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HAL Id: hal-03472284

https://imt-mines-ales.hal.science/hal-03472284

Submitted on 9 Dec 2021

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Abstract. Understanding, simulating and forecasting dynamic and nonlinear natural phenomena are necessary in a climate change context and increased sensitivity of societies to natural hazards. Nevertheless, even though powerful computing tools and algorithms have been widely used to understand and to predict natural disasters, these tasks are still challenging for scientists. Indeed, one of the most dangerous natural phenomena, flash floods keep being a challenge for modelers, despite (i) the existence of some effective hydrological simulating tools, and (ii) the increasing availability of descriptive data, especially rainfall and discharge. In particular, on one hand, environmental data contain an important amount of noise leading to additional uncertainties and on the other hand, physically based models strongly depend on assumptions about the behavior of the basin, that is often more variable in space and time than what is modelled. With the objective of applying data assimilation to improve forecasting properties of the physical model, it is necessary to dispose of a differentiable model. In order to mitigate this issue, a hybrid physical and statistical approach is proposed in this study. It was shown in previous works that deep neural networks are able to identify any differentiable function by using the universal approximation property. Deep neural networks are also good candidates to perform the digital twin of the physical model. Thus, three different neural networks models were designed in this study, and each one is implementing a different type of non-linear filter model, in order to achieve the dynamic character of the catchment area (recurrent, feedforward and static models). The study area is located in the Gardon de Sainte-Croix basin (France), which is known for its sudden and violent floods that caused casualties and a lot of damage. The chosen physical-based model is semi distributed conceptual hydrological SOCONT model, RS Minerve (https://www.crealp.ch/down/rsm/install2/archives.html). Neural networks design was done by using a rigorous complexity selection and regularization methods to promote a good generalization. The three models obtained were thus compared. The feed forward model gave the best results on tests events (Nash score=0.98-0.99), making full use of the inputs with previous observed discharges whereas the recurrent model gave interesting results representing satisfactorily the dynamics of the physical model (Nash score=0.8-0.97). The static model, whose inputs contain only rainfall, is less efficient, showing the importance of dynamics in that kind of system (Nash score=0.62-0.84). Beyond data assimilation, these results open paths of inquiry for building digital twins of physical model, allowing also a great reduction of computing time.

1. Introduction

Flash floods are one of the most destructive natural hazards. Southern France, as many Mediterranean regions, has experienced, in the past few years, catastrophic flash flood episodes causing fatalities and damages, that could both increase in a global warming context [1]. Hydrologists have used various models, from traditional mass balance hydrologic models to data-driven statistical models, both applied to various catchments, to solve the forecasting of such phenomena issue. Heterogeneity and intensity of both rainfall and hydro-physical processes, and uncertainty in short-term rainfall forecasts are the main issues encountered by authors. Consequently, models' performance often suffers from uncertainties on past and future rainfall as well as on their parameters, sometimes showing a lack of representativeness. Besides, in the case of physically-based models, calculation time may not be compatible with operational use.

Digital twins, originally proposed for manufacturing industry, is defined as the representation of an object, a process or a closed physical system with an empirical or numerical approach [2]. Some of the challenges of hydrology could be met by this approach, especially concerning calculation time and uncertainties reduction. In this study, we propose to reproduce a physically-based model using artificial neural networks models (ANN). ANN are chosen to identify digital twins due to their universal approximation property, allowing to identify any differentiable function. Moreover, ANNs are known to be relevant for representing nonlinear complex relationships that underlies hydrological responses. Thus, three deep multilayer perceptron inspired by [3, 4] and dedicated to reproduce a previously calibrated physically-based model are evaluated in this study.

In the first section, the study area and the database will be described as well as the physically-based model and the neural networks. Then, the results and performance of both physically-based model calibration and ANN twins will be presented and discussed.

2. Materials and methods

2.1 Study area

The study area is the *Gardon de Sainte-Croix* in *Pont-Ravagers* basin, located in the *Cévennes* range, in Southern France. It covers 47 sq. km and its elevations ranges from 350 to 1100 m.a.s.l., inducing very steep slopes demonstrated in 'figure 1'. As most of the basins of the *Cévennes* range, this basin is known to generate flash floods due to heavy rainfall events that can exceed 500 mm in only one day. These events mainly occur during autumn, after hot and dry summers. Most of the surface of the basin is occupied by a micaschist bedrock and it is mainly covered by forests and natural landscapes.

2.2. Database presentation

The database provided by the local flood forecasting service (SPC Grand Delta) and Météo-France is composed of 6 rain gauges, one temperature station and one hydrometric station at *Pont Ravagers*, each sampled at a 30 minutes' time step from 2002 to 2019. The rain gauges are *Barre-de-Cévennes* (BDC), *Saint-Roman-de-Tousque* (SRDT), *Mialet* (MIA), *Saumane* (SAU), *La-Croix-de-Berthel* (BER), *Sainte-Cécile-d'Andorge* (SCA), and the temperature station is located in *Générargues* (GENE). Descriptive statistics about the database are given in 'table 1'.
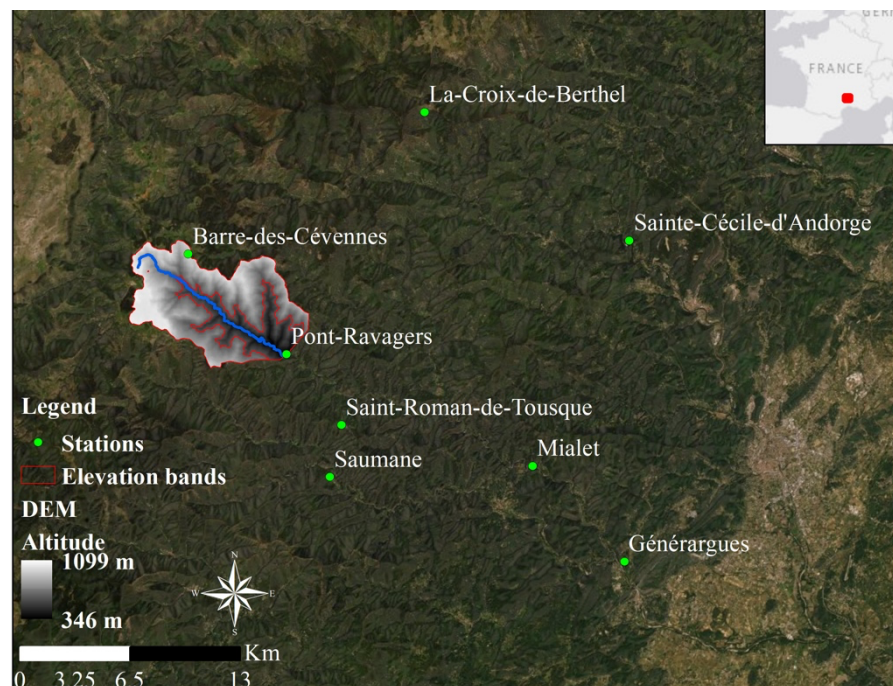
Figure 1. Map of the study area with the meteorological and gauge stations.

Table 1. Descriptive statistics of the database over the 2002 to 2019 period.

	Rainfall [mm]						Temperature [°C]	Discharge [m³s⁻¹]	Specific discharge [m³.s⁻¹.km⁻²]
	BDC	SRDT	MIA	SAU	BER	SCA	GENE	Pont-Ravagers	
Maximum	32	565	79.5	63	43.5	51.5	31	108	2.3
Minimum	0	0	0	0	0	0	-5.1	0	0
Average	0.09	0.08	0.09	0.08	0.09	0.08	14.4	0.79	0.02
Median	0	0	0	0	0	0	14.3	0.32	0.01

This database is dedicated to the calibration of the physically-based model (named hereafter phy-model). From the result of the run of the phy-model over the 17 years' period, we extracted 7 relevant autumns (e.g. including major flood events). This second database is composed of the inputs used by the phy-model (interpolated rainfall and temperature, and calculated evapotranspiration) and of the output that it produces (discharge). This second database is dedicated to the ANN training, test, and validation.

2.3. Physically based model

The SOCONT rainfall-runoff conceptual semi-distributed model, incorporated in the RS Minerve software developed by CREALP [6, 7, 8, 9, 10] have been used to simulate the discharges over 17 years.

The phy-model design requires dividing the basin in elevation bands (300 meters in this study) in order to spatially distribute the rainfall and temperature signals. The SOCONT model is composed of a Snow-SD model [9] that remains mostly unused is this case, due to the rarity of significant snowfall, a GR3 infiltration reservoir model [6, 7], and a SWMM (Storm Water Management Model) surface runoff model [10] as shown in 'figure 2'. The whole model will be called the "RS Model" to ease reading and writing.
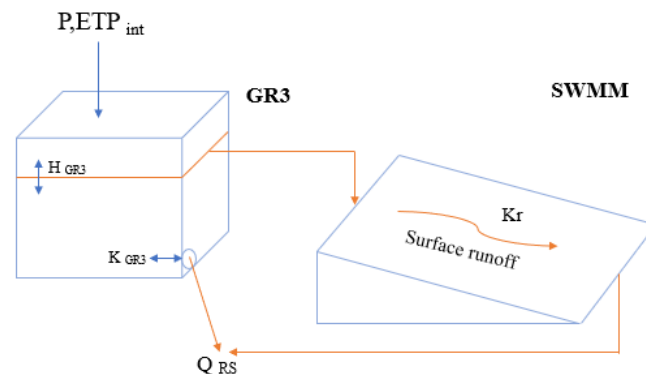
Figure 2. Illustration of phy-model with the main calibrated parameters. P and ETP refer respectively to rainfall and evapotranspiration, HGR3 is the level of water in the soil reservoir, KGR3 is the release coefficient of this reservoir, Kr is the surface roughness of the slopes and QRS is the resulting discharge.

The GR3 model operates as an infiltration reservoir storing water that is driven to the output with a discharge depending on the storage and draining rates. The infiltration reservoir in the GR3 model [8, 9] calculates the base flow while the SWMM model, developed by [8], converts net rainfall intensity into surface runoff over an impervious surface when the reservoir is full. Q_{RS} in 'figure 2' is the total discharge calculated at the basin outlet. The model is fed by virtual stations at the gravity center of each sub-basin (elevation band). These virtual stations interpolate the values from real stations using an inverse distance weighting interpolation combined to elevation gradients. It needs precipitation and temperature and it calculates evapotranspiration using the well-known Turc formula.

The model calibration is performed by adjusting the following parameters:

- H_{GR3} and K_{GR3}, respectively the infiltration reservoir capacity and the water release coefficient of this reservoir for the GR3 part,
- K_r, the Strickler coefficient of the slopes for the SWMM part,
- A precipitation multiplicative coefficient, a temperature additive coefficient and a potential evapotranspiration multiplicative coefficient,
- Precipitation, temperature and potential evapotranspiration gradients.

2.4. Search for a digital twin: deep multi-layer perceptron

The neural networks have the capacity to identify any differentiable function; thus it should be possible to use them to carry out a digital twin of the phy-model. Being themselves differentiable, it will be also possible to implement data assimilation on the digital twin of the phy-model, in order to be able to correct the input variables most prone to uncertainties, using data assimilation. This section describes the realization of the numerical twin of the phy-model [11].

2.4.1. Artificial neural networks models. Artificial neural networks are composed of neurons that are mathematical operators, first calculating their potential (the weighted sum of their inputs) and then their output, by transforming their potential using a nonlinear activation function. Combined in networks, the neurons are of two types: (i) hidden neurons, in hidden layers, whose outputs are not the output of the model and (ii) output neurons, whose outputs are outputs of the model. One of the most common type of neural network is the multilayer perceptron (MLP). It is chosen in this study, due to its two main properties: universal approximation and parsimony. Universal approximation is the ability of the ANN to approximate any differentiable function, with an accuracy depending on the number of hidden neurons [12]. Parsimony defines the need of fewer parameters, compared to linear statistical models [13].

The role of time in modelling a dynamic system is crucial and lead to design different types of architectures, some of them having a dynamic behavior [14]. Three types of models are presented here,

where $y(k)$ is the estimated output at the discrete time k; $\boldsymbol{x}(k)$, the vector of input variables; n, the sliding window width; $y_p(k)$, the observed output at k, ; $\boldsymbol{w}$, the vector of parameters; r, the order:

- The *static model* is considered as a finite impulse response model. It receives only exogenous variables (1). In this type of model, time has no functional role.

$$y(k) = g_{NN}(x(k), \mathbf{x}(k-1) \ldots, \mathbf{x}(k-n+1), \mathbf{w}) \tag{1}$$

- The *recurrent model* differs from static model by having at least one feedback input in addition to the exogenous variables (2). It is thus an infinite impulse response filter, showing a dynamic behavior. This model is recommended if the noise on observed outputs is more important than the noise affecting exogenous inputs [14].

$$y(k) = g_{NN}(y(k-1), \ldots, y(k-r), \mathbf{x}(k), x(k-1) \ldots, \mathbf{x}(k-n+1), \mathbf{w}) \tag{2}$$

- The feed-forward model receives as input the measured value of the outputs at the previous time steps. These inputs play the role of a state variable and allows the model to simulate a dynamic behavior (3) even if the model is static.

$$y(k) = g_{NN}(y_p(k-1), \ldots, y_p(k-r), \mathbf{x}(k), \mathbf{x}(k-1) \ldots, \mathbf{x}(k-n+1), \mathbf{w}) \tag{3}$$

2.4.2. Overfitting and regularization methods. Training consists in calculating the parameter vector that minimizes a cost function on a subset of data called the training set. In this study the cost function is the mean squared error and the Levenberg-Marquardt algorithm is used for training [15].

[16] showed that the training error is an unreliable estimator of the generalization error, and that the difference between both errors increases when the complexity of the model, i.e. the number of free parameters, increases. The design of a neural network model thus consists in defining the optimal complexity of the model that will maximize the generalization performance. This is done by using regularization methods. After the model design, the quality of the model is also evaluated on another subset of the data called the test set, strictly independent of the training set. The test set is used to evaluate the ability of the model to "generalize" to real unseen data.

Three regularization methods are used in this study. First, the cross-validation was proposed by [17] and allows determining the set of optimal inputs and the number of hidden neurons. First proposed by [18] early stopping is another regularization method, controlling the number of "active parameters". It stops the training process before the generalization error increases. To this end, an additional subset, independent of the training and test sets, called the stop set is introduced. Finally, [19] and [20] show that creating an ensemble model, differing only by the parameters' initialization before training, also plays the role of regularization. In this case, the ensemble output at each time step is the median of the ensemble members outputs.

2.4.3. Database. The database devoted to design the neural network twin contains the same variables than the phy-model:

- Inputs consist in interpolated temperatures and precipitations, and calculated evapotranspiration, for three elevation bands (300 to 600 m.a.s.l., 600 to 900 m.a.s.l. and above 900 m.a.s.l.
- The accumulated precipitation is also applied as input. This allows providing an estimation of the soil moisture to the ANN.
- The output is the discharge simulated by the RS model.

The twin database has a smaller duration than the total database in order to specialize the twin-model on floods. It contains 7 autumns, which is the season when flash floods preferentially occur (from September to half of November). Selected autumns contain important and/or numerous flood events. Each of these autumns provides one subset, and the subsets are spread in training, test and stop sets. Five of them are used for training, one for testing and one for stopping.

2.4.4. Model selection. About architecture - Remember that the RS model is a model distributed according to three elevation bands. This concept is transposed to the neural network using three groups of inputs. Each group applies to the model: temperature, rain, cumulated rain and evapotranspiration as in 'figure 3'. Each group feeds a "branch" that calculates a nonlinear combination of its inputs using a deep subnetwork (a multilayer perceptron). Finally, these three branches are connected to a shallow subnetwork (also a multilayer perceptron) providing the output. The model is thus a kind of cascading multilayer perceptrons.

About model selection - The length of the exogenous inputs sliding time windows, n in equations 1, 2, 3, have been set using cross correlations between the considered input (rains, ...) and the output (phy-model discharge), as explained in [20]. They are set respectively to the delay corresponding to the maximum of the cross correlation. The cumulated rainfall is accumulated over the delay corresponding to the memory effect introduced by [21]. This allows providing an information about the previous rains using only one value.

For the feedforward model (eq.3), the length of the time-window related to state inputs (observed discharge at previous times-steps), corresponding to r in eq.3, was selected by cross-validation. For the recurrent model (eq. 2), r was calculated using auto correlation. Nevertheless, as the value of r is very high, feedback inputs were not taken into account directly but using several windows grouping the recurrent values in several time scale, as done in [22]. Each of these windows is connected to a linear neuron before being introduced to the hidden layer in order to diminish the number of parameters and, by this way, the complexity of the model. This contributes to improve de generalization ability of the model.
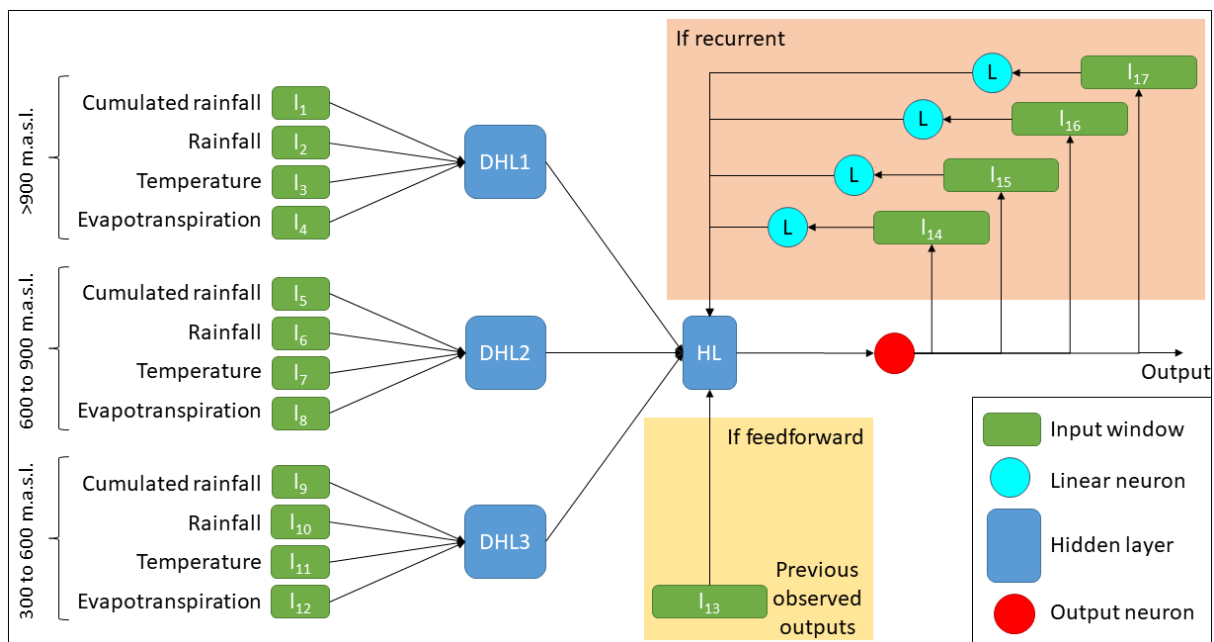

Figure 3. Neural network models. The brown part is added for the recurrent model and the yellow part for the feedforward model. Deep hidden layers are numbered from DHL1 to DHL 3 whereas input windows length are numbered from l_1 to l_{17} in which l_{14} to l_{17} are the order of the recurrent model. HL is for the shallow hidden layer.

As discharges are always positive, the output neuron has a RELU activation function, preventing the model providing negative values. In the hidden layers, sigmoid functions are implemented.

2.5. Performance criteria

Two criteria are used to assess the quality of the models. With the same notations than before and with $\overline{y_p}$ the average of observed values and *n* the number of values of the considered dataset.

- The Nash criterion. It varies between -∞ and 1 where the latter is the best possible value (4).

$$Nash = 1 - \frac{\sum_{k=1}^{k=n}(y(k) - y_p(k))^2}{\sum_{k=1}^{k=n}(y_p(k) - \overline{y_p})^2} \qquad (4)$$

- The relative volume bias. It represents the difference between the estimated water volume and the observed water volume at the outlet (5). 0 is the best possible value. This criterion is more relevant for the RS model, as it explicitly takes into account water volumes transfers.

$$Relative\ volume\ bias = \frac{\sum_{k=1}^{k=n}(y(k) - y_p(k))}{\sum_{k=1}^{k=n} y_p(k)} \qquad (5)$$

3. Results and discussions

3.1 Performance analysis for the phy-model

The simulations over the 17 years' database were not excellent, but convincing enough for a semi distributed physically-based model, for a continuous simulation having to represent hydrological extremes for floods a well as for droughts, on this complex Mediterranean pluvial basin. The Nash criterion is equal to 0.61, which could be considered as low, but do not prevent the identification by the twin model.

Table 2. Quality of hydrological modeling for 2015 autumn episode.

Criteria	Values for 2015	Values for the whole dataset
Nash	0.9	0.61
Relative volume bias	0.84	0

An example of the results over the 2015 autumn is presented in 'figure 4' and the corresponding performance is presented in 'table 2'. In this period including intense events, as for most of the other autumns, the criteria are higher than on the whole dataset. Peaks are reached, which is important for the purpose of the study, but the recessions are reproduced relatively worse.
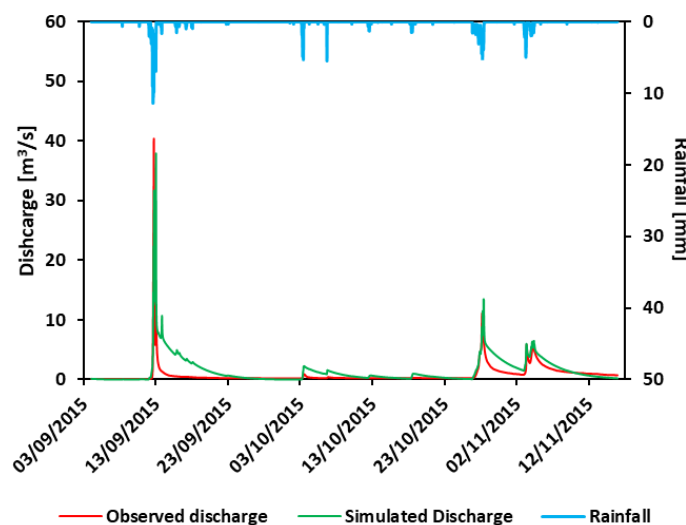

Figure 4. Simulation result of hydrological model for autumn 2015.

3.2 Model selection

The input windows width were selected according to the method described in section 2.4.4. Ensemble models were built with 10 member having different random initializations of parameters. For all hidden layers, the range of cross validation investigation was between 2 to 6 neurons. This thus makes a total of 6,250 cross validation experiences for each type of architecture (static, recurrent, feedforward). The selected models are described in 'table 3', in which elements refer to 'figure 3'.

Table 3. Model selected (elements of the model refer to 'figure 3')

Elements of the model	Static	Recurrent	Feed-forward
Neurons on DHL1	2	2	2
Neurons on DHL2	5	2	2
Neurons on DHL3	3	2	4
Neurons on HL	5	6	4
l_1 Cumulated rainfall higher-band	1	1	1
l_2 Rainfall-higher band	5	5	5
l_3 Temperature higher band	1	1	1
l_4 Evapotranspiration higher band	1	1	1
l_5 Cumulated rainfall medium-band	1	1	1
l_6 Rainfall-medium band	5	5	5
l_7 Temperature medium band	1	1	1
l_8 Evapotranspiration medium band	1	1	1
l_9 Cumulated rainfall lower-band	1	1	1
l_{10} Rainfall-lower band	2	2	2
l_{11} Temperature lower band	1	1	1
l_{12} Evapotranspiration lower band	1	1	1
l_{13} Previous observed outputs	none	none	3
order l_{15} Scale 2-24 ½ hours	none	23	none
order l_{16} Scale 25-54 ½ hours	none	29	none
order l_{17} Scale 55-102 ½ hours	none	102	none

3.3 Simulations

The results are presented in 'figure 5' for autumn 2015 (test set) and for the three models. They show that the feed-forward model simulations are by far the best, followed by the recurrent and the static model simulations.
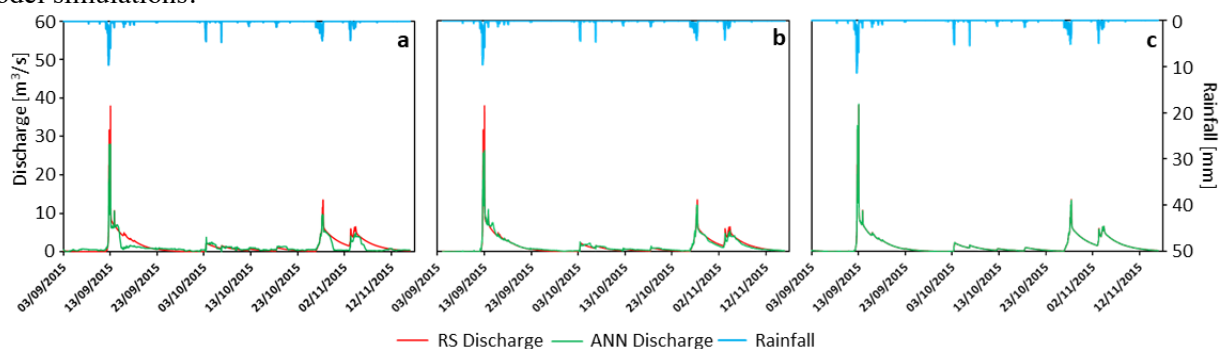

Figure 5. Hydrographs for flood concerning 2015 autumn produced (test set) by static (a), recurrent (b) and feed-forward models (c).

Table 4. Nash scores for all the cross tested episodes.

Season	2002	2003	2006	2011	2015	2016
Static	0.84	0.62	0.84	0.66	0.8	0.82
Recurrent	0.97	0.85	0.89	0.76	0.96	0.80
Feed-forward	0.998	0.993	0.98	0.998	0.999	0.997

Once the model optimized, cross tests have been performed to observe the behavior of the model on other events. Rigorously, another model selection would have been necessary for each new test set to practice these cross tests, but the calculation time would have been very high whereas the scores presented here are very close to the ones of these subsets when they were in cross validation during cross validation stage. The results for all the events in test are presented in 'figure 4'. They show the same increasing values as in 'figure 5' and that the 2011 and 2003 autumns are less accurately modeled.

These results are graphically represented in the scatter plots of 'figure 6'. They confirm the best performance of feedforward and recurrent models. In all cases, on average, the ANN twins tend to slightly underestimate the RS model discharges.
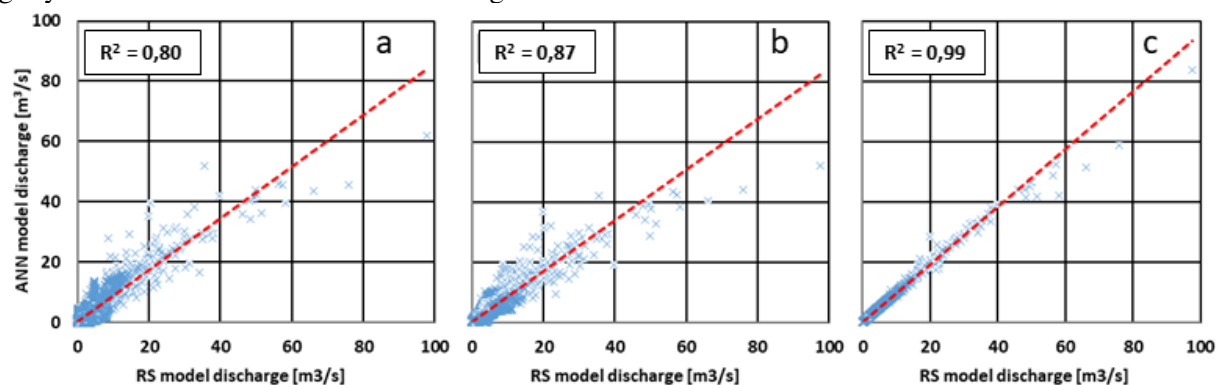

Figure 6. Scatter plots of all the cross-tested events for static (*a*), recurrent (*b*) and feed-forward (*c*) models. The red line shows the linear regression and its determination coefficient is indicated on each plot.

4. Conclusions

Flash floods remain a challenge for modelers but some alternative approaches, as the one developed in this paper, progressively lead to enhance their simulation. Here, we show that using a rigorous model selection, we can reproduce the discharge simulated by a physically based model using ANN digital twins. We also highlight differences between several architectures, which takes into account the role of time in different ways. First, the static model shows poor performance, mainly because it lacks the consideration of the system dynamics, whereas the recurrent model is better. Unsurprisingly, the feed-forward model performs significantly better than the two others and proposes very high-fidelity simulations, probably strongly relying on previous observed values. In the cases explored in this paper, data are free of noise because they come from a physically based model. This will allow using these results in future research to practice data assimilation on rainfall in a free of noise context before implementing it on a real basin. It is thus an important milestone on the path of reducing uncertainties related to inputs.

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