_d(t) = \max [0, 0.1 f_{q,3} \times P_r(t) + f_{q,4} \times F(t)]$;
Total outflow: \( Q_{\text{lat}}(t) = Q_{ft}(t) + Q_d(t) \).

**Kinematic wave routing** (adapted from Te Chow, Maidment, and Mays (1988)):

This routing module is based on a conceptual 1D kinematic wave model that is numerically solved with a linearized implicit numerical scheme (Te Chow et al., 1988). The discharge routing problem is classically reduced to a 1D problem by considering a 8 direction (“D8”) drainage plan \( D_\Omega(x) \), obtained by terrain digital elevation model processing with the condition that a unique pixel has the highest drained area.

The kinematic wave model is obtained by simplifying the 1D Saint-Venant equations assuming that the momentum reduces to flow friction slope equal bottom slope. Using a conceptual parameterization of the momentum \( A = a_{kw}Q^{b_{kw}} \), with \( A \) the flow cross sectional area, \( Q \) the discharge, \( a_{kw} \) and \( b_{kw} \) two constants to be estimated, and injecting it into the mass equation \( \partial t A + \partial x Q = Q_{\text{lat}} \), with \( Q_{\text{lat}} \) the lateral discharge (total runoff produced at a pixel from GR operators presented above), a one equation model is obtained:

\[
\frac{\partial Q}{\partial t} + \frac{1}{a_{kw}b_{kw}} Q^{(1-b_{kw})} \frac{\partial Q}{\partial x} = \frac{1}{a_{kw}b_{kw}} Q_{\text{lat}} Q^{(1-b_{kw})}
\]

This model is expressed as follows in order to be discretized with a finite difference approach (Te Chow et al., 1988):

\[
\partial x Q + a_{kw}b_{kw} Q^{(b_{kw}-1)} \partial t Q = Q_{\text{lat}}
\]

Given \( N_u \) adjacent upstream cells within \( \Omega \) flowing into cell \( x \) as imposed by flow direction map \( D_\Omega \), the upstream runoff is:

\[
Q_u(x, t) = \sum_{k=1}^{N_u} Q(k, t)
\]
Then, the numerical solution of the simplified mass equation by a finite difference approach, using a linearized implicit scheme (Te Chow et al., 1988), is:

$$Q(t) = \frac{\Delta_t}{\Delta x} Q_u(t) + a_{kw} b_{kw} Q(t - 1) \left( \frac{Q(t-1)+Q_u(t)}{2} \right)^{b_{kw}-1} + \frac{\Delta_t}{\Delta x} \frac{Q_{lat}(t-1)+Q_{lat}(t)}{2}$$

**Text S4. Model setup**

The study zone in the Eastern Mediterranean region features 9 gauged catchments that are used for calibration while 6 others are considered as pseudo-ungauged for validation of spatial extrapolation capabilities (regionalization) (Figure S1). The SMASH model is run on a $dx = 1$ km spatial grid at $dt = 1$ h time step, i.e., at the same resolution as rainfall data. The model is forced by: (i) observed rainfall grids based on hourly ANTILOPE J+1 radar-gauge rainfall reanalysis from Météo-France (Champeaux et al., 2009); (ii) potential evapotranspiration (PET) estimated using the formula of (Oudin et al., 2005); and (iii) temperature data from SAFRAN reanalysis produced by Météo-France on a $8 \times 8$ km$^2$ spatial grid (Quintana-Seguí et al., 2008) downscaled to a $1 \times 1$ km$^2$ spatial grid. The model initial state $h_0$ is not calibrated here and simply set such that relative saturation of production and transfer reservoir is 0.5. Discharge data at gauges over the calibration period P1 (August 2009 to July 2013) and the validation period P2 (August 2013 to July 2016) are obtained from preprocessed data sourced from SCHAPI-DGPR. Seven spatially distributed physical descriptors (Figure S2), resampled at $dx = 1$ km on the model grid, are considered as input for the regionalization algorithm, i.e., as input of the neural network $\phi_2$. 
Figure S1. Study zone located in the Southeast region of France, comprising multiple gauges downstream of both nested and independent catchments. The gauged catchments (highlighted in red) are used for multi-site calibration, whereas the pseudo-ungauged catchments (highlighted in blue) serve for spatial validation. The selection of catchments is based on the availability of extensive time series with high-quality observed flow and minimal anthropogenic impacts. Nine gauged catchments are employed for calibration, with an additional six considered pseudo-ungauged for spatial validation. This area presents a challenging modeling case due to diverse hydrological properties, such as steep topography and highly heterogeneous soils and bedrock. The region is susceptible to intense rainfall, leading to nonlinear flash flood responses, and is characterized by a significant proportion of karstic zones.
Figure S2. Maps of physical descriptors in the study area, including various types such as topography, morphology, land use, and hydrogeology. A set of seven descriptors at 0.01° in the WGS 84 projection is used as inputs for the regionalization mapping \( \phi_2 \), consisting of: \( d_1 \) the local slope (in degrees) from the Copernicus database (version of 2016) and preprocessed by Odry (2017); \( d_2 \) the drainage density from Organde et al. (2013); \( d_3 \) the percentage of basin area in karst zone from Caruso et al. (2013); \( d_4 \) the forest cover rate and \( d_5 \) the urban cover rate both from the Corine Land Cover database (version of 2012); \( d_6 \) the potential available water reserve (in mm) from Poncelet (2016); \( d_7 \) the high storage capacity basin rate from Finke et al. (1998). Before the optimization process, all descriptors are standardized between 0 and 1 using min-max scaling.
Figure S3. Boxplot of KGE scores computed over the full time series across gauged and pseudo-ungauged catchments in calibration (number of catchments in parenthesis), spatial validation, and temporal validation for four regionalization methods (reg), alongside a reference obtained from two locally calibrated methods (loc). The comparison assesses the performance in simulating discharges of different methods, hybrid models with process parameterization pipeline $\phi_1$ in darker colors (S-GRNN), with regionalization pipeline $\phi_2$ in different shades of pink (reg.NN).
Figure S4. Distribution over 161 flood events of relative error, with an optimal value of 0, for four flood event signatures (Ebf - base flow, Eff - flood flow, Erc - runoff coefficient, Epf - peak flow). The median, mean, and standard deviation errors are respectively denoted $m$, $\mu$, $\sigma$. The evaluation takes place in gauged catchments during P1 (2009-2013) for calibration.
Figure S5. Distribution over 93 flood events of relative error, with an optimal value of 0, for four flood event signatures (Ebf - base flow, Eff - flood flow, Erc - runoff coefficient, Epf - peak flow). The median, mean, and standard deviation errors are respectively denoted $m$, $\mu$, $\sigma$. The evaluation takes place in pseudo-ungauged catchments during P1 (2009-2013) for spatial validation.
Figure S6. Distribution over 95 flood events of relative error, with an optimal value of 0, for four flood event signatures (Ebf - base flow, Eff - flood flow, Erc - runoff coefficient, Epf - peak flow). The median, mean, and standard deviation errors are respectively denoted $m$, $\mu$, $\sigma$. The evaluation takes place in gauged catchments during P2 (2013-2016) for temporal validation.
References


