The eWaterCycle platform for Open and FAIR Hydrological collaboration, Reply to reviewers

We like to thank the reviewers for their time and their kind words describing our work. We are proud that the reviewers agree with us that our work “is a very welcome development to hydrology because computational hydrology suffers from a lack of reproducibility, time “lost” to coding, and a preference for models already used in the research group” (reviewer #1) and is an “interesting and significant advancement in hydrologic modeling” (reviewer #2).

Below we address the comments of the reviewers. We have pasted the original comments in *italics* and our response in regular type. Suggested additions or changes to the manuscript are presented as indented blocks of text.

Comments by reviewer #1

The ewatercycle platform presented in this paper is a very welcome development to hydrology because computational hydrology suffers from a lack of reproducibility, time “lost” to coding, and a preference for models already used in the research group (because this is easiest and not because they are scientifically most appropriate). ewatercycle (partially) addresses these problems and thereby could be a very valuable contribution to hydrological sciences.

The presented paper provides an introduction and overview of ewatercycle, and gives a few examples of how the platform can be used for various experiments. The description there is largely clear. In its current form, the paper seems to be publishable but sharpening the writing may benefit the readers and thereby also the uptake of the platform.

The paper is largely an overview description of the framework, and some examples, without any science being presented. My comments therefore largely focus on how the framework can better serve its users. I hope the authors find these comments useful, and I also invite them to disagree in case they do not think the suggestions will better the paper/framework.

We thank the reviewer for their kind words. The paper has the purpose to give an overview of the framework and we are therefore grateful for the comments, questions and suggestions provided below that we believe will make the paper better.

Main comments.

How does ewatercycle support studies that use multiple (many) catchments at once? The current interface of selecting a catchment seems to be useful for studies of individual catchments, but not really optimal for studying multiple catchments at once (which is common in many hydrological experiments).

In the manuscript we do indeed provide fairly basic examples to show the capabilities of the platform and the reviewer is totally correct in pointing out that most current modeling studies are more complex indeed. The platform fully supports those more complex multi catchment studies. For example co-author Jerom Aerts has studied the impact of different spatial scales in WFLOW over the CAMELS dataset. The typical workflow for those type of studies is to start with an example notebook that already runs the model in question and build from there. We will add the following to the case-study part of the manuscript to make this clear:

> The case studies presented here are chosen to demonstrate the features of the platform in a clear way. They all feature only a single catchment. Current hydrological modeling studies often include many catchments in their analysis. The platform fully supports those more complex studies as is shown in Aerts 2021 where the impact of different spatial resolutions of the same model are studied for 454 catchments from the CAMELS dataset.

In addition, most scientific modeling studies in hydrology will use some other sources of data that are not provided in ewatercycle. How will ewatercycle facilitate such studies and their reproducibility? This would be isotope data, groundwater levels, etc. In addition, the paper talks about ERA-5 and ERA-interim being available as forcing. I understand that such gridded global gridded "data" products are the most convenient to work with, but most published catchment-scale studies will require data from actual observation stations in and around the catchments. How will ewatercycle facilitate such studies? I do not think this is possible with the ESMValTool?

Regarding forcing data: ESMValTool has been developed as a tool to help the geoscientific communities standardize their data. If users of eWaterCycle want to work with additional datasources that are not (yet) available through ESMValTool, they should follow the steps described in the ESMValTool documentation to 'CMOR-ize' their datasets. Station data is supported by the CF-Conventions for NetCDF files that ESMValTool builds upon, see chapter 9 of the CF-conventions (https://cfconventions.org/Data/cf-conventions/cf-conventions-1.9/cf-conventions.html#discrete-sampling-geometries). The EMSValTool community is currently discussing supporting station data. This discussion is available in ESMValtool GitHub issues: https://github.com/ESMValGroup/ESMValTool/issues/1119 , https://github.com/ESMValGroup/ESMValTool/issues/496 , and https://github.com/ESMValGroup/ESMValTool/issues/1655 .

The beautiful thing is that once hydrologist have added their data, their datasets become available as forcing for all models in eWaterCycle. The ESMValTool documentation can be

found here: https://docs.esmvaltool.org/en/latest/input.html. To make this clear to the readership we will add to section 3.4:

> If hydrologists want to work with their own datasources as forcing for their models within the eWaterCycle platform they can follow the steps on the ESMValTool documentation (https://docs.esmvaltool.org/en/latest/input.html) to make their data available. Making their data available for one model, given the way EMSValTool is set up, makes it immediately available for other models as well.

Regarding observations and other data sources: as mentioned in the text of the manuscript: commonly used discharge observations from GRDC and USGS are automatically available through the ewatercycle.observations submodule of the python package. If hydrologists want to add further datasets they can of course import them to their jupyter environment, or dynamically link them if the dataset facilitates that. It is on the user in this case to make sure that any dataset imported is available to other for reproducibility.

ewatercycle ties together many existing components, largely from services provided by others. How does ewatercycle ensure that past simulations are also feasible to repeat in the future (for example when those outside services have been updated, or become unavailable)?

This is an important point to us and one that we have thought long about in the process of designing and building eWaterCycle. For the core of eWaterCycle: the models that we share with the hydrological community, this is solved by using container technology. When a container image is created all dependencies are wrapped inside the container. As long as a container engine remains available, these models will be run-able. By archiving the containers also on a platform that guarantees long term storage like zenodo we hope to maximize the lifespan of those containers. For other parts of the complete system we are indeed dependent on developments from other projects (like ESMValTool). By making sure we always link to specific archived versions of those third party resources we make sure that even if those resources move to a newer, incompatible, version, our platform would still function.

The paper states that "the technologies developed for the eWaterCycle platform are portable to other domains of (geo)science where researchers work with each other's models and datasets". This is an interesting and relevant thought, but to what extent this statement is accurate seems to really depend on the field and the type of data used. In sciences where data is gridded and standardized this seems to be the case, but in sciences that use more soft data, and unique (and less structured) field info for their models the approach seems not to be transferable?

We fully acknowledge that in building eWaterCycle, even though we tried to remain as domain agnostic as possible, we must have inadvertently taken decisions that would make the platform un-usable to some domains of science. The central part of the platform: a jupyter hub environment that runs models in containers through a programming language agnostic remote procedure call method, is portable to other domains. The BMI interface is defined very broadly such that models from widely different fields of science can be linked to each other. As a first

step to test how many hidden assumptions we have taken on board in building eWaterCycle we want to test how easy it is to add groundwater models like MODFLOW.

The examples provided give an indication of how a hydrological model (or more models) are run in various set-ups. I would argue that most hydrological science nowadays (hopefully) goes far beyond running a rainfall-runoff models and comparing observed and simulated hydrographs. How would the ewatercycle platform facilitate modeling studies that go beyond this "simple task". For example:

- *Investigating water age: Harman, C. J. (2015). Timeâ variable transit time distributions and transport: Theory and application to storageâ dependent transport of chloride in a watershed. Water Resources Research, 51(1), 1-30.*
- *Investigating human water interactions: Elshafei, Y., Coletti, J. Z., Sivapalan, M., & Hipsey, M. R. (2015). A model of the socioâ hydrologic dynamics in a semiarid catchment: Isolating feedbacks in the coupled humanâ hydrology system. Water Resources Research, 51(8), 6442-6471.*
- *Coupled water and vegetation dynamics: Kyongho, S., & Tague, C. (2019). A top–down soil moisture and sap flux sampling design of a rain–snow transition mountain watershed. Hydrological Processes, 33(11), 1553-1568.*
- *Coupled hydrology and landscape dynamics: Hancock, G., & Willgoose, G. (2001). The interaction between hydrology and geomorphology in a landscape simulator experiment. Hydrological Processes, 15(1), 115-133.*

The reviewer is absolutely right that most studies are indeed more complicated and involve additional processes or datasources not provided out of the box in eWaterCycle. We would argue that the tools provided in eWatercycle are ideally suited for the studies mentioned above since using ewatercycle takes away part of the (computer / technological) complexity of coupling different models and has done the heavy lifting for the hydrological models used in these studies. Zooming in on Elshafei et al and Hancock et al: BMI is originally built and (thus) ideally suited for coupling different models together into a larger coupled model. By adding a BMI layer to the geomorphological model this study could be (re)done in a way where the experiment and the two coupled models are clearly separate (research) objects. The CSDMS has a collection of models from all over the geosciences on their portal which already include BMI. To emphasize that eWatercycle is able to facilitate research like this we will add the following text to section 4.3:

> While this example shows the coupling of two hydrological models, the eWaterCycle platform facilitates coupling of any models that incorporate a Basic Model Interface (BMI), including those not describing hydrology. Work where hydrological models are connected to, for example, models describing human behavior (Elshafei et al) or geomorphological processes (Hancock et al) can be done using the eWaterCycle platform.

In addition, Hutton and colleagues stated that "some form of code is used to produce the vast majority of hydrological research papers, from data processing and quality analysis [Teegavarapu, 2009; Mcmillan et al., 2012; Coxon et al., 2015], regionalization and large-scale statistical analysis across catchments [Blöschl et al., 2013; Berghuijs et al., 2016],". This part of (still) computational hydrology provides a large part of the hydrological literature, but remains undiscussed in the current manuscript. I understand that eWaterCycle cannot solve all our problems, but I think it would be unfair to say the framework solves the problems raised by Hutton, while it is really at present only a solution for a small subset of computational hydrology.

Proud though we are on what we have built in the eWaterCycle platform, the reviewer is right that our platform does not solve all of the issues that Hutton (2016) raised. We focus on providing a solution that moves us in the right direction for a subset of the hydrological community: those that work with hydrological models to do their work. To clarify this we will change the statement at the end of the manuscript thusly (main changes in **bold)**:

Hutton et al. (2016) argued that computational hydrology can only be a proper science if the hydrological community makes sure that hydrological model studies are executed and presented in a reproducible manner. We replied that to **improve current practices for hydrologists using hydrological models in their work**, hydrologists shouldn't 're-invent the water wheel' but rather use existing technology from other fields, such as containers and the ESMValTool, and open interfaces, such as BMI, to do their computational science (Hut et al., 2017). With this paper and the release of the eWaterCycle platform we are putting our money where our mouth is and provide the hydrological community with a 'FAIR by design' platform to do our science.

At times the paper is rather unspecific about how things are done. The paper for example states "can be easily added to" without specifying how this is done. I would encourage the paper to state how it's done, rather than a vague description that it is easy. This applies to many steps presented in the paper.

We will scrutinize the paper for these issues of vagueness and improve by either explaining or pointing to references to make things more clear.

Abstract:

L2: There is an inconsistency between the "we" in for example, "We replied" (where "we" refers to Hut and 2 colleagues" and the author list of the current manuscript. Please rephrase to avoid confusion.

The reviewer is absolutely right that there is a mismatch between the team behind the platform, who are all co authors on this paper, and the small team that wrote Hut 2017. I find this one hard to change without making the opening sentences of the abstract unreadable but I suggest to change this into:

> Hutton et al. argued that computational hydrology can only be a proper science if the hydrological community makes sure that hydrological model studies are executed and presented in a reproducible manner. Hut, Drost and van de Giesen replied that to achieve this, hydrologists shouldn't 're-invent the water wheel' but rather use existing technology from other fields (such as containersand ESMValTool) and open interfaces (such as BMI) to do their computational science (Hut et al., 2017).

L6: Personally, I would omit: "our"

Agreed that removing our makes this sentence better

L11: "MARRMoT" is not a model, but a set of other existing models?

We will add 'and model suites' after 'models in L10 to make this clear.

L27-31: The main message of this paragraph seems clear, but the wording is rather convoluted and imprecise. Also, do we really understand how water moves through soils locally (See e.g., Evaristo & McDonnell 2015)? Do we really understand how water moves through plants if the sources of this plant water use remain uncertain even at extensively studied sites?

Very valid point that we do also lack knowledge on fundamental processes and are constantly improving our understanding. To make sure the focus of this manuscript stays on the work presented we will change L28 to read:

> We may have adequate descriptions of how water moves through plants and soils at small scales but the medium is never the same from one spot to the next.

And will purposefully leave the definition of 'adequate' to be discussed by the hydrological community in other publications or (preferably) with each other at coffee breaks during conferences.

L33: why the ""? with Beven?*

This is an artifact from our (mis)use of LaTeX and will be fixed in production.

L33: are hydrologists "forced" or do they "choose" to work with effective parameters? (or ignorantly "pick"?).

Will change to "Hydrologist often work with" to avoid this becoming a point of discussion.

The second part of the introduction (section 1) already reads like a description of the Ewatercycle. I do not think this adds to the clarity of the paper, by already integrating that here.

We choose to introduce eWaterCycle at this point so that we can contrast it with other platforms and similar efforts by others in the community starting at L92. We feel that moving the introduction of eWaterCycle further down would make it harder for the readership to read that part of the introduction and understand how we try to position eWaterCycle within that landscape.

Section 1.1. Would the paper benefit from making this a supplement at the end?

Given how much the definition of seemingly simple terms like ‘model’ can change between scientists (Venhuizen 2019) we want to make sure that the readership sees this list before diving into the detailed description of the platform. However, we do agree that providing a long list of definitions in a paper in this way is unconventional. We would like to explicitly ask the handling editor to provide advice on where to put the glossary and will act according to this advice.

L170. If I understand this section correctly, ewatercycle is currently not yet really operational for foreign users. In that case, this needs to be reflected in how the abstract and other key summary parts of the paper are written.

This is understood incorrectly and that is on us for not making this clear enough. The platform can be installed on any machine. The instructions for installation by admins are provided in Verhoeven 2021. To make this clear we will change the text of L169 - 172 into:

> At the time of writing, the eWaterCycle platform is hosted on infrastructure from SURF, the infrastructure provider of the Dutch Academic Community (surf.nl). Anyone collaborating with a Dutch partner can access this infrastructure. This is demonstration infrastructure intended to show the capabilities of the platform. Anyone with a budget on the SURF Research Cloud can start up an instance of eWaterCycle there. Those without access to this resource can install the software of the eWaterCycle platform on their own infrastructure, see Verhoeven 2021 for details. See section 5 for future plans regarding making the platform more broadly accessible to the hydrological community

L388: “of BSc student Thomas Albers” is OK, but I think conventionally we remove such irrelevant clauses (because we do also not include that with any of the other references in the paper).

We added this very deliberately to demonstrate that this type of research, which hitherto would not have fitted in the scope of a BSc thesis project, can now be done within that scope and would therefore suggest to let this one pass.

Figure 9: what is “the MARRMoT model”? In my understanding, MARMMoT is a suite of models.

This is correct and will be changed into “The simplest one-bucket model from the MARRMoT suite of models”

Many figure legends are placed outside the hydrographs. I understand that this is easier, but it gives a lot of whitespaces that seems unnecessary.

All hydrographs in the paper are generated using the ewatercycle.analysis.hydrograph() function from the python package. In building this function we made the design choice to place the legend outside of the main graph area since we can not predict which part of the area will be taken up by data. We agree it would save whitespace in this publication to manually move the legends around, but we chose not to do so to make sure that any figures used in this publication come directly from the platform.

Reviewer #2

This mansucript summarizes an interesting and significant advancement in hydrologic modeling. The e-water cycle platform uses open source, modern tools to provide access to a range of hydroligic models, input datasets and observations for comparison. I have some comments below, but they are only suggestions. I recommend this manuscript be accepted as-is.

We thank the reviewer for their kind words. “I recommend this manuscript be accepted as-is.” made our day when we received the review. We will of course still reply to the points raised.

I thought the discussion of other platforms was helpful. This puts e-water cycle in context with related efforts.

I particularly liked the glossary and careful definition of terms. While many of these terms are not new to the readership of GMD, some of them are, and all these terms are new to someone who is just starting the process of learning to use hydrologic models. Aspects like this for the manuscript (and the platform itself) broaden the scope of this manuscript beyond simply a documentation of the work but also a how-to guide for new users.

In the list of models to be added (line 205+), I'm curious what makes the models listed "different" from the set of models included? Is this a technical difference, or something in the way the equations solved are developed?

There is no fundamental differences between the models already included and those still on our list to be added. This is merely a matter of available time (and associated funding). We see how the use of “these” in L206 is a dangling modifier and causes confusion. We will replace ‘These’ in L206 with ‘The models already in eWaterCycle and those still to be added’

-While by no means a verification of the platform, I did review the website and read the docs for getting started with e-water cycle. The instructions seemed clear and complete. I did notice some platform specific language (e.g. the use of wget instead of curl) that might cause issues for more novice users.

We specifically included all documentation and links to the website with the manuscript for the reviewers and are happy you took the effort to look into these. The platform specific language is a blind spot on our side and we will update it to be more platform inclusive.

-With respect to the explorer (line 157+ / S2.1), I could not find a link to where or how run this part of the platform? Is this hosted somewhere? Something that needs to be installed locally? The explorer concept is very intetesting and I liked the automatic notebook generation concepts, but was left wanted more detail.

We apologize for not making this clear enough. When the platform is installed using the instructions provided in Verhoeven 2021 the explorer is automatically installed as well. The url is the standard entry point (for example https:/<machine>/) for the machine where this is running.

-I'm curious about the limitations of the BMI. Does this require access to the models as a subroutine via python, as a wrapper around the models, or something else? How are the differences in model file structure handled?

BMI is very forgiving for model structure and is defined for many languages, see https://csdms.colorado.edu/wiki/BMI for more details. By using GRPC4BMI we can call any model that has implemented BMI from our python platform. We are currently supporting C/C++, Fortran, R, Octave (Open Source version of MATLAB) and R but can add support for any language that has a gRPC library.