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Reply on RC1

Raphael Kriegmair et al.

Author comment on "Using neural networks to improve simulations in the gray zone" by
Raphael Kriegmair et al., Nonlin. Processes Geophys. Discuss.,
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This article presents an application of a neural net to represent a parametrization of features that are not resolved by a low-resolution numerical model but that can occur at a similar scale than the low-resolution. The method is applied to the forecast of the state of a 1D shallow-water model (height, wind speed, rain mass fraction). The effect of adding a physical constraint is addressed. The article is a valuable contribution to the field of machine learning-based parametrization. It is well written, easy to follow, and the conclusions are convincing and physically interpreted. In my opinion, this work deserves publication. Nevertheless, I have 2 main comments and other secondary comments.

We thank the reviewer for his important comments. These and other reviewer's comments have led to significant changes in the manuscript:

- ***The partition of training/validation data has been changed. All plots are updated accordingly. The main conclusions remain unchanged.***
- ***A new Figure was added showing the trajectory of both nature runs.***
- ***A new section (section 3: Verification methods) was introduced to clarify our verification metrics.***
- ***The bar plots for the single time step predictions (In the new manuscript Figures 4,7 and 8) are displayed differently and contain more information.***

1. about to construction of the datasets and the ANN:

- L90-91: This choice of train/validation split is very surprising. If you select one of every two points in the training, how can you be sure the training/set and the validation set are independent? On the contrary, I would expect that one state on the training is very close to the corresponding step of the validation (one time step further for example). I would be concerned about data leakage that would make you score over the validation dataset overconfident and would be unable to detect overfitting. Can you expand a bit on this choice of train/Val split?

***We agree with reviewer and have changed our experiments accordingly. All the plots have been redone with the new data. The conclusions have not changed.
We write:***

"A time series of $T=200\ 000$ time steps, which is equivalent to approximately 57

days, is generated for both orographies. The first day of the simulation is discarded as spin up, the subsequent 30 days are used for training and the remaining 26 days are used for validation purposes. The decorrelation length scale of the model is roughly 4 hours."

- section 2.2 is there a test set? (see the following point about hyperparameters tuning)
As the learning process of our ANNs does not depend on the validation data (we don't apply any regularization such as early stopping), a test data set is less important. We also did not rigorously tune our ANNs, for which the validation data set would serve as indicator. For example, we did not change the ANN architecture and hyperparameters for our new training/validation data set. We do agree that tuning and regularization could help optimize our ANNs, in which case we would need a test data set. However, optimizing/tuning the ANNs is not the focus of this work, as this is an idealized setup.

- section 2.3 Did you need to tune the hyperparameter of the ANN (e.g. size of layers, learning rate, ...)? If so did you use the validation set or did you use a part of the training set? I think it would be nice to have a bit more details about this point...

\ We did loosely check out sensitivities to the architecture and hyperparameters on both the training data set and validation data set, but detected no strong sensitivities. We did not test the sensitivity to the size of the training data set. Reducing the size of the data set to the minimum required would probably increase the sensitivity to the ANN architecture. However, as argued before, optimizing the efficiency of the ANNs is not the focus of this work. We added the following sentence:

"The ANN architecture and hyperparameters were selected based on a loose tuning procedure, where no strong sensitivities were detected."

2. about physical constraint

- Eq.(1) It seems relatively "easy" to enforce strictly the water mass constraints (just remove uniformly the mean Δh at the last layer of the ANN.). Why not test this hard constraint here? First, it seems more "natural" as the weak constraint, because it is expected that the mass is strictly conserved. Second, results suggest that despite a "strong" mass constraint there is still a mass drift that makes the model diverge (Figure 9).

Good idea. We have actually tried this, but the results were not as good. We believe this is because the ANN corrects at very specific locations (depending on the state of the convection), so taking out the mass violation uniformly would also take out or add mass where the ANN did not correct anything, creating local biases. We also tried spatially splitting the ANN corrections into negative and positive corrections and multiplying the positive (or the negative, depending on the sign of the mass violation) part with the appropriate scalar to remove the total mass violation. Unfortunately this also did not lead to improvements. We added the following in the beginning of section 3.2:

"Instead of including mass conservation in the training process of the ANN, it is natural to first try to correct the mass violation by post processing the ANN corrections. We tested two approaches: homogeneously subtracting the spatial mean of the h corrections, and multiplying the vector of positive (negative) h corrections with the appropriate scalar when the mass violation is positive (negative). Neither of these simple approaches led to improvements. We therefore included mass conservation in a weak sense in the training process of the ANN, as described equation (1)."

Other comments:

- L27-28 "but the resolution of 2-4 km does not give accurate results for typical convective cloud structures are often less than 10 km in size". I am not a native English speaker, but this sentence is a bit unclear to me.

We have rewritten the paragraph to more explicitly the problem of poorly resolved convection in km-scale models, as follows:

"An important example of the gray zone in practice is the simulation of deep convective clouds in kilometer-scale models used operationally for regional weather prediction. The models typically have a horizontal resolution of 2-4 km, which is not sufficient to fully resolve the cumulus clouds with sizes in the range from 1 to 10 km. In these models, the simulated cumulus clouds collapse to a scale proportional to the model grid length, unrealistically becoming smaller and more intense as resolution is increased (Bryan et al., 2003; Wagner et al., 2018). In models with grid lengths over 10 km, the convective clouds are completely subgrid and should be parameterized, while models with resolution under 100 m will accurately reproduce the dynamics of cumulus clouds provided that the turbulent mixing processes are well represented. In the gray zone in between, the performance of the models depends sensitively on resolution and details of the parameterizations that are used (Jeworrek et al., 2019)."

- L71-L72 "In this study, a small but significant model intrinsic drift in the domain mean of u is accounted for by adding a relaxation term." Do you mean there is a systematic drift of u in the model? Is this at all resolutions? When it says "accounted for", does it mean that the drift is corrected?

Yes, there is a systematic drift in the model for both resolutions used in this work. Accounted for indeed means corrected in this case. We substituted "accounted for" by "removed".

- L72, you could say here that the overbar designs the domain average.

Fixed.

- L89 the index of the time t is 'i' but it was 'n' few lines above. This is still correct of course, but I feel that consistency in the notation can make the article even clearer.

Very confusing indeed. We have fixed this.

- Table 1: Is the time step the same for the LR and HR run? Due to CFL, I would expect the time step to be smaller for HR.

Thank you for pointing this out. The output time step (that is, the time step that we save as model output) is the same for both resolutions. However, the modRSW model internally computes a dynamical model time step length at each iteration, taking into account the CFL criterion. We have added the following two sentences in training data generation section:

"The dynamical time step of the model is determined at each iteration based on the Courant–Friedrichs–Lewy (CFL) criterion. To achieve temporally equidistant output states for both resolutions, the time step is truncated accordingly when necessary. "

- L85. it is mentioned that 2 orographies are used, but I don't understand what are the 2 orographies setups here, there seems to be an ensemble of orography. It is a bit clearer in the conclusion, but I think it should also be detailed here.

We describe the generation of the orography in section 2.1 now and modified the text. We also added a Figure (Figure 1) to show the different behavior of the simulations resulting from the two orographies.

" Depending on the orography used, this model yields a range of dynamical organization between regular and chaotic behaviour. Orography is defined as a superposition of cosines with wavenumbers $k = 1/L, \dots, k_{\max}/L$ (L domain length). Amplitudes are given as $A(k) = 1/k$, while phase shifts for each term

are randomly chosen from $[0, L]$. In this work, two realizations of the orography are selected to represent regular and more chaotic dynamical behavior. Figure \ref{fig:00} displays a 24 hour segment of the simulation corresponding to each orography. "

- L118: "...with the standard loss function, the MSE": maybe you could add "($w_{mass}=0$)" here (instead of mentioning it L149)

We rephrased:

"In section 3.1 we first explore the performance of the ANNs trained with the standard MSE as loss function ($w_{mass}=0$ in equation (1))."

- L128: How do you define the LR_ANN simulation? Is it the average of the 25 LR simulations? (Maybe this is what is meant L131, but I am not sure to understand)

To clarify this, we decided to add an entire section (verification methods), where we define more precisely the simulations that we do and how we verify them.

- L130: Initial conditions being selected every 2 hours, do you expect them to be independent? If they are not, that could bias the average and standard deviation.

We expected them to be independent, but 2 hours is indeed somewhat tight. We adjusted our experiments accordingly:

" The 48-hour forecasts are generated from a set of 50 initial conditions ($T_{veri}=50$) taken from the validation data set. To ensure independence, the initial conditions are set 4 hours apart, which is roughly the decorrelation length scale of the model."

- Figure 4: It seems that, after around 20 hours, the dispersion of the RMSE around the mean is greater for LR_{ANN} than for LR . Could you comment on that?

We added the following:

"Also, the SD_{total} of LR_{ANN} is rapidly exceeding that of LR . This is because, in contrast to LR , the shaded region for LR_{ANN} includes the variability due to the ANN realizations which significantly contributes to the total variability. This is seen in Figure 12 and discussed further in the next section. "

- L155-160: Maybe it is worth mentioning that the overall effect of w_{mass} on the RMSE is very low as the improvements are similar (e.g. between 97.55% and 97.70% for h , regular case)

We have rephrased this paragraph. We now say:

"A clear, convincing correlation between the reduction in SME and bias for h and any other field and/or metric is not detected, with possibly the exception of the SME for u in the chaotic case.

A trade-off between increasing RMSE and decreasing MSE for increasing w_{mass} was expected, but is not observed. The RMSE even tends to decrease a minimal amount for the chaotic case."

- Figure 10, that's a really nice point!

- L178 "Based on the subjective interpretation of the human brain of a a hand full of animations of the forecast evolution, it appears that convective events produced in the LR run are wider and shallower". Would it be some theoretical reason or literature to support this assertion?

This behavior is expected since the convergent flow narrows the convective elements until their size is close to the grid length where the collapse is stopped by numerical diffusion. A similar collapse to the grid size is typical of km-scale numerical weather prediction models, as noted in the revised introduction (see response to the first "other comment" above). The sentence at L178 has been rewritten:

"A visual examination of animations of the forecast evolution suggests that convective events produced in the LR run are wider and shallower than in the coarse grained HR run. This behavior mimics the collapse of convective clouds towards the grid length that is typical of km-scale numerical weather prediction models, as noted in the introduction."

- Figure 12: what are the dotted red lines?

We added to the caption:

"The dotted red line are the convection threshold H_c and rain threshold H_r ."

- Figure 12: Is the example taken from the training set/validation set/test set?

From the validation data set. We included this information in the caption.