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Interactive comment on "Simulating Coupled Surface-Subsurface Flows with ParFlow v3.5.0: Capabilities, applications, and ongoing developmentof an open-source, massively parallel, integrated hydrologic model" *by* Benjamin N. O. Kuffour et al.

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Response to Anonymous Referee #2 Comments for "Simulating Coupled Surface-Subsurface Flows with ParFlow v3.5.0: Capabilities, applications, and ongoing development of an open-source, massively parallel, integrated hydrologic model"

We would like to thank the Editor and the Anonymous Referee #2 for the comments and suggestions made to improve our manuscript. The original text of the Anonymous

Referee #2 comments are given below with author responses provided with headings "Authors Response".

NB: The responses below were provided by the corresponding author (first author) on behalf of all the co-authors. Additional information may be provided by co-authors.

Anonymous Referee #2 The motivation (and objective) of the paper is stated as (Lines 71-74) : "The purpose of this manuscript is to provide a current review of the functions, capabilities, and ongoing development of one of the open-source integrated models, ParFlow, in a format that is more accessible to a broad audience than a user manual or articles detailing specific applications of the model". I am very familiar with integrated hydrologic models, but not with ParFlow, and I therefore belong to the target audience. However, after very carefully reading the paper (some sections more than once because they could be clearer), I conclude that the paper does not reach its objective and does not provide a clear review of the code's functions, capabilities, and ongoing development. Overall, the organization and writing should be improved to make the text much clearer. Some sections provide too much information on peripheral details and too little on some important points. That is especially the case for the coupling section (section 5), which does not provide a clear picture of the code's capabilities with respect to its coupling with other codes. I provide below more detailed comments on specific sections of the paper.

Title The title is not representative of the content of the paper. With respect to coupling, a good portion of the paper focuses on describing the coupling of ParFlow with other codes. The focus is therefore not so much on coupled surface and subsurface flow as the title suggests. Actually, the surface and subsurface coupling could be described more clearly (see comment below). The capabilities are described but the paper does not provide a clear picture of the applicability limits of the model. The ongoing development is not really addressed. The paper rather lists past developments

Authors Response The applicability of ParFlow has been well discussed in section

6 (Discussion and Summary) highlighting challenging hydrologic projects or research works where ParFlow was employed. For example, the code has been applied to simulate surface and subsurface flows at varying spatial scales i.e. from mouth of continental river basins at high resolutions, evaluate relationship between topography and groundwater flow, assess resilience of water resources and anthropogenic stressors, and simulate atmospheric, surface and subsurface energy and water budgets involving complex parameterization when coupled with other models. The manuscript has been revised to add ongoing development plan in the last paragraph such as incorporation of new formulations of both kinematic and diffusive wave approximations, and advanced parallelization support (GPU'S and heterogeneous compute architectures).

Anonymous Referee #2 Comment Introduction The introduction does not fit with the purpose of the paper, which is to present an overview of ParFlow's capabilities. There are some very broad statements on integrated hydrologic models (IHMs) in the first paragraph that are not really required since the intended audience will likely be already aware of IHMs and will not need to be convinced of their usefulness.

Authors Response We disagree with the referee #2 that our statements on integrated hydrologic models (IHMs) are not needed. Our intended audiences are not only those well-vested or with broader knowledge in numerical or hydrologic modeling but include those looking to learn more about IHMs (e.g. graduate students) of which we want ParFlow to be their choice. We believe it would be useful to such potential code users and readers to know what IHMs do and why ParFlow belongs to that class of simulation platforms.

The second paragraph (lines 75-94) provides a short summary of ParFlow's surface and subsurface flow capabilities. It is somewhat confusing to provide this summary in the introduction since the main goal of the paper is to provide a much broader overview of the code.

Authors Response Generally, ParFlow is an IHM that basically simulates coupled

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Discussion paper

surface-subsurface flow so we could not have completed the introduction of this manuscript without talking about surface-subsurface flow capability of the code. A brief introduction was provided to lead our readers to what is to be discussed in the paper in terms of surface-subsurface flow simulation by ParFlow.

Lines 95-103 provide a list of previous studies but the description of the scale of application is confusing (large domains, small catchments, complex terrain, large watersheds, continental scale. . .). Also, the main conclusions or results of these studies are not mentioned. Just citing papers is not helpful. It would be better to comment on these studies to provide the reader with a clearer understanding of the code's applicability. There are several other instances where a list of ParFlow applications is given, without much detail, (example are lines 132-139, lines 161-163, lines 870-875), which generates repetition.

Authors Response The manuscript has been revised according to the referee #2 suggestions to give numerical evidences to the use of description of the scale of application such as large domains, small catchments, and large watersheds. This is fully exemplified in Table 2 where all of these descriptions are given values of lateral and vertical extents based on the referenced studies.

Section 1.1 on the development history is interesting and relevant (although lines 132-139 can be removed).

Authors Response Section 1.1 gives a general trajectory of the code's development based on periodic modifications and applications enhancing the code's capabilities. Lines 132-139 end the section with brief recount of some of the recent tested additional modifications and applications which were discussed in subsequent sections of the manuscript. So, we view the presentation in those lines very necessary in the manuscript.

Anonymous Referee #2 Comment Core functionality It is not clear why variably-saturated and steady-state saturated modes are identified separately. Equation 1 is the transient variably-saturated flow equation and equation 3 is derived from the same equation by setting the time derivative to zero and both relative permeability and saturation 1.0. Why treat them separately, especially since a common solution method is used (line 148)? I would only present equation 1 to avoid confusion.

Authors Response The two equations (1 and 3) were presented to elaborate the fact that the steady-state saturated flow can be derived from the variably saturated flow. This was done for the purpose of simplification and clarity of the equations.

Lines 179-185 are out of place and probably not necessary. If they are kept, they should go into an introduction. Same comment for lines 293-300.

Authors Response Referee #2 finds lines 179-185 and 293-300 unnecessary and out of place, but we kindly disagree with the referee #2. We found it highly essential to begin each section or subsection with a brief introduction or background to lead our readers into what is it we'd be discussing in the said section of the manuscript. So, we think it is necessary we have such a start in these sections.

The description of the coupling between surface and subsurface (pages 8-9) is confusing and should be clarified. I think that there is two-way coupling in ParFlow but the text suggests that there is only flow from surface to subsurface (see lines 204-206: "To account for vertical flow (into the subsurface from the surface), a formulation that couples the system of equations through a boundary condition at the land surface becomes necessary"). Figure 1 suggests the same one-way flow direction.

Authors Response We agree with the referee #2 that there exists two-way coupling of the surface and subsurface flows in ParFlow. The manuscript has been revised to make that explicit.

It is also not clear if surface and subsurface are coupled everywhere during a simulation or only at limited locations. Section 3.4, which describes the solution for the coupled surface and subsurface flow system, seems to suggest that surface flow is not solved everywhere (although I am not entirely sure because section 3.4 would have to be written more clearly).

Authors Response Surface-subsurface coupling occur everywhere during a simulation.

I do not see the usefulness of section 2.4. There is no evidence that the multiphase flow capabilities are used and the explicit time-weighting scheme used for transport is extremely restrictive for real applications, as well as the absence of dispersion or diffusion. It seems like these options are seldom used.

Authors Response We agree with the referee #2 that the multiphase flow capabilities of ParFlow are seldom used in recent times. However, we provided this functionality of the code to prompt or alert potential code users of the existence of that essential inherent capability of ParFlow.

Anonymous Referee #2 Comment Equation discretization and solvers The writing style is clearer for this section, compared to the rest of the paper, but there are still some inconsistencies. For example, the method used to solve the variably-saturated flow equation is mentioned in 3 different places, but it is not consistent Lines 365-367: for variably saturated subsurface flow, ParFlow does this with the inexact Newton-Krylov method implemented in the KINSOL package Lines 372-373: For variably saturated subsurface flow, ParFlow uses the GMRES Krylov method Lines 409-410: For variably saturated subsurface flow, ParFlow uses the NewtonâĂŘKrylov method coupled with a multigrid preconditioner

Authors Response The different solvers mentioned in section 3.1 are all options in ParFlow capable of solving variably saturated flow equation. The choice of a solver depends on the specific problem(s) being solved, and the code user reserves the right to select which solver to use. For example, for a particular problem, one solver may provide faster convergence compared to the other. In that case, the solver may be the choice of the code user.

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Discussion paper

Similarly, for saturated flow, it is written Lines 415-416: For saturated flow, ParFlow uses the conjugate gradient method also coupled with a multigrid method Lines 430-431: ParFlow uses the multigrid-preconditioned conjugate gradient (CG) solver to solve the groundwater equations under steady-state, and fully saturated flow conditions Either the conjugate gradient method coupled with a multigrid method and the multigrid-preconditioned conjugate gradient represent the same solution method (in which case there is unnecessary repetition) or they are different solution methods (in which case some more information is required).

Authors Response Conjugate gradient method coupled with multigrid method and the multigrid-preconditioned conjugate gradient for saturated flow are different ways of presenting the solver in the performance of its function and not necessarily repetition.

Anonymous Referee #2 Comment Coupling Section 5 on coupling is the section that requires the most careful revision. PF.CLM: It is mentioned that a modified version of CLM was incorporated into ParFlow. There is no clear description of the modified CLM (only some examples of capabilities, as listed starting on line 552). There is also no mention of the differences between the modified CLM and the original CLM published by Dai et al. (2003). Considering the aim of the paper, it would be useful to at least list the main capabilities and types of applications, instead of referring to previous work (lines 566-567). There is a mention of comparison to uncoupled models (line 588) but no identification of what the uncoupled models are. Also, since the modified CLM has been integrated into ParFlow, PF.CLM is not really a coupled model in the same sense as the other coupled models presented in section 5.

Authors Response There is not much of a functional change between the original CLM and the modified version integrated into ParFlow. The difference is that the modified version incorporates subsurface pressure values from ParFlow in select computations. All features or input/output file structure remain functional as in the original CLM. The manuscript has been revised to highlight this difference. It may not be feasible to enlist all the capabilities and application of ParFlow presented in the previous research works in detail. Highlighting essential capabilities and /or applications such as the capability of PF.CLM to predict accurately root-depth soil moisture and referring readers and potential code users to those resources where tested and primary applications are detailed would be useful. The phrase “uncoupled model” simply meant a stand-alone model used in a simulation i.e. performing a simulation with CLM (land surface model) to compute soil moisture content without coupling with other model (ParFlow), then CLM is an uncoupled model in that regard. We have explained this in the revised version of the manuscript.

ParFLowE.CLM : The section mentions that a 3D heat transport equation has been added to ParFlow, which becomes ParFLowE. Since heat transport appears to be a core feature, why is it only mentioned here instead of being presented much earlier in Section 2? Is it because ParFlowE is a different ParFlow? Also, it is really not clear if the CLM used in ParFlowE.CLM is the same as in PF.CLM. Is ParFlowE available to use with the other models listed in Section 5?

Authors Response ParFlowE was not included to section 2 because it is a modification made to ParFlow for a specific application. It is included in section 5 because ParFlowE is essentially ParFlow with 3D heat transport formulation addition and coupled to the CLM. It was explicit in the manuscript the original CLM was used in the coupling.

ParCrunchFlow: That section is confusing. There is a description of CrunchFlow and its solution methods (lines 769-794) but it looks like only the reaction terms computed by CrunchFlow are used by ParFlow and the advective-dispersive transport capabilities are not used. If that’s the case, I would not describe all the CrunchFlow features, only those used. It would also be interesting to indicate why CrunchFlow’s advective-dispersive transport capabilities are not used and the advection-only capability of ParFlow is used instead, with its restrictive explicit time-weighting scheme. I assume that it’s a question of dimensionality but it is not clearly stated. Also, the reader has to guess that ParCrunchFlow is only applicable for subsurface simulations (it should be clearly stated). The whole section would need to be rewritten more clearly.

Authors Response The document has been revised to highlight that ParCrunchFlow is applicable only in the subsurface.

The terminology used to describe the coupling of ParFlow with other codes is not consistent and can be confusing. There is a mention of offline and online couplings in section 5, which are fairly clearly described, but those terms are not used after that. It would be clearer if a constant terminology was used to describe the type of coupling.

Authors Response The entire section 5 has been revised for consistency in the use of terminologies “online” and “offline” couplings.

Anonymous Referee #2 Comment Discussion and Summary That section does not contribute much to the paper. Some sentences and statements are too general. One example is the first paragraph of the section. The very last paragraph provides some practical information about ParFlow. From the point of view of a potential user or developer, it would be interesting to develop that aspect. For example, there is a mention that a software development and sustainability plan exists. It would be very interesting to provide a summary of that plan. Also, community models have their challenges. For example, how is the model verified once modifications have been made? Is there a series of verification examples? Is there a single version or have many “branches” been developed over the years? If there are many branches or versions, how are they managed? Who is responsible for maintaining the code and designing the development and sustainability plan? What6 are the main issues faced by a user (new or experienced)?

Authors Response We have included further descriptions to the software development and sustainability plan for ParFlow such as new formulations of both kinematic and diffusive wave approximations, and advanced parallelization support (GPU’S and heterogeneous compute architectures). Sources to all versions and/or releases of the code has been provided in the “code availability and data policy” section where code developers and contributors can be found. This is not included in the main text to prevent redundancy.

Tables and Figures Table 2 provides an overview of coupling studies but with very little information and one has to refer to the individual publications to have a better understanding of these simulations (and ParFlow's capabilities). In that table, The simulation scale is not clear since there are mentions of watershed and catchment but it is not clear what size they are. There is also a mention of regional scale but no indication on how it is different from catchment or watershed. I suggest that some information on the size of the model (for example the area and perhaps the depth) be given.

Authors Response Table 2 has been revised to define the sizes (i.e. lateral and vertical dimensions) of catchment, watershed, regional scale as used in the original articles mentioned in the manuscript.

It would be informative, for a potential user, to indicate which studies are conceptual (e.g. model development, numerical methods) and which are application to real systems, with a mention if there was a model calibration to observations.

Authors Response Table 2 was revised to indicate whether the original study was model development and if there was a model calibration to observations.

Figure 7 is not referenced in the text.

Authors Response The paper has been revised to reference Figure 7 in the text.

Anonymous Referee #2 Comment Symbols and equations The symbols used in the equations have to be checked for consistency. There are several instances where the same letter or symbol designates different quantities and cases where the same quantity is identified with a different symbol (one example is hydraulic conductivity). Also, some variables (one example is porosity) are defined more than once. I am not providing an exhaustive list but some examples are: Equation 2: x is not defined

Authors Response Equations 2 has been revised to define all variables appropriately.

In equation 2, p is pressure head but it is hydraulic head in equation 4

Authors Response The symbols for pressure head and hydraulic head in Equations 2 and 4 have been revised. Different symbols have been used.

Units for qs in equation 1 are given as L3T-1, which is not consistent with the units for equation 1. qs is used in both equations 1 and 5 but it is not the same quantity since the units are different in the two equations.

Authors Response The units of qs in Equations 1 and 5 have been revised to be equal.

Equation 5 could be deleted and replaced by equation 9

Authors Response Equation 5 is a lead to equation 9 so we believe it does not make it less important including it.

Equations presented in section 5 should be carefully reviewed because they have obviously been copied from other documents and have not been checked for consistency with respect to the ParFlow equations presented in section 2.

Authors Response Equations in section 5 have been revised for consistency in the equations where appropriate.

Anonymous Referee #2 Comment Writing Careful proofreading is required because there are several instances where words are missing or where a sentence or expression is not clear. I am not providing an exhaustive list but some illustrative examples in the beginning of the paper are: Line 57: “vadose flow”. Should be something like vadose zone flow.

Authors Response Line 57 is revised to include “zone” to vadose flow.

Lines 58-59: “process domains”. Not sure what process domains are.

Authors Response Lines 58-59 have been revised.

Lines 62-63: “hydraulically-linked interconnected” is redundant

Authors Response Text in Lines 62-63 are revised to eliminate redundancy. The phrase "hydraulically-connected" is used.

Line 64: "feedback between the components". Components is not defined and it is not clear what it refers to.

Authors Response Components represented surface and subsurface flow systems, and the text has been revised as such.

Lines 75-76: "surface, unsaturated, and groundwater flow". There should not be any distinction between unsaturated flow and groundwater flow. Flow in the unsaturated zone is groundwater flow.

Authors Response "Unsaturated" has been removed

Line 77: "surface and overland flow". Is surface flow different from overland flow? The paper uses both terms without specifying if they are synonyms or represent different flow processes (which this sentence is suggesting). The paper should be checked for consistency in using surface and/or overland flow.

Authors Response The paper is revised to use surface or overland flow appropriately.

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