Authors' Response to Editors/Reviewers of

Hybrid physics–AI and neural ODE approaches for spatially distributed hydrological modeling

Huynh et al.
GMD,

Dear Editors and Reviewers,

We greatly appreciate your time and effort in reviewing our manuscript.

We sincerely thank the two reviewers for their positive feedback highlighting the timeliness and innovation of our contribution, as well as for their very constructive suggestions, which will help us enhance the manuscript. We fully agree with the reviewers that several details and clarifications on different components of the proposed hybrid framework are needed, including a schematic presentation to better illustrate the compared models and improve clarity for a wider audience.

Responses to other points are provided in a detailed, point-by-point manner below.

Thank you again for your careful and constructive review.

N. N. T. Huynh and P.-A. Garambois, on behalf of the authors.

1. Reviewer 1

1.1. Summary

RC: The manuscript proposes a hybrid physics–AI framework for spatially distributed rainfall–runoff modeling. It builds on a differentiable, continuous state-space GR-type hydrological core with 1D routing based on a D8 drainage scheme, augmented by two neural components: (i) a regionalization network that maps physical descriptors to spatially varying hydrological parameters, and (ii) a flux-correction network that adjusts internal model fluxes using meteorological inputs and prior model states. Because state evolution is governed by ODEs, the flux-correction component is trained jointly with an implicit ODE solver in a neural-ODE fashion. Across case studies, the hybrid configurations deliver more accurate and stable streamflow predictions than the classical GR baseline. Overall, this is a timely and valuable contribution to robust, differentiable coupling of process-based hydrology with machine learning.

AR: Thank you for your positive and encouraging feedback on the timeliness and value of our contribution. We appreciate your recognition of the proposed hybrid physics-AI rframework and its potential impact.

1.2. Major comments

RC: Self-contained presentation and background: The current manuscript would benefit from a concise background on rainfall–runoff modeling (empirical/black-box, conceptual, and distributed approaches; recent ML-based advances and their limitations) to situate the contribution and clarify what is new versus prior work.

AR: Thank you for this suggestion, we will enrich the already existing background on black-box to distributed hydrological approaches, ML-based advances and limitations. This will better highlight the main novelty of our work that lies in its generalizability when integrating NNs into an implicit numerical scheme instead of an algebraic approach (Huynh et al., 2025) to resolve the ODEs, within a hybrid regionalization framework previously developed in Huynh et al. (2024).

RC: High-level system overview: Given the number of interacting components (regionalization network, flux-

correction network, ODE state evolution, PDE/routing), please add a clear schematic that shows data flow for the different configurations listed in Table 1.

AR: Thank you very much for this comment. We will definitely include a schematic view of the models compared in Table 1 to provide a clearer representation of the methods compared.

RC: Roles of the two neural networks and learned quantities: Different parts of the manuscript appear to attribute different parameter sets to the regionalization network. Please make explicit, in one place, which parameters each network predicts or corrects, their units and ranges, and how parameter scaling/normalization is handled to avoid ill-conditioning due to heterogeneous magnitudes.

AR: Thank you for this comment. The two NNs are described in Eq. 3, but the learned quantities and their units were not explicitly detailed as you mentioned. We will include this information in one place (probably a table) in the revised manuscript, along with their ranges and the parameter scaling/normalization approach as suggested.

RC: Notation and naming: Since the two networks serve distinct purposes, consider replacing generic labels (ϕ_1, ϕ_2) with intuitive names.

AR: Thank you for this remark. We agree and will replace the notations (ϕ_1, ϕ_2) with more intuitive names such as $(\phi_{flux}, \phi_{reg})$.

RC: Numerical solver choices and stability: You motivate the implicit ODE solver, which in turn needs Jacobians calculations. Please compare against an explicit solver (e.g., RK methods) in terms of accuracy, stability, computational cost, and training convergence, at least on a representative subset. Also, please report typical Newton–Raphson iteration counts, convergence criteria, and any damping/line-search strategies used to ensure robustness.

AR: Thank you for this insightful comment on the method. In fact, an explicit ODE solver was initially coded and tested in smash. We did not include this solver in the experiments and results for the following reasons:

1. Initial experiments on a simple case study showed significant errors and reduced numerical stability. This finding is consistent with previous studies (e.g., Santos et al. (2018), which employed a lumped state-space GR model—very similar to our GR-like operator distributed model—and Song et al. (2024)). It also aligns with the demonstrations in Clark and Kavetski (2010), which showed that among 8 time stepping methods for 6 hydrological model structures, the implicit Euler method provides a good solution (with a fixed time step in their study and adaptive time steps in Santos' lumped GR model, as we also implement). We will clarify this point in the revised version.

2. For model comparison, we already evaluated 9 configurations. Adding explicit solvers would introduce 6 additional configurations (3 explicit ODE solvers and 3 explicit neural ODE solvers corresponding to the 3 regionalization mappings), which would make the comparison too heavy and distract from the main focus of the paper.

For these reasons, we prefer to keep the focus on the implicit solver, but we agree that other details such as Newton-Raphson iterations, convergence criteria, etc. are important and would be more clearly reported in the revised version.

RC: PDE and differentiability: If the routing/finite-difference step (Eq. 7) is part of the training graph, please clarify whether gradients are backpropagated through the routing solver in addition to the ODE solver, and outline how this is implemented.

AR: Thank you for pointing this out. The routing is chained after the production module, and this complete forward modeling chain is differentiated to obtain the adjoint model enabling to compute cost gradient with respect to high dimensional control parameters (either hydrological ones and/or neural network ones) . This

is one of the original aspects and strength of the proposed spatially distributed modeling framework, which explicitly includes spatialized routing model (here the kinematic wave mdoel which is a hydraulic-based PDE) and hybridization possibility with neural networks adapted to predicitng quantities of a spatilized dynamic model. We will detail this point in the revised manuscript.

RC: Definition of "neutralized" inputs: Please define precisely what is meant by "neutralized" inputs and where this is applied in the pipeline.

AR: Neutralized rainfall or evapotranspiration, corresponds to the neutralization of original rainfall or evapotranspiration by the interception reservoir. This terminology is specific to GR models, as referenced in Perrin et al. (2003) and Santos et al. (2018). We will add this clarification to the revised manuscript.

RC: Closure and derivations: Provide a short derivation or a clear reference for the closure relation in Eq. (6).

AR: Thank you for this comment. The closure relation in Eq. 6, which will be more clear with the foward-inverse model flowchart that will be added, follows a simple flux summation under our GR-like hypothesis at each pixel (detailed algebraic model statement in Colleoni et al. (2025) and smash documentation: `https://smash.recover.inrae.fr/math_num_documentation/forward_structure.html#hydrological-operator-mathcal-m-rr`). We will clarify this in the revised manuscript.

RC: Model capacity and regularization: Specify the architecture sizes (layers, hidden units, activations) for both networks, parameter counts, and any regularization used.

AR: Thank you for this comment. We will add all information related the NN architecture as suggested.

RC: Training strategy: During the pre-calibration phase, have you considered training the regionalization network with the original conceptual model (i.e., without the flux-correction)? Also, how crucial was the pre-calibration to the overall training performance?

AR: Yes, during the pre-calibration phase, we train only the regionalization network (i.e., without the flux-correction). This phase is important to ensure the physical consistency of the model (i.e., meaningful parameter values) before training the flux-correction network. We will clarify this point in the revised manuscript.

2. Reviewer 2

RC: The authors embed a small neural network inside a physically based, gridded rainfall–runoff model and solve the resulting neural ODEs using an implicit Euler/Newton–Raphson scheme. They also learn spatially varying parameters from physical descriptors via MLPs/CNNs. In the Aude basin (France), hybrid models generally calibrate better than classical GR4 variants, and the neural-ODE approach moderates extreme runoff more plausibly during floods.

This research highlights the significance of physics-based deep learning, specifically developing a neural network to estimate fluxes and localized parameters in ODEs. It is innovative enough to be relevant to this journey. In the AI for science field, physics-guided AI is becoming increasingly important because it can be more interpretable and reliable. Additionally, it can significantly enhance the performance of traditional models based solely on physics rules.

To be honest, I am not an expert in the field of river runoff, although I have some knowledge of hybrid modeling. Therefore, for readers like myself, despite an understanding of the overall methodology, I still find it challenging to fully grasp your methods. Additionally, I would find it difficult to accept that calibrating and validating your advanced model solely within limited areas of the Aude Basin is sufficient. It would be preferable to present results from a different location to demonstrate the model's generalizability, unless one-area testing is a standard procedure in runoff modeling. Consequently, I recommend a major revision prior to the acceptance of this paper. The authors should enhance the clarity of their wording, improve the

presentation of results, and include additional validation and calibration tests.

AR: Thank you very much for your positive review and constructive suggestions. We will use them to improve the clarity of our wording and presentation so that the methodology can be more easily understood by a wider audience. The presented case is sufficient to validate the numerical consistency of the algorithm and is suitable for this software-focused journal. The proposed hybrid model formulation was built on the simpler algebraic model structure (analytically integrating the ODE set) and tested over a large sample, as reported in a previous paper. This article focuses on a numerical solver adapted to hybrid ODE systems with neural networks dependent on the model statel—a challenge especially for spatially distributed model operator. While the ODE solver's response unsurprisingly closely matches that of the algebraic model, it entails greater technical challenges and necessitates the novel methodological developments presented here.

Regarding the study area (Aude river basin), we understand your concern about relying on a medium-sized basin ($\approx 5,000\text{km}^2$) to demonstrate our approach. We would like to highlight, however, that our previous studies have already tested related hybrid methods on large datasets: for example, the hybrid regionalization method, HDA-PR, in Huynh et al. (2024) over a study zone covering one-quarter of France and in Colleoni et al. (2025) on the CONUS dataset across the US, and the hybrid flux-correction method for the algebraic GR model structure in Huynh et al. (2025) over 235 French catchments. This technical paper focuses on model development, where the main novelty lies in a solver adapted to ODE including neural networks depending on statge, in the generalizability of the numerical scheme. Therefore, we chose to illustrate the approach on the Aude basin, a medium-sized basin with a multi-catchment setup including 25 catchments, as a representative case study.

We also note that extensive benchmarking of the different hybrid configurations against large-sample datasets requires significant computational effort, especially when integrating into a coupled 1D hydrologic–hydraulic modeling chain. Such benchmarking studies, including comparisons with purely physics-based and purely ML approaches, are already planned and will be carried out in the near future.

2.1. Major comments

RC: As a paper on hybrid modeling, the authors should first present the general problem with a clear governing equation. Then, explicitly show what the neural networks are doing, using clear subscripts for terms predicted by NNs, such as "QNN1" and "QNN2" in this study. Next, clearly demonstrate how the NN-predicted terms are used in the governing equations. Afterwards, show the optimization process and iterations. The authors may reorganize section 2.1 to focus their system on equations (3) and (5), removing the redundant ones, and can follow examples like Brenowitz and Bretherton (2019), Yuval and O'Gorman (2020), and Yuval et al. (2021). The goal is to make this section easier for readers to understand quickly.

AR: Thank you for this comment. Our presentation flow is as follows: Sect. 2.1 introduces the general problem (forward model and governing equations, including NN components), and Sect. 2.2 details the numerical scheme used in Sect. 2.1, with the Jacobian matrix combining NN backpropagation for the Newton–Raphson method, which is one of the key novelties of this work. The flow is organized from a view of physics and hydrological modeling, but we agree that some details on the NN components are not sufficiently reported, as also noted by Reviewer 1. We will therefore enhance the clarity of the method representation in the revised manuscript by adding details on NN architectures, learned outputs, and their physical ranges and units. However, we prefer to keep the notations of the outputs as $\boldsymbol{f}_q$ and $\boldsymbol{\theta}$, since they explicitly represent physical quantities that we aim to learn.

RC: From lines 84 to 91, what are the differences between GR4 and ODE? In their first appearance, it seems like GR4 functions like the host model. But later, it is all about NODE. However, the author also replaces many processes and parameterizations in GR with neural networks, resulting in GR.MLP and GR.CNN. The authors should be more straightforward about why they introduce both GR4 and ODE simultaneously—are they trying to show that one is better? What implications does that have? The authors should also explain GR4 and ODE more from a physics perspective at the beginning, clearly stating their purposes rather than just

referencing them. It would be helpful to include a diagram to illustrate the workflow of GR.NN, NODE.NN, and their variants.

AR: Thank you for this comment. We confirm that all models evaluated in this work are fundamentally based on the hydrological operators of the classical GR4 model. The difference between models labeled "GR" and those labeled "ODE" lies in the method used to resolve the ODEs of the state update (Eq. 5). While the original GR4 model proposes an algebraic approach (an explicit solution that only exists under specific assumptions), these ODEs can also be solved more generally with a numerical scheme (Santos et al., 2018), which we denote as "ODE" in our notations. When NNs are incorporated into this solver, we obtain a neural ODE, denoted "NODE."
The notation after the dot specifies the type of regionalization mapping used to estimate model parameters, for example, "MLP" in "NODE.MLP." These explanations are already mentioned in the manuscript, but we will rewrite them for greater clarity. As also suggested by Reviewer 1, we will add an additional diagram/flowchart to illustrate the workflow and all 9 model configurations.

RC: Include at least one subsection about neural networks, such as MLPs or CNNs. Most importantly, I still do not know what the input variables are for both NNs. Even though they are not complex neural networks, please write about their basic architecture and hyperparameters. I know some information is already in section 2.3. Please refine it and make it easier to see, such as by adding a small table, rather than hiding it within lines.

AR: Yes, we totally agree with this remark, more details on NN components will be added in the revised version of the manuscript.

RC: Although this paper focuses on hybrid models, comparing them to a pure-ML baseline would be beneficial. If it requires too much work, including references to give readers a concept of the accuracy of pure-ML models in simulating river runoffs would also be valuable.

AR: Thank you for this suggestion. We would first like to emphasize that the scope of this paper is the development of a new and more generic hybrid modeling approach (enabling to solve ODE embedding neural networks depending on states), building upon approaches that we have already rigorously tested on large-sample datasets. Our primary focus here is on resolving mathematical and numerical challenges in hybrid modeling, as well as ensuring physical interpretability, rather than on performance benchmarking.
As mentioned above, a more comprehensive evaluation of model performance (including comparisons with pure ML approaches) on larger datasets has already been planned and will be carried out shortly. We agree that such comparisons are important and appreciate your suggestion, which we will take into account in the design of our upcoming benchmarking study.

RC: The authors have shown the horizontal resolution is 500m or 1km, and a time step of 1 hour. Could they also state how many grid cells are in the region for calibration? Also how much of the GPU/CPU time are used for GRs and NODEs? Will adding the neural net components significantly add to the computational burden of the host model? In Newton iterations, please show the convergence tolerances and the usual iteration steps.

AR: Thank you for this comment. We will add all of these details about the size of the study zone, computational time, convergence criterion, etc. in the revised manuscript.

RC: It is better to add multi-basin tests (at least one contrasting basin) to demonstrate the generalization capability and robustness of the NN parameters and the NODE system.

AR: Thank you for this suggestion. While we agree that testing on multiple contrasting basins can further demonstrate the generalization capability of our methods, we emphasize that the Aude basin test case is already a medium-sized, multi-catchment setup (25 catchments) representing diverse hydrological conditions. We believe that this area provides a sufficiently complex and realistic scenario to demonstrate the proposed algorithms and their methodological innovations, particularly for a software-focused journal like GMD.
As highlighted in previous responses, the primary goal of this paper is the development and rigorous testing of the hybrid modeling framework, including the implicit solver for neural ODE and NN integration, rather

than comprehensive performance benchmarking. Extensive generalization tests across multiple basins and comparisons with pure ML and hybrid approaches are planned and will be addressed in a dedicated follow-up study, which will require significant computational effort, especially when incorporating a coupled 1D hydrologic–hydraulic modeling chain.

RC: Are the physical budgets constrained? For example, water conservation. In the runoff scenario, it would be storage = rainfall – ET – runoff. So, plot the cumulative rainfall – ET – storage – runoff closure and show how the NNs affect them.

AR: Thank you for this remark. The physical constraints are ensured by the ODE system underlying the hydrological model (with reservoir storage), which could be replaced by other physical laws within the proposed framework. Mass conservation using the same model structure—except for the ODE solver, which is one of the key novelties presented here—has been investigated in detail in Huynh et al. (2025) over a large sample. We will clarify this in the revised manuscript.

2.2. Minor comments

AR: We greatly appreciate your detailed minor comments in addition to the major concerns mentioned above. We will address each of these minor comments with a thorough explanation in the revision. Thank you again for your careful and constructive review of our manuscript.

References

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