

Short comment – Astrid Kerkweg

Dear authors,

In my role as Executive editor of GMD, I would like to bring to your attention our Editorial version 1.1: <http://www.geosci-model-dev.net/8/3487/2015/gmd-8-3487-2015.html>

This highlights some requirements of papers published in GMD, which is also available on the GMD website in the 'Manuscript Types' section:

http://www.geoscientific-model-development.net/submission/manuscript_types.html

Discussion Paper

In particular, please note that for your paper, the following requirement has not been met in the Discussions paper:

"All papers must include a section, at the end of the paper, entitled 'Code availability'. Here, either instructions for obtaining the code, or the reasons why the code is not available should be clearly stated. It is preferred for the code to be uploaded as a supplement or to be made available at a data repository with an associated DOI (digital object identifier) for the exact model version described in the paper. Alternatively, for established models, there may be an existing means of accessing the code through a particular system. In this case, there must exist a means of permanently accessing the precise model version described in the paper. In some cases, authors may prefer to put models on their own website, or to act as a point of contact for obtaining the code. Given the impermanence of websites and email addresses, this is not encouraged, and authors should consider improving the availability with a more permanent arrangement. After the paper is accepted the model archive should be updated to include a link to the GMD paper." Please note that your statement "The code of TerrSysMP-PDAF will be made available on the HPSC-TerrSys website (www.hpsc-terrsys.de) for academic and noncommercial use." does not fulfil the criterion, as it is only a declaration of intent what will happen in the future and does not allow the reviewers or interested readers to access the code now. Please make sure, that at least in your revised submission a working way to access the code is given.

We understand that our declaration of the code availability was not in line with the requirements for papers to be published in GMD. Therefore, we will add the source code as a supplement to the GMD article. We modified the 'Code availability' section to:

"The source code of TerrSysMP-PDAF is added as a supplement to this article."

Reviewer I

General Comments

The paper “TerrSysMP-PDAF (version 1.0): A modular high-performance data assimilation framework for an integrated land surface–subsurface model” by W. Kurtz, G. He, S. Kollet, R. Maxwell, H. Vereecken, and H.-J. Hendricks Franssen, presents efforts to couple the TerrSysMP model to the PDAF assimilation library. Overall, the paper is clear and provides an adequate level of description of the new system. This paper will be an important future reference for upcoming assimilation studies performed using this system.

We wish to thank the reviewer for pointing out the clarity, contribution and novelty of our work.

In the introduction, I'd like to see comparisons with other similar modelling systems (coupled Atmosphere, Land Surface, and Groundwater) capable of assimilation. How does the TerrSysMP-PDAF compare with other assimilation capable systems? Ultimately, to answer the question: what makes the TerrSysMP-PDAF unique?

One major difference between TerrSysMP-PDAF and other already established data assimilation systems is that TerrSysMP-PDAF includes a physically-based integrated groundwater model (ParFlow) which solves the 3D-Richards equation and coupled surface-subsurface water movement. Most other data assimilation systems (e.g., CaLDAS, GLDAS, WRFDA) usually rely on a simplified representation of the surface water/ groundwater component inherent in land surface models. In these land surface models, 1) water movement is usually only calculated in vertical direction (no lateral flow), 2) surface water and subsurface flow are not coupled and 3) the influence of lateral groundwater flow is not explicitly taken into account.

An exception is the data assimilation system for the physically-based integrated groundwater model MIKE-SHE (Ridler *et al.*, 2014) which also includes lateral groundwater flow and surface water-groundwater exchange. However, unsaturated flow in MIKE SHE is still calculated in 1D only and the vegetation is simplified compared to CLM. Another difference here is how the data assimilation module is coupled to the flow model. For MIKE-SHE, the OpenMI framework is used to couple the model to the data assimilation utilities of OpenDA. In TerrSysMP-PDAF, the data assimilation algorithms of PDAF and the models of TerrSysMP are coupled in a more integrated fashion, which is more efficient especially for large data assimilation problems.

Another advantage of TerrSysMP-PDAF is its modularity. With TerrSysMP-PDAF it is possible to perform data assimilation with different (combinations of) component models depending on the needs of the actual data assimilation problem. This allows the user to be more flexible with respect to the process description (i.e., the utilized forward models) and the computational demand of the data assimilation problem.

Furthermore, we would like to stress that TerrSysMP-PDAF is also capable of performing joint state-parameter estimation. Although there is a growing body of literature on the utilization of data assimilation techniques to estimate parameters in land surface models and especially in groundwater models, this functionality is, to our knowledge, still not found in any published data assimilation system. However, we deem parameter estimation important especially for land surface and subsurface models because a large part of model uncertainty is related to the parametrization in these kinds of models.

We modified the last part of the introduction and include now the above mentioned differences and novelties of TerrSysMP-PDAF compared to other data assimilation frameworks (parameterization of groundwater flow, joint state-parameter update, computationally efficient coupling between model and data assimilation) (line 121-166):

“There is a number of already existing data assimilation frameworks that can be utilized to perform data assimilation for specific earth system compartments. Examples for the land surface compartment are the Canadian Land Data Assimilation System (CaLDAS) (Carrera et al., 2015) or the Global Land Data Assimilation System (GLDAS) (Rodell et al., 2004). An example for an atmospheric data assimilation system is provided by Barker et al. (2012) who developed a data assimilation system for the numerical weather prediction model WRF (WRFDA). For the assimilation in the subsurface compartment, Ridler et al. (2014) developed an assimilation system for the integrated hydrological model MIKE SHE. However, these data assimilation systems usually rely on a simplified representation of groundwater dynamics because the process description in the utilized land surface models does not include lateral flows and surface water-groundwater interactions. Hence, these models do not include a sufficient process description to take the dynamic feedbacks between land surface and subsurface processes into account. An exception is the data assimilation system for the groundwater model MIKE SHE which also includes lateral groundwater flow and surface water-groundwater exchange. However, unsaturated flow in MIKE SHE is still calculated in 1D only and the vegetation is simplified compared to other land surface models. Additionally, the above mentioned data assimilation frameworks do not provide the possibility to perform joint state-parameter estimation which has been shown to be important in the context of subsurface and land surface data assimilation.

Besides the above mentioned data assimilation systems for certain earth system compartments, there is also a number of generic data assimilation frameworks which are not tailored to a specific simulation model. Examples of such generic data assimilation frameworks are the Data Assimilation Research Testbed (DART) (Anderson et al., 2009), the Parallel Data Assimilation Framework (PDAF) (Nerger and Hiller, 2013) or the OpenDA framework (OpenDA, 2013). These different frameworks provide various data assimilation algorithms and the necessary computational infrastructure to operate with any kind of simulation model. Ridler et al. (2014) demonstrated the use of the OpenDA framework to establish a data assimilation system for the integrated hydrological model MIKE SHE. This was achieved by connecting both components with the Open Modelling Interface (OpenMI) software. This kind of interfacing is based on Java and .NET technology and can also be used for other OpenMI compliant models. However, the utilized communication approach between model and data assimilation may not be efficient enough to be applied for large data assimilation problems.

In this paper, we present a data assimilation system for the terrestrial system modelling platform TerrSysMP (Shrestha et al., 2014). This model consists of three component models for the subsurface (ParFlow), the land surface (Community Land Model) and the atmosphere (COSMO-DE). The data assimilation is established with the PDAF library (Nerger and Hiller, 2013). Currently, the data assimilation system is restricted to the land surface–subsurface part of TerrSysMP (CLM and ParFlow) and provides the possibility to perform state as well as joint state-parameter updates. The data assimilation framework uses a memory based communication between model and data assimilation routines and avoids frequent re-initializations of the model which is beneficial for the scalability and the application to large scale hydrological systems. The paper is structured as follows: In Sects. 2 and 3 we first introduce the modelling platform TerrSysMP and the data assimilation software PDAF. In Sect. 4 the technical implementation of the data assimilation system with TerrSysMP and PDAF is described in detail. Section 5 provides an illustrative example of the designed data assimilation framework for a simple land surface–subsurface setup with a focus on hydrological model states and fluxes. In this section also the scaling behaviour of the data assimilation framework and its applicability for high-resolution modelling problems is tested and presented in detail. Finally, Sect. 6 provides conclusions and an outlook on possible further developments.”

The modularity of TerrSysMP-PDAF is highlighted in the conclusions (line 766-771):

“The data assimilation system for TerrSysMP is designed in a modular fashion, i.e., assimilation can either run with the coupled land surface–subsurface model (ParFlow + CLM coupled via OASIS-MCT) or with one of the standalone models (ParFlow or CLM). This provides the user with some flexibility regarding the model choice because for certain modelling purposes the use of a single compartment model (subsurface or land surface) may be sufficient in the context of data assimilation whereas in other situations a fully coupled approach may be more adequate.”

References:

Ridler, M.E., van Velzen, N., Hummel, S., Sandholt, I., Falk, A.K., Heemink, A., Madsen, H. (2014), Environ. Modell. Softw., 57, 76-89, doi:10.1016/j.envsoft.2014.02.008

The writing style - although understandable can be clumsy to read due to long sentences without commas. I've listed a few cases below. A word processor (like MS Word) will pick up most of these run-on sentences. Overall, I found the paper to be worth publication once the comments above and below are taken into account.

Thank you for pointing this out. We corrected the cases you mentioned. We also made every effort to revise the manuscript for clarity throughout (see manuscript with track changes for details).

Specific Comments

p.9632 ln.4 → It's unclear where does the observation to model index mapping fit into the system? Is the observations handled by the PDAF and assumed to be fixed in location with known model indices? More explanation is required here.

We agree that the mapping of observations onto the model grid was not very clear from our description. Basically, TerrSysMP-PDAF reads in a separate observation file (netCDF format) at each assimilation cycle. This observation file only contains information on the currently available observations. This information includes the measurement values, the estimated measurement errors (optional) and the location of the observations in the model grid. The latter information is given in the form of model grid cell indices. This means that the user needs to determine the grid cells which match the observation locations beforehand. The grid cell indices provided in the observation files are then handed over to PDAF, which will use these indices to extract the simulation results at observation locations from the state vector. We clarified this point in the description of the observation mapping in the revised manuscript (line 371-378):

“Then the observation data are read from netCDF files which hold the measurement values, the corresponding measurement errors and information on their spatial location. The spatial location of observations has to be provided in the form of model grid cell indices, i.e. the user needs to determine the grid cells which match the observation locations. The grid cell indices provided in the observation files are then handed over to PDAF which will use these indices to extract the simulation results at observation locations from the state vector. Note that by using grid cell indices, no interpolation or other kind of measurement operation is performed because the observations are simply clipped to the nearest model grid cell.”

p.9632 ln.13 → Why is the TerrSysMP restricted to the EnKF? Will it not work with a deterministic (non-localized) filter? Localization is often useful (essential in some cases) in assimilation applications. Is that not implemented?

In principle, the PDAF library includes various filter variants (e.g., EnKF, ETKF, SEIK, LETKF). For the coupling of PDAF and TerrSysMP (or any other kind of model) it is

necessary to provide several user-specified functions in order to define the data assimilation problem for PDAF (e.g., definition of the state vector, definition of the observations, etc.). Some of these user-specified functions are shared among different filter variants (e.g., reading of observations) and others are specific for certain kinds of filters (e.g., specification of grid cell coordinates for local filter variants).

Currently, the main focus of our research is to perform data assimilation with TerrSysMP at the catchment scale using the Ensemble Kalman Filter. As such, TerrSysMP-PDAF is currently configured to work with EnKF, however we are also intending to test deterministic filters for this kind of data assimilation problem in the near future.

We also agree that localization is useful or even mandatory for certain assimilation problems. For example, we are planning to assimilate remote sensing soil moisture data with TerrSysMP-PDAF as one of the next steps. This will make it necessary to use filter variants with localization (e.g., LETKF).

You will surely understand that systems like TerrSysMP-PDAF are always a work in progress and the development is usually driven by the needs of the actual users. Our goal is to provide the full functionality of PDAF with respect to filter variants and filter options in the near future. This is acknowledged now in the conclusions section (line 791-793):

“It is also planned to extend the data assimilation system to make full use of the functionality of PDAF with respect to filter variants and assimilation options (e.g., localization and smoothing).”

Figure 8 shows four time series plots of Soil moisture at four locations. Are these four locations where there are observations. It’s not very informative to validate using the same measurements that were used in the assimilation. Could you not find 4 points distal (or in between the assimilated measurements) for validation?

You are right. Fig. 9 shows predicted soil moisture values at four observation locations. In order to make this comparison more objective, we also used four independent points for verification which are in between the observation points ($x=2500m$, $y=1500/2500/3500/4500m$, see modified Fig. 5 in revised manuscript). The results for these independent verification points are now shown in Fig. 9 in the revised manuscript (see also Fig. 1 below). However, the conclusions for these different verification points are quite similar to the ones from the previous figure.

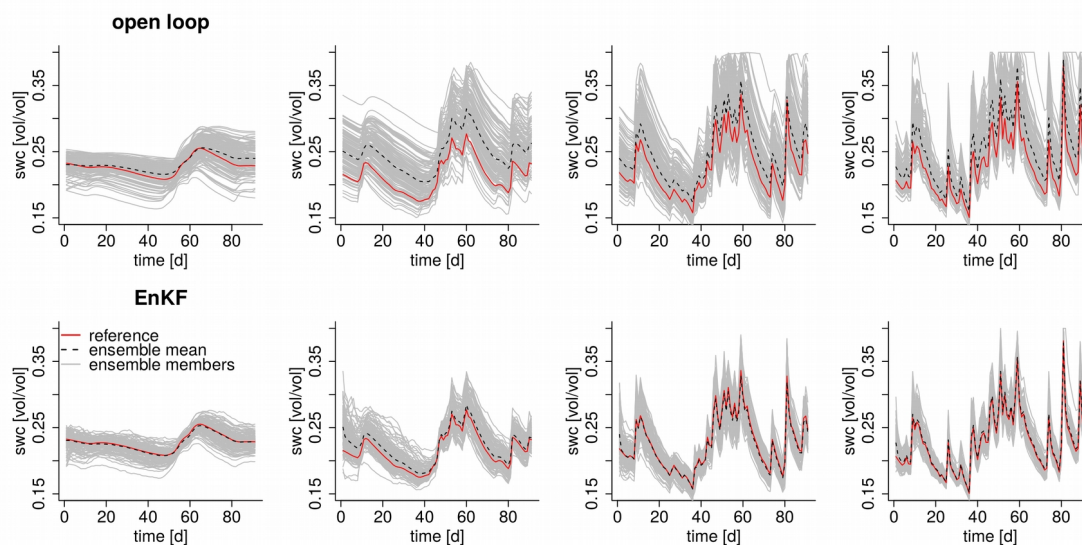


Figure 1. Simulated soil water content at four verification nodes ($x=2500m$, $y=1500/2500/3500/4500m$, from north to south) for April–June 2013 (91 days). Upper row shows results for open-loop simulations and lower row for assimilation.

p.9643 In. 20 *It is surprising that there is such little change in the energy fluxes after assimilation. Especially in the grassland area (right) as this regions seems to be where the impact of the assimilation is greatest for both corrections of soil moisture and the hydraulic conductivity. I'm not convinced that the minimal effect is solely due to the high groundwater (as you say) especially for a plant type with short roots.*

We already mentioned in the manuscript that the errors of land surface fluxes were relatively low even for the open loop runs (p.9643 line 15ff). The total AAE values (averaged over all grid cells and time steps) for sensible (latent) heat were 1.003 (1.212) W m^{-2} in the open-loop run. Two possible reasons for these relatively low errors have been nicely pointed out by reviewer 2: (1) Plant physiological parameters were not perturbed (2) Meteorological forcings that affect stomatal conductance were not perturbed. Results from these open-loop simulations show that in our setup the variability of soil moisture content only had a limited effect on land surface fluxes and most of the model domain is not affected by water limitation. With the assimilation of soil moisture contents, the total AAE values of sensible (latent) heat fluxes were reduced to 0.730 (0.876) W m^{-2} . In relative terms, the assimilation of soil moisture data improved land surface fluxes by about 27% but still the absolute values are relatively low ($\sim 1 \text{ W m}^{-2}$ on average). If one looks at the patterns of land surface flux errors, one can indeed see that most of the improvement by data assimilation can be found in the grassland area. We modified the results section on land surface fluxes and discussed the above mentioned reasons for the low absolute improvement of land surface fluxes in more detail (line 678-694):

“The effect of soil moisture assimilation on land surface fluxes (latent and sensible heat flux) was also analysed for this setup. The total AAE values (averaged over all grid cells and time steps) in the open-loop run were 1.003 Wm^{-2} for sensible heat flux and 1.212 Wm^{-2} for latent heat flux. The spatial pattern of errors in land surface fluxes is closely related to those of AAE_θ in Fig. 10. In principal, the calculation of land surface fluxes within TerrSysMP can be affected by: (1) plant physiological parameters (2) meteorological forcings that affect stomatal conductance and (3) the availability of water in the subsurface. In the chosen setup neither plant physiological parameters nor meteorological forcings (with the exception of precipitation) were perturbed, so the variability of land surface fluxes is mainly influenced by the availability of water in the rooting zone. The relatively low errors in the open-loop simulation indicate that the variability of soil moisture content only had a limited effect on land surface fluxes in the chosen setup and that most of the model domain is not affected by water limitation. With the assimilation of soil moisture contents, the total AAE values of sensible (latent) heat fluxes were reduced to 0.730 (0.876) Wm^{-2} respectively which is a relative improvement of about 27%. Nevertheless, the absolute magnitude of land surface flux errors and the improvements by data assimilation are relatively low due to the fact that the system was not affected by water limitation throughout the simulation period.”

The scaling factor and processor time is measured using two cases (identical ensemble and a more realistic case). It would be interesting to see results (or at least the author's thoughts) on the impact of using a model with a varying topography and thus overland flow calculations on the scaling factor.

We think that our section on the scaling of TerrSysMP-PDAF is already quite detailed. The comparison of the 'ideal' (identical ensemble members) and the 'heterogeneous' (different ensemble members) test case nicely illustrated the effect of ensemble perturbations on the scaling behaviour of TerrSysMP-PDAF. Even for this setup without overland flow, the results very much depend on the model specification and the ensemble perturbations. So this scaling test is not meant to be a benchmark for the system, but it's rather an illustrative example how

the scaling could typically behave under realistic conditions.

Overland flow would, of course, add some additional complexity to the system and then also has the potential to alter the results of this scaling exercise. However, this again is highly case sensitive because the temporal evolution of overland flow (and the corresponding convergence properties) depends on factors like model geometry, model discretization and model parametrization.

Our experience is that especially the onset and offset of overland flow at particular grid cells (due to heavy rainfall or recession events) can be computationally very demanding. This is due to the fact that overland flow has much faster time scales than the water movement in the subsurface which can lead to convergence issues at the onset/offset of coupling of the two domains. Such events can have a negative influence on the scaling behaviour of the deterministic forward model because the computationally demanding onset/offset of overland flow only occurs in certain parts of the model domain and the utilization of more CPU's only has a limited effect on speeding-up convergence in these particular areas (see also *Kollet & Maxwell (2006)* and *Osei-Kuffuor et al. (2014)*).

A negative influence of overland flow on the scaling behaviour of the data assimilation system could be expected when only certain realisations experience convergence problems due to the onset/offset of overland flow (e.g., through the chosen perturbations of subsurface parameters or meteorological forcings). In this case, a few realisations might dominate the total runtime of the system which then has a negative impact on the overall scaling of the data assimilation system.

However, such problems are not only restricted to overland flow coupling but could also occur, e.g., when there are strong spatial gradients in model parameters (e.g., hydraulic conductivities) which may pose a problem to the numerical solver.

Generally, the scaling behaviour of ensemble-based data assimilation systems will depend on the numerical robustness of the deterministic forward model towards ensemble perturbations. Therefore, it is important to configure the deterministic forward model well with respect to numerical stability and execution time. This can be achieved, e.g., through the correct choice of solver parameters, an adequate spatio-temporal discretization of the problem and a proper choice of model parameters and ensemble perturbations.

We believe that for a well configured overland flow problem, the scaling results might be quite similar to the 'heterogeneous' example without overland flow. However, in cases where the ensemble perturbation affects the overland flow convergence for a limited amount of realizations, a negative influence on the scalability of the data assimilation run could be expected.

We added a paragraph to Sect. 5.2 that discusses the potential effects of overland flow on the scaling results (line 641-655):

“The scaling results for the more realistic heterogeneous ensemble are also promising for the application of TerrSysMP-PDAF for more complex land surface-subsurface data assimilation problems. Generally, for any given model setup, the scaling behaviour of the data assimilation problem will particularly depend on the numerical robustness of the deterministic forward model towards ensemble perturbations. Critical situations with respect to convergence could occur, e.g., for strong heterogeneities in the subsurface parameterization (e.g., hydraulic conductivities) or for the coupling of overland and subsurface flow. For the latter case, especially the computationally demanding onset and offset of overland flow at particular grid cells (e.g., due to heavy rainfall or recession events) can have a negative influence on the scaling behaviour of the deterministic forward model (Kollet & Maxwell (2006); Osei-Kuffuor et al. (2014)). If only a subset of realisations is affected by such convergence problems, also the scalability of the ensemble propagation might be influenced negatively. Therefore, it is important to configure the deterministic forward model well with respect to numerical stability and execution time. This can be achieved, e.g., through the correct choice of solver parameters, an adequate spatio-temporal

discretization of the problem and a proper choice of model parameters and ensemble perturbations.”

References:

Kollet, S.J., Maxwell, R.M. (2006), Adv. Water Resour., 29, 945-958, doi: 10.1016/j.advwatres.2005.08.006

Osei-Kuffuor, D., Maxwell, R.M., Woodward, C.S. (2014), Adv. Water Resour., 74, 185-195, doi: 10.1016/j.advwatres.2014.09.006

Technical Corrections

Assess instead of access (3 times at least) In abstract, p9638 ln 1, and p 9638 ln 21

Replaced as recommended.

p9619 l.18 ... in the model input, which allows to...

Changed.

p9619 l.21 ... model states, which are ...

Changed.

p9619 l.24 . terrestrial system, including

Changed.

p9620 l.9 Typically in these cases, point ...

Changed.

p9622 l.10 integrated view of the terrestrial

Changed.

p9622 l.23 are performed at a high

Changed.

p9622 l.24 realisations are needed ...

Changed.

p9622 l.25 There are a number of

Changed.

p9624 l.9 only in a vertical

Changed.

p9624 l.10 ie. there is no lateral.

Changed.

p9624 l.27 allows it to solve

Changed.

*p9626 l.8 allows **for an integrated view *of the**

Changed.

p9626 l.12 Awkward sentence → another important point that is noteworthy is that

Changed to: "Another interesting feature of TerrSysMP is its modularity: apart from ..."

p9626 l.16 has already shown to be highly scalable on the massively...

Changed.

p9629 l.12 remove the ":" and replace with ".", then First.. the Secondly and Thirdly in the paragraph should be Second and Third .

Changed.

p9634 l.2 CLM except for the special ...

Changed.

p9635 l.2 ten layers, pressure, ...

Changed.

p9636 l.8 DWD hasn't been introduced yet. What is it?

DWD is an acronym for the German Weather Service. his abbreviation has been added in line 457-458:

"...are taken from reanalysis data of the German Weather Service (DWD) for the year 2013..."

p.9638 assessed instead of accessed.

Changed.

Reviewer II

General comments

This paper by Kurtz et al. introduces a modular high performance data assimilation framework for a coupled land surface groundwater model (part of the TerrSysMP model). This paper introduces the technical implementation in great detail, analyzed the computational efficiency of the parallel framework, and provides an illustrative example. The paper is generally well written. Both data assimilation and coupled modeling systems have become increasingly popular in the hydrometeorology community in recent years. The coupling technique and the implementation of data assimilation technique introduced in this paper could be expanded to other data assimilation method and other coupled modeling systems.

We thank the reviewer for pointing out the relevance of our work.

Specific comments

1. P9622, L12 *“However, while such integrated modelling approaches provide a better description of model physics which effectively reduces model structural errors that often occur in single compartment models through the parameterization of lower or upper boundary conditions. . .”* I don't quite agree. Sometimes coupled models could introduce model structural errors. However, this is minor.

We believe that one of the main purposes for coupling different geoscientific compartment models is the better physical description of processes at the compartment interfaces. Therefore, we think that our statement is generally valid. Of course, if the coupling is not done in a consistent way or if the coupling violates some underlying assumptions in the parameterization of the forward models, one could easily introduce model structural errors. However, if the coupling is done in a physically consistent manner, the model error should decrease.

2. P9627, L24 *“For example, local filter variants like LETKF need special routines to infer the position of each element of the state vector in the model domain in order to perform the localization which is not needed by global filter algorithms like EnKF.”* I understand that localization is not needed by EnKF. However, covariance localization could be important for a large-scale multi-watershed application. Is there a way to account for localization in the data assimilation system?

Sorry, our formulation was a bit misleading here. We wanted to express that this special routine (determination of distances between state vector elements) is not used by the EnKF formulation in PDAF. The reason is that localization for EnKF is currently not implemented in the release version of PDAF.

We certainly agree that localization could be a very important factor for the data assimilation results. However, this is currently not possible with EnKF in PDAF. Alternatively, PDAF provides local variants of several other filters (e.g., ETKF/LETKF). This functionality is not yet available in TerrSysMP-PDAF but will be provided in the near future.

In order to avoid confusion, we removed the misleading formulation “[...] which is not needed by global filter algorithms like EnKF.” from the sentence.

3. P9633, L6 *“In this case, pressure values in ParFlow are indirectly corrected with the incoming soil moisture measurements through the correlations between soil moisture and pressure. This is necessary, because the prognostic variable in ParFlow is pressure and soil moisture (or saturation) is a derived quantity which is not directly used as a state variable for the next time step.”* I understand that soil moisture is a derived variable but not a prognostic variable in ParFlow. But

the pressure values could easily be converted into soil moisture using the van Genuchten equation. So why not convert the pressure values into soil moisture values, update the soil moisture values, and convert them back into pressure values?

You are certainly right. There are basically two ways how pressure can be updated with soil moisture data in ParFlow: (1) The one we described in the manuscript is to use an augmented state vector composed of soil moisture and pressure. Pressure is then indirectly updated through the correlations with soil moisture. (2) Alternatively, as you mentioned, one can also use saturation/ soil moisture as the solely state variable in the filtering step and then transfer the updated saturation/ soil moisture values back to pressure via the 'inverse' van Genuchten function. In fact, this second variant of updating soil moisture/ pressure is also included in TerrSysMP-PDAF for testing purposes. As we are using the first method in the verification example, we did not mention that there are two options in TerrSysMP-PDAF for assimilating soil moisture data, in order to avoid confusion. Nevertheless, we changed the description of the soil moisture assimilation to include both updating options (line 397-413):

“In the coupled (ParFlow+CLM) and uncoupled (ParFlow standalone) TerrSysMP configuration, measurements of pressure or soil moisture can be assimilated in ParFlow. The assimilation of both measurement types involves an update of pressure values in ParFlow because this is ParFlow's prognostic variable and soil moisture (or saturation) is a derived quantity which is not directly used as a state variable for the next time step. For the assimilation of pressure data, simulated pressure values in ParFlow are directly modified by the pressure observations. For the assimilation of soil moisture data, two options are implemented in TerrSysMP-PDAF to update pressure values with soil moisture observations: (1) The state vector consists of soil moisture and pressure values of ParFlow. In this case, pressure values in ParFlow are indirectly corrected with the incoming soil moisture measurements through the correlations between soil moisture and pressure. (2) The state vector solely contains soil moisture values and the updated soil moisture values are transformed back to pressure values via the 'inverse' van Genuchten function before the next time step. Besides the state update, it is also possible to include permeability values or Mannings coefficients of ParFlow in the state vector (both log-transformed) and thus to correct these model parameters with incoming pressure or soil moisture measurements. In case the data assimilation framework is only applied with the CLM component, the state vector is constructed with the soil moisture provided by CLM which can be corrected with incoming soil moisture measurements.”

4. The system can be used to estimate parameter values. Is there a way to constrain the parameter values (and state variables) in their physically plausible ranges? This could be important as some “bad” parameter values could break the model.

Currently, TerrSysMP-PDAF does not include a plausibility check for updated state or parameter values. We agree that an update towards implausible state/parameter values could pose a problem to model performance. However, an update towards implausible parameter values can also hint to some problems in the overall model/ data assimilation configuration. Restricting the updated values to predefined bounds will possibly not solve these problems but will just mask them from the user. From our perspective, a better solution is to identify the reasons for too extreme state/parameter updates (e.g., spurious correlations due to limited ensemble size) and then try to take actions that reduce this problem (e.g, increasing ensemble size, localization).

5. P9643, L18 “The improvements made by assimilating soil moisture content are relatively limited for land surface fluxes which is related to the shallow ground water table in the simulations

guaranteeing that actual evapotranspiration is equal to potential evapotranspiration.” I don’t think the actual evapotranspiration is equal to potential evapotranspiration in this case. The plant stomatal conductance is affected by visible solar radiation (S), air temperature (T_{air}), air humidity (RH), and soil moisture (Θ). In this case, although soil moisture is close to saturation, S , T_{air} and RH still limit the actual ET which may not reach the potential ET . The reason that the AAE is small for H and LE is because (1) S , T_{air} , and RH are the same in the ensemble as in the reference run; (2) in both the ensemble and the reference run, soil moisture is close to saturation, and (3) the other parameters affecting ET are not perturbed (e.g., the minimum stomatal conductance).

We would argue that potential ET is limited by the amount of energy available for evapotranspiration. According to this definition, S , T_{air} and RH affect potential ET , but not so much the ratio actual ET /potential ET (although this ratio can be affected by the absolute value for potential ET). We agree that stomata resistance is affected by T_{air} and RH , which could reduce evapotranspiration under stress conditions like very high temperatures and extremely dry air, which is hardly an issue for the case presented in this paper. Nevertheless, otherwise we agree with the reviewer. Concerning the land surface fluxes, we only focused on the hydrological aspects but did not take into account plant physiology and the meteorological forcings.

We modified the paragraph on land surface fluxes to address the reasons for the relatively low errors and improvements of land surface fluxes. We also removed the statement that actual ET is identical to potential ET (line 678-694):

“The effect of soil moisture assimilation on land surface fluxes (latent and sensible heat flux) was also analysed for this setup. The total AAE values (averaged over all grid cells and time steps) in the open-loop run were 1.003 Wm^{-2} for sensible heat flux and 1.212 Wm^{-2} for latent heat flux. The spatial pattern of errors in land surface fluxes is closely related to those of AAE_{θ} in Fig. 10. In principal, the calculation of land surface fluxes within TerrSysMP can be affected by: (1) plant physiological parameters (2) meteorological forcings that affect stomatal conductance and (3) the availability of water in the subsurface. In the chosen setup neither plant physiological parameters nor meteorological forcings (with the exception of precipitation) were perturbed, so the variability of land surface fluxes is mainly influenced by the availability of water in the rooting zone. The relatively low errors in the open-loop simulation indicate that the variability of soil moisture content only had a limited effect on land surface fluxes in the chosen setup and that most of the model domain is not affected by water limitation. With the assimilation of soil moisture contents, the total AAE values of sensible (latent) heat fluxes were reduced to 0.730 (0.876) Wm^{-2} respectively which is a relative improvement of about 27%. Nevertheless, the absolute magnitude of land surface flux errors and the improvements by data assimilation are relatively low due to the fact that the system was not affected by water-limitation throughout the simulation period.”

Technical corrections

1. P9619 L1 “20 Mio. Unknowns” Should be “unknowns”.

Changed.

2. P9619 L10 “precipitation, hydraulic properties” Could be more clear if change this to “soil hydraulic properties”.

Changed.

3. P9620, L4 “. . . and to a lesser extend also concentration” Not clear concentration of what.

Liu et al. (2008) and *Li et al. (2012)* used solute concentrations in a groundwater model and *Gharamti et al. (2014)* used molar fractions in a reservoir model. We changed this sentence to (line 49-53):

“In groundwater hydrology, usually pressure head data are assimilated (Chen and Zhang, 2006; Hendricks Franssen and Kinzelbach, 2008; Nowak, 2009) and to a lesser extend also transport related data, like solute concentrations (Liu et al., 2008; Li et al., 2012), molar fractions of chemical constituents (Gharamti et al., 2014) or groundwater temperatures (Kurtz et al., 2014). “

4. L9622, L7 “like, e.g., . . .” “Like” is redundant.

Removed 'like'.

5. P9623, L22 “Finally, 6 provides. . .” Change this to “Section 6”.

Changed to: 'Finally, Sect. 6 provides ...'.

6. P9624, L10 “i.e., the is no lateral exchange. . .” Change this to “there is no lateral exchange”.

Changed.

7. P9625, L21 “recharge values” Do you mean infiltration values? Are they the same?

The recharge values q_{inf} are composed of the infiltration values at the top soil layer and the transpiration losses from the root zone (first ten soil layers).

8. P9627, L21 “for e.g.” “For” is redundant.

Removed 'for'.

9. P9635, L6 “The poroity is set to a value of 0.4 and . . .” Unit is missing for porosity.

Changed to: "The porosity is set to a value of 0.4 m³m⁻³ and ...".

10. P9641, L11 “A more detailed information . . .” “A” is redundant.

Changed to: "More detailed information...".

11. P9642, L13 “. . . stays above > 0.8” The greater than symbol is redundant.

Greater than symbol was removed.

12. P9644, L15 “Therefore, it was also tested whether the . . . framework is also applicable . . .” “Also” appear twice in this sentence.

The second 'also' was removed from the sentence.

13. Figure 9 Legend is missing. The ensemble mean is not shown in the figure.

A line for the ensemble mean and a legend are now included in Fig. 9. Additionally, Fig. 9 now shows data for four verification points instead of the observation points.

14. Figure 10 There is a phantom line at $y = 1500$ m. Not sure if this is a pdf rendering problem.

Unfortunately, we found that there was a problem in the calculation of the AAE fields (time shift between the reference and the ensemble mean of soil moisture). Based on the new calculations, the discontinuity at $y=1500$ m vanished and the background AAE value of 0.03 was decreased to zero (see Fig. 1 below). Other results were not affected by this calculation error.

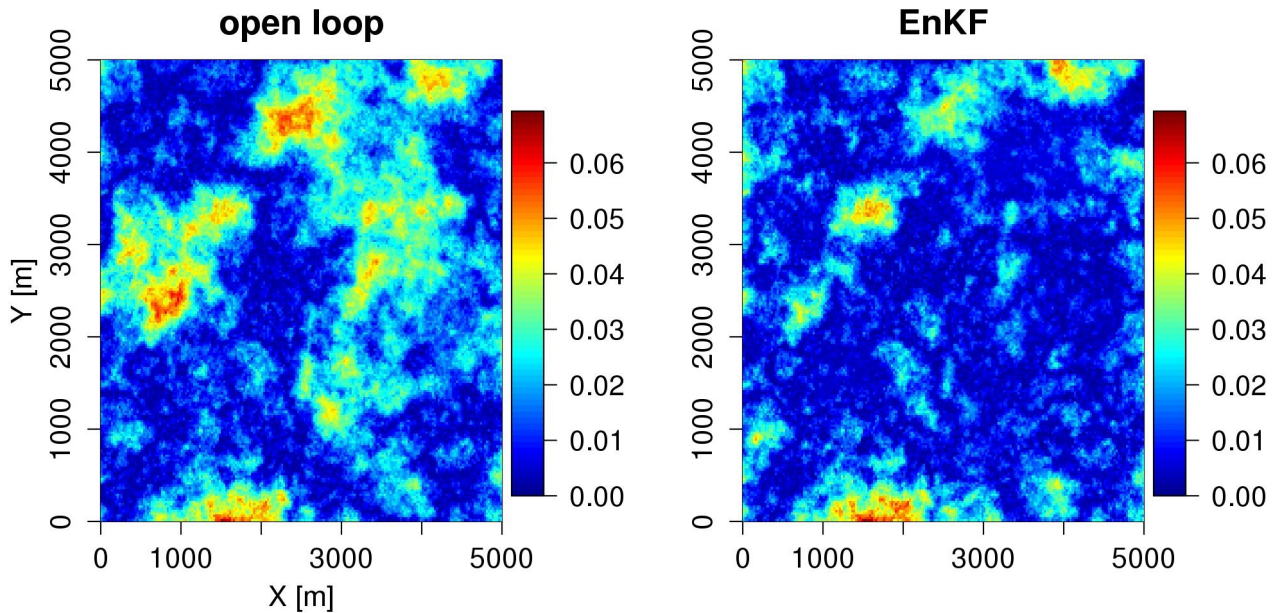


Figure 1. Absolute average error of soil water content AAE_{θ} for open-loop (left) and assimilation (right) at a depth of -65 cm from April–June 2013.

Reviewer III/ Short comments by Kao-Shen Chung

General Comments

The paper of the “*TerrSysMP-PDAF (version 1.0): a modular high-performance data assimilation framework for an integrated land surface–subsurface model*” by W. Kurtz et al. present the work of coupling the model to the assimilation system. The manuscript focuses on the introductions of the technical implementation, computational efficiency of the parallel framework, and also examines the performance of the data assimilation.

Overall, the manuscript provides proper information and description of the new system, and could be a important reference for upcoming studies in the future. In the introduction, it would be nice to mention other similar system such as “*The Canadian Land Data Assimilation System (CaLDAS)*”. In addition, authors may want to point out the uniqueness of their compared to others. Once authors revise the manuscript based on the comments/suggestions here, I believe that the paper is worth to publish.

We thank the reviewer for recognizing the contribution of this work. We modified the last part of the introduction and mention now several established data assimilation systems used in the earth system modelling community. Additionally, we highlight differences and novelties of TerrSysMP-PDAF compared to other data assimilation frameworks (parameterization of groundwater flow, joint state-parameter update, computationally efficient coupling between model and data assimilation) (line 121-166):

“There is a number of already existing data assimilation frameworks that can be utilized to perform data assimilation for specific earth system compartments. Examples for the land surface compartment are the Canadian Land Data Assimilation System (CaLDAS) (Carrera et al., 2015) or the Global Land Data Assimilation System (GLDAS) (Rodell et al., 2004). An example for an atmospheric data assimilation system is provided by Barker et al. (2012) who developed a data assimilation system for the numerical weather prediction model WRF (WRFDA). For the assimilation in the subsurface compartment, Ridler et al. (2014) developed an assimilation system for the integrated hydrological model MIKE SHE. However, these data assimilation systems usually rely on a simplified representation of groundwater dynamics because the process description in the utilized land surface models does not include lateral flows and surface water-groundwater interactions. Hence, these models do not include a sufficient process description to take the dynamic feedbacks between land surface and subsurface processes into account. An exception is the data assimilation system for the groundwater model MIKE SHE which also includes lateral groundwater flow and surface water-groundwater exchange. However, unsaturated flow in MIKE SHE is still calculated in 1D only and the vegetation is simplified compared to other land surface models. Additionally, the above mentioned data assimilation frameworks do not provide the possibility to perform joint state-parameter estimation which has been shown to be important in the context of subsurface and land surface data assimilation.

Besides the above mentioned data assimilation systems for certain earth system compartments, there is also a number of generic data assimilation frameworks which are not tailored to a specific simulation model. Examples of such generic data assimilation frameworks are the Data Assimilation Research Testbed (DART) (Anderson et al., 2009), the Parallel Data Assimilation Framework (PDAF) (Nerger and Hiller, 2013) or the OpenDA framework (OpenDA, 2013). These different frameworks provide various data assimilation algorithms and the necessary computational infrastructure to operate with any kind of simulation model. Ridler et al. (2014) demonstrated the use of the OpenDA framework to establish a data assimilation system for the integrated hydrological model MIKE SHE. This was achieved by connecting both components with the Open Modelling Interface (OpenMI) software. This kind of interfacing is based on Java and .NET technology and can also be used for other OpenMI compliant models. However, the utilized communication approach between model and data assimilation may not be efficient

enough to be applied for large data assimilation problems.

In this paper, we present a data assimilation system for the terrestrial system modelling platform TerrSysMP (Shrestha et al., 2014). This model consists of three component models for the subsurface (ParFlow), the land surface (Community Land Model) and the atmosphere (COSMO-DE). The data assimilation is established with the PDAF library (Nerger and Hiller, 2013). Currently, the data assimilation system is restricted to the land surface–subsurface part of TerrSysMP (CLM and ParFlow) and provides the possibility to perform state as well as joint state-parameter updates. The data assimilation framework uses a memory based communication between model and data assimilation routines and avoids frequent re-initializations of the model which is beneficial for the scalability and the application to large scale hydrological systems. The paper is structured as follows: In Sects. 2 and 3 we first introduce the modelling platform TerrSysMP and the data assimilation software PDAF. In Sect. 4 the technical implementation of the data assimilation system with TerrSysMP and PDAF is described in detail. Section 5 provides an illustrative example of the designed data assimilation framework for a simple land surface–subsurface setup with a focus on hydrological model states and fluxes. In this section also the scaling behaviour of the data assimilation framework and its applicability for high-resolution modelling problems is tested and presented in detail. Finally, Sect. 6 provides conclusions and an outlook on possible further developments.”

Specific Comments

P9642, line 27-28: “Assimilation of soil moisture data leads to a reduction of . . .” In Fig.9, you show the soil water content for each member compared to the reference value. This only demonstrates the reduction of the ensemble spread after data assimilation. However, we do not see the reduction of the bias. In data assimilation, it is common to show the root mean square error (RMSE) and the bias of the control variable(s). I suggest authors examine the performance of DA/without DA in this way.

We agree that the term “bias” is a bit misleading here and that Fig. 9 only provides examples of the temporal evolution of soil moisture which do not give an indication on the overall model performance. Therefore, we replaced “...a reduction of the bias between the ensemble mean...” with “...a reduction of the mismatch between the ensemble mean...” (line 662) and we also added a line for the ensemble mean to Fig. 9 which makes the improvement of the ensemble mean by data assimilation (for the verification points) more readily visible. In order to provide also a global goodness-of-fit measure, we added information on the summary error statistics of soil moisture (line 668-671):

“AAE_θ averaged over the uppermost ten model layers reduced from 0.0135 m³m⁻³ (open-loop simulation) to 0.0096 m³m⁻³ (assimilation experiment) through the assimilation of soil moisture data (the ten lower model layers were excluded from this calculation because they are constantly saturated during the whole simulation period).”

P9643, line 6-7: “This can again be related to the lower observation density at the model borders.” I agree with authors’ explanation. However, why it does not occur in other boundaries? The results present in Fig 9 are based on four points from north to south at x=2000m. Based on my previous comments and suggestions, it would be nice if you can select different points other than x=2000m and examine the results. This could also verify your explanation of the boundary issue.

In fact, this phenomenon can also be observed for the boundary grid cells of the western and the eastern face of the model domain. The only difference is that the magnitude of AAE is larger at the southern and northern boundary. Please note, that there were problems in the calculation of the AAE fields in Fig. 10 (see below). However, the spatial patterns of AAE still remain, only the magnitude changed slightly.

For Fig. 9, we also checked four independent points for verification which are in between the

observation points ($x=2500\text{m}$, $y=1500/2500/3500/4500\text{m}$, see modified Fig. 5 in the revised manuscript). However, the conclusions for these different verification points are quite similar to the ones from the previous figure.

We show the results from the independent verification points now in the modified Fig. 9 in the revised manuscript (see also Fig. 1 below).

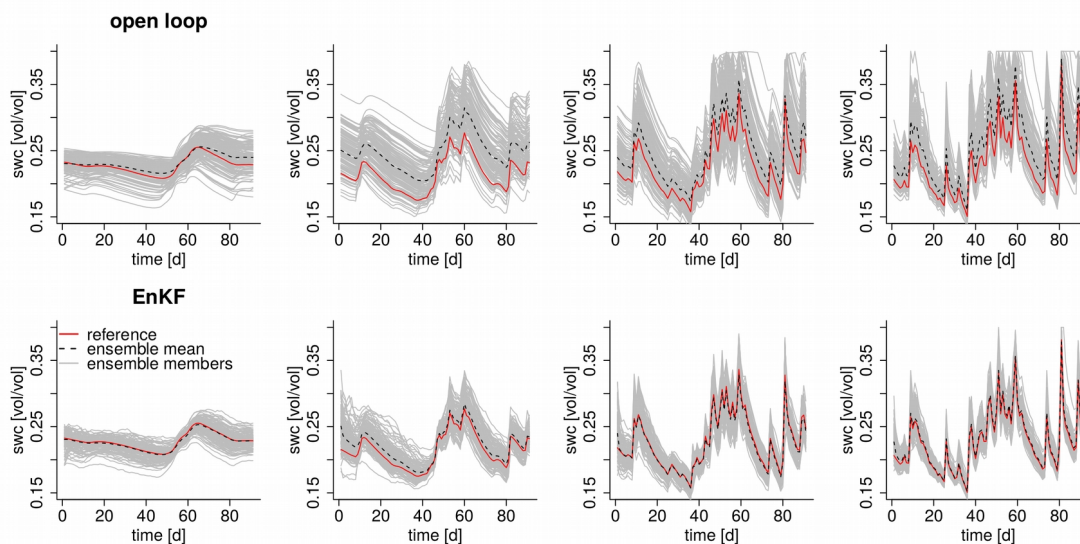


Figure 1. Simulated soil water content at four verification nodes ($x=2500\text{m}$, $y=1500/2500/3500/4500\text{m}$, from north to south) for April–June 2013 (91 days). Upper row shows results for open-loop simulations and lower row for assimilation.

In section 5.4, you performed the results of higher resolution. Are there any different setups of the EnKF between 25-m and 5-m resolutions?

The basic setup is the same for both model resolutions. For the 5m-resolution model, the input data were re-gridded from the 25m-resolution model input. The re-gridded $\log(K)$ -fields of the reference and the ensemble members were additionally perturbed with small-scale noise, which is the only difference between both models. The setup for the 5m-resolution model is described in paragraph p.9644 line 20 – p.9645 line 4 of the discussion paper.

In addition, P9627, line 24, authors state that there is no need for localization by global filter algorithms like EnKF. Please clarify this statement. As my understanding, as long as you have limited members for ensemble, localization is necessary and could perform better result.

Sorry, our formulation was a bit misleading here. We wanted to express that this special routine (determination of distances between state vector elements) is not used by the EnKF formulation in PDAF. The reason is that localization for EnKF is currently not implemented in the release version of PDAF.

We certainly agree that localization could be a very important factor for the data assimilation results. However, this is currently not possible with EnKF in PDAF. Alternatively, PDAF provides local variants of several other filters (e.g., ETKF/LETKF). This functionality is not yet available in TerrSysMP-PDAF but will be provided in the near future.

In order to avoid confusion, we removed the misleading formulation "[...] which is not needed by global filter algorithms like EnKF." from the sentence.

Fig. 10 a) There is a discontinuity at $y=1500\text{ m}$, and the values of the AAE is also Discontinuous. Is this caused by MPI? b) How to explain the values of AAE in the south boundary ($x=1000-2000$,

$y=0$) is larger in the EnKF (with DA) than in the open loop (no DA)?

Unfortunately, we found that there was a problem in the calculation of the AAE fields (time shift between the reference and the ensemble mean of soil moisture). Based on the new calculations, the discontinuity at $y=1500\text{m}$ vanished and the background AAE value of 0.03 was decreased to zero (see Fig. 2 below and modified Fig. 10 in the revised manuscript). Other results were not affected by this calculation error.

Although there is an overall decrease of AAE values for soil moisture within the model domain, there is indeed a slight increase with data assimilation around $x=1000\text{-}2000\text{m}$, $y= 0\text{-}200\text{m}$. If one compares the reference field of hydraulic conductivity (Fig. 11), one can see that the reference values are relatively low especially for this region. Additionally, one can see that this patch of low conductivity values is outside of the observation network. So, in fact, there is no information in the observations that indicates low permeability values for that region. So this is essentially a sampling problem. If one looks at the updated hydraulic conductivity field for this region, the filter even slightly increased the average parameter value for this part of the model domain which leads to the slightly higher soil moisture errors after the update.

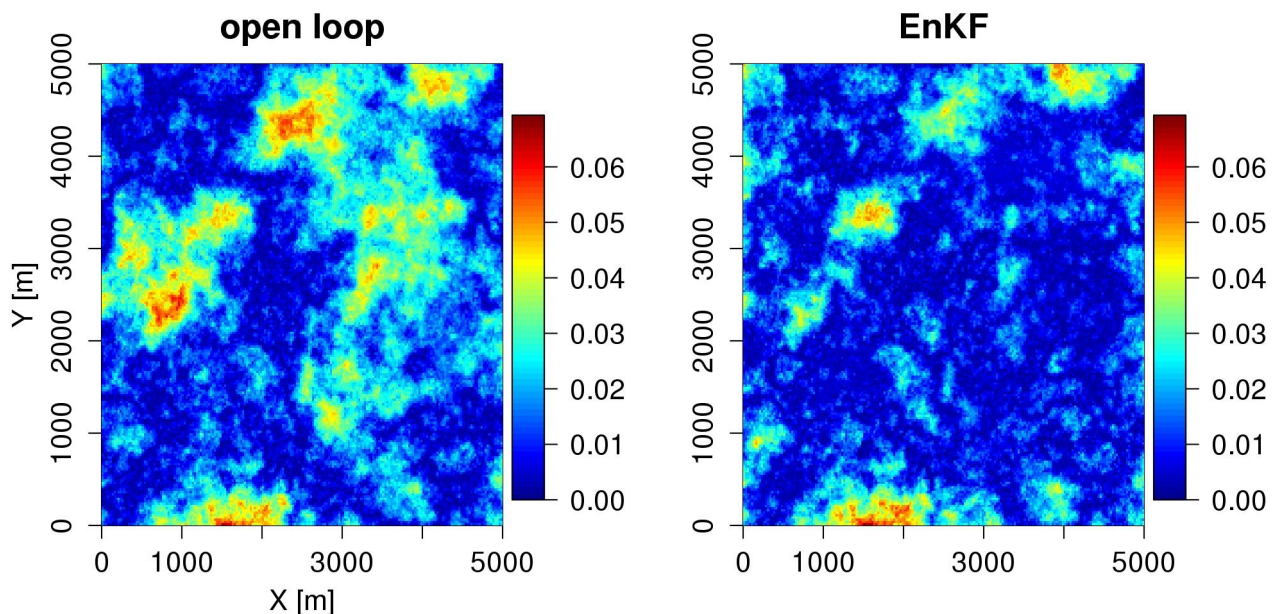


Figure 2. Absolute average error of soil water content AAE_{θ} for open-loop (left) and assimilation (right) at a depth of -65 cm from April–June 2013.

Technical Corrections

P9624, Line 10: “i.e. the is no lateral” should be “i.e. there is no lateral”

Changed.

The captions in Fig. 5 are not complete. Only sub-figure in the left is translated.

The caption of Fig. 5 was changed to:

“Synthetic setup for the twin experiment. The left hand figure shows boundary conditions of the subsurface model (ParFlow) and the location of observation (crosses) and verification (filled circles) points. Grey numbers indicate the depth of observation and verification nodes which are constant in W-E-direction. The right hand figure shows the spatial distribution of plant functional types used in the land surface model (CLM).”

The captions in Fig. 9 are not complete. What is red line and what is grey line?

A legend was added to Fig. 9.

Fig. 11 versus Fig. 12: For inter-comparison of these two figures, please use the same maximum and minimum for the color bar.

The colour bars of both figures were adjusted to the same range of values.

Additional changes

The description of the offline/ online coupling was slightly modified. The sentence *“If the model source code is not available and the model is only present as a single executable, the model is integrated forward by system calls from within PDAF. If the model source code is available, the coupling routines for PDAF can be included in the model source code.”* (p.9626 line 26ff in discussion paper) was removed from the manuscript. Instead, the explanation of offline/ online coupling was extended to (line 248-263, see also manuscript with track changes):

“The first method (offline coupling) is more ad hoc and also applicable when the source code of the model is not available. In this case, the user needs to take care of the execution of the model forward runs to the next assimilation cycle. An additional executable containing calls to PDAF routines is then used to perform the data assimilation. Within this executable, PDAF reads the state vector from the model output files, performs the assimilation and writes out the assimilation results in the form of input files for the next model integration. One drawback is that this coupling method produces a lot of I/O overhead because a huge amount of files has to be read and written at each assimilation step. Another drawback of the offline coupling is that the model needs to be re-initialised after each assimilation step. In the second variant (online coupling), PDAF is directly integrated into the model source code. This enables a direct data transfer between the model and the data assimilation algorithms of PDAF via main memory. Additionally, the model only needs to be initialised once because the model integration is only paused for the data assimilation with PDAF within the time stepping loop of the model. This coupling variant is significantly faster in terms of CPU-time but requires more programming effort and the availability of the model source code. The model coupling for both coupling variants (offline and online) is defined by the user through the aforementioned generic interface routines that are provided by PDAF. These routines include:”

TerrSysMP-PDAF (version 1.0): a modular high-performance data assimilation framework for an integrated land surface–subsurface model

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Abstract. Modelling of terrestrial systems is continuously moving towards more integrated modelling approaches where different terrestrial compartment models are combined in order to realise a more sophisticated physical description of water, energy and carbon fluxes across compartment boundaries and to provide a more integrated view on terrestrial processes. While such models can effectively reduce certain parameterization errors of single compartment models, model predictions are still prone to uncertainties regarding model input variables. The resulting uncertainties of model predictions can be effectively tackled by data assimilation techniques which allow to correct model predictions with observations taking into account both the model and measurement uncertainties. The steadily increasing availability of computational resources makes it now increasingly possible to perform data assimilation also for computationally highly demanding integrated terrestrial system models. However, as the computational burden for integrated models as well as data assimilation techniques is quite large, there is an increasing need to provide computationally efficient data assimilation frameworks for integrated models that allow to run on and to make efficient use of massively parallel computational resources. In this paper we present a data assimilation framework for the land surface–subsurface part of the Terrestrial System Modelling Platform TerrSysMP. TerrSysMP is connected via a memory based coupling approach with the pre-existing parallel data assimilation library PDAF (Parallel Data Assimilation Framework). This framework provides a fully parallel modular environment for performing data assimilation for the land surface and the subsurface compartment. A simple synthetic case study for a land surface–subsurface system (0.8 Mio. unknowns) is used to demonstrate the effects of data assimilation in the integrated model TerrSysMP and to ~~access~~ [assess](#)

the scaling behaviour of the data assimilation system. Results show that data assimilation effectively corrects model states and parameters of the integrated model towards the reference values. Scaling tests provide evidence that the data assimilation system for TerrSysMP can make efficient use of parallel computational resources for > 30 k processors. Simulations with a large problem size (20 Mio. ~~unknowns~~unknowns) for the forward model were also efficiently handled by the data assimilation system. The proposed data assimilation framework is useful in simulating and estimating uncertainties in predicted states and fluxes of the terrestrial system over large spatial scales at high resolution utilizing integrated models.

1 Introduction

30 Terrestrial system model predictions are often associated with a considerable degree of uncertainty. These uncertainties stem from a limited knowledge of the governing model forcing terms and model parameters which is, for example, related to the spatial and temporal variability of certain model input like precipitation, soil hydraulic properties or vegetation parameters. In addition, the determination of adequate initial conditions for terrestrial system simulations is often highly
35 uncertain. Ensemble based data assimilation (DA) techniques are gaining increasing attention in the geoscientific community as a tool to merge such uncertain model predictions with uncertain observation data. These techniques follow a Monte Carlo approach in which an ensemble of different model realisations is integrated forward in time. The different model realisations can include various uncertainties in the model input, which then allows to approximate the variability
40 of model predictions for different model state variables given the different uncertainty sources. These uncertain model predictions are then sequentially conditioned to available observation data where predictions and data are optimally combined according to their uncertainties. This results in updated model states, which are merged closer towards the measurements and provide an improved model forecast for the following time steps. Data assimilation has already been
45 applied to a wide variety of models in different compartments of the terrestrial system, including atmosphere, land surface and groundwater using various kinds of observation data. In this overview we focus on the water and energy cycles of the terrestrial system. The most commonly applied data assimilation algorithm in such systems is the Ensemble Kalman Filter (EnKF) (Evensen, 1994; Burgers et al., 1998) and its deterministic variants (e.g., Anderson, 2001; Bishop et al.,
50 2001; Tippett et al., 2003). In groundwater hydrology, usually pressure head data are assimilated (Chen and Zhang, 2006; Hendricks Franssen and Kinzelbach, 2008; Nowak, 2009) and to a lesser extend also ~~concentration~~ (Liu et al., 2008; Li et al., 2012; Gharamti et al., 2014) or ~~temperature~~ (Kurtz et al., 2014) data transport related data, like solute concentrations (Liu et al., 2008; Li et al., 2012), molar fractions of chemical constituents (Gharamti et al., 2014) or groundwater temperatures (Kurtz et al., 2014). Data assimilation has also been applied for variably

saturated conditions in synthetic model setups (e.g., Erdal et al., 2014; Song et al., 2014; L. Shi et al., 2015) as well as for real-world data (e.g., Li and Ren, 2011; Wu and Margulis, 2011, 2013). ~~In these cases typically~~ Typically in these cases, point measurements of pressure or soil moisture are assimilated. Data assimilation techniques were also used in the context of coupled
60 surface–subsurface flow (Camporese et al., 2009; Bailey and Baù, 2012; Rasmussen et al., 2015) where the focus is mostly on the assimilation of pressure head and discharge data. In land surface data assimilation the most commonly assimilated data types are remotely sensed soil moisture products or brightness temperatures (Crow and Wood, 2003; De Lannoy et al., 2007; Han et al., 2013) but also land surface temperature (Kumar and Kaleita, 2003; Ghent et al., 2010; Reichle
65 et al., 2010; Han et al., 2013), snow cover data (Andreadis and Lettenmaier, 2006; Su et al., 2010; Xu and Shu, 2014) or leaf area index (Sabater et al., 2008; Ford and Quiring, 2013; Barbu et al., 2014). The assimilation of such observation data into either land surface or subsurface models usually leads to an improvement of the predictive capability of the respective model. Besides the correction of model state variables, it has become common especially in subsurface and land
70 surface data assimilation to also correct model parameters jointly with model states. The reason is that the parametric uncertainty in such models is rather high compared to other compartments, like the atmosphere, where initial value problems dominate the uncertainty. Examples for the joint correction of model states and parameters in land surface and subsurface models are the correction of hydraulic subsurface parameters like hydraulic conductivity (Chen and Zhang, 2006; Hendricks
75 Franssen and Kinzelbach, 2008; Rasmussen et al., 2015; Pasetto et al., 2015), porosity (Li et al., 2012, 2015), leakage coefficients (Kurtz et al., 2013; Rasmussen et al., 2015), van Genuchten parameters (Li and Ren, 2011; Montzka et al., 2011; Y. Shi et al., 2014; L. Shi et al., 2015), dispersion parameters (Li et al., 2015) or textural information (Han et al., 2014). Other examples in the context of land surface modelling include the estimation of vegetation parameters like stomatal
80 resistance and canopy water storage (Y. Shi et al., 2015) or the estimation of parameters related to land surface flux partitioning (Bateni and Entekhabi, 2012). In most cases, this joint updating of model states and model parameters leads to better simulation results than a correction of model states alone because the uncertainties coming from a wrong parameterization are reduced.

Data assimilation in the above mentioned examples is often performed within an individual, iso-
85 lated geoscientific compartment, e.g., either for the land surface, the subsurface compartment or the atmosphere. However, there is a growing number of publications that emphasise the dynamic feedbacks between different geoscientific compartments. For example, Kollet and Maxwell (2008) demonstrated the sensitivity of land surface fluxes on the depth of the groundwater table. They found a critical water table depth of 1–5 m where the influence on the energy balance is most pronounced and where the influence also depends on soil heterogeneity and land use type. Similar effects of wa-
90 ter table depth on land surface fluxes have been found by Rihani et al. (2010) who used an idealised simulation setup to infer the effects of topography, land cover, atmospheric forcings and subsurface

heterogeneity on land surface fluxes. Ferguson and Maxwell (2010) investigated the feedback between groundwater table and energy fluxes under changing climate conditions and found that such interactions depend on the prevailing hydrological conditions (energy-limited vs. water-limited). Tian et al. (2012) also found a significant influence of water table depth on land energy fluxes for simulations of the Heihe catchment (China). Williams and Maxwell (2011) investigated the propagation of heterogeneity of subsurface parameters and the corresponding soil moisture distribution into the atmosphere and found a strong dependency of land surface fluxes and wind fields on uncertainty in subsurface parameters. Butts et al. (2014) showed that the two-way coupling of a groundwater and a regional climate model leads to different precipitation and evapotranspiration estimates compared to the standalone regional climate model especially during summer time. Maxwell et al. (2011); Shrestha et al. (2014) and Rahman et al. (2015) provide further examples how subsurface dynamics affect the development of the atmospheric boundary layer.

Due to these various feedbacks, there is a growing number of modelling platforms that integrate different compartment models for subsurface, land surface and atmosphere. ~~like~~, e.g., ParFlow-CLM (Maxwell and Miller, 2005; Kollet and Maxwell, 2008), ParFlow-WRF (Maxwell et al., 2011), COSMO-CLM² (Davin et al., 2011), AquiferFlow-SiB2 (Tian et al., 2012), TerrSysMP (Shrestha et al., 2014) or HIRHAM-MIKESHE (Butts et al., 2014). Such models allow a more integrated view ~~on~~ of the terrestrial system and water cycle in particular and the coupling leads to a physically more consistent description of processes across compartment scales. However, while such integrated modelling approaches provide a better description of model physics which effectively reduces model structural errors that often occur in single compartment models through the parameterization of lower or upper boundary conditions, the parameter and forcing uncertainty still remains in such models. Therefore, data assimilation methods may also help to quantify the uncertainties of integrated modelling approaches and to improve their forecast capability through the merging with observation data. Integrated models are usually computationally expensive and often need to be run on a high-performance computational infrastructure. Therefore, there is a need to establish data assimilation frameworks that can efficiently cope with the high computational burden of integrated terrestrial system models. This is especially relevant when simulations are performed ~~on~~ at a high spatial resolution and when a relatively high number of model realisations ~~is~~ are needed which is typically the case for ensemble based data assimilation with land surface and subsurface models.

There is a number of already existing data assimilation frameworks that can be utilized to perform data assimilation ~~also with terrestrial system modelling platforms~~ for specific earth system compartments. Examples for the land surface compartment are the Canadian Land Data Assimilation System (CaLDAS) (Carrera et al., 2015) or the Global Land Data Assimilation System (GLDAS) (Rodell et al., 2004). An example for an atmospheric data assimilation system is provided by Barker et al. (2012) who developed a data assimilation system for the numerical weather prediction model WRF (WRFDA). For the assimilation in the subsurface compartment,

130 Ridler et al. (2014) developed an assimilation system for the integrated hydrological model MIKE
SHE. However, these data assimilation systems usually rely on a simplified representation of
groundwater dynamics because the process description in the utilized land surface models does
not include lateral flows and surface water-groundwater interactions. Hence, these models do not
include a sufficient process description to take the dynamic feedbacks between land surface and
135 subsurface processes into account. An exception is the data assimilation system for the groundwater
model MIKE SHE which also includes lateral groundwater flow and surface water-groundwater
exchange. However, unsaturated flow in MIKE SHE is still calculated in 1D only and the vegetation
is simplified compared to other land surface models. Additionally, the above mentioned data
assimilation frameworks do not provide the possibility to perform joint state-parameter estimation
140 which has been shown to be important in the context of subsurface and land surface data assimilation.

Besides the above mentioned data assimilation systems for certain earth system compartments,
there is also a number of generic data assimilation frameworks which are not tailored to a specific
simulation model. Examples of such generic data assimilation frameworks are the Data Assimila-
145 tion Research Testbed (DART) (Anderson et al., 2009), the Parallel Data Assimilation Framework
(PDAF) (Nerger and Hiller, 2013) or the OpenDA framework (OpenDA, 2013). These different
frameworks ~~are well tested and all have a generic structure which means that they~~ provide various
data assimilation algorithms and the necessary computational infrastructure to operate with any kind
of simulation model. Ridler et al. (2014) demonstrated the use of the OpenDA framework to estab-
150 lish a data assimilation system for the integrated hydrological model MIKE SHE. This was achieved
by connecting both components with the Open Modelling Interface (OpenMI) software. This kind of
interfacing is based on Java and .NET technology and can also be used for other OpenMI compliant
models. However, the utilized communication approach between model and data assimilation may
not be efficient enough to be applied for large data assimilation problems.

155 In this paper, we present a data assimilation system for the terrestrial system modelling platform
TerrSysMP (Shrestha et al., 2014). This model consists of three component models for the sub-
surface (ParFlow), the land surface (Community Land Model) and the atmosphere (COSMO-DE).
The data assimilation is established with the PDAF library (Nerger and Hiller, 2013). Currently,
the data assimilation system is restricted to the land surface–subsurface part of TerrSysMP (CLM
160 and ParFlow) and provides the possibility to perform state as well as joint state-parameter updates.
The data assimilation framework uses a memory based communication between model and data
assimilation routines and avoids frequent re-initializations of the model which is beneficial for the
scalability and the application to large scale hydrological systems. The paper is structured as follows:
In Sects. 2 and 3 we first introduce the modelling platform TerrSysMP and the data assimilation soft-
165 ware PDAF. In Sect. 4 the technical implementation of the data assimilation system with TerrSysMP
and PDAF is described in detail. Section 5 provides an illustrative example of the designed data as-

simulation framework for a simple land surface–subsurface setup with a focus on hydrological model states and fluxes. In this section also the scaling behaviour of the data assimilation framework and its applicability for high-resolution modelling problems is tested and presented in detail. Finally, [Sect.](#)
170 6 provides conclusions and an outlook on possible further developments.

2 Terrestrial System Modelling Platform (TerrSysMP)

The recently developed Terrestrial System Modelling Platform (TerrSysMP) (Shrestha et al., 2014) is a modular scale-consistent terrestrial system model consisting of three already well established models for the atmosphere, the land surface and the subsurface (see Fig. 1).

175 Atmospheric processes are simulated with COSMO-DE (Baldauf et al., 2011) which is the operational forecast model of the German weather service. COSMO-DE is convection permitting and utilizes a terrain following coordinate system with variable vertical layer thickness. For more details on the model physics see Shrestha et al. (2014).

The land surface part of TerrSysMP consists of the Community Land Model (CLM) version 3.5
180 (Oleson et al., 2004, 2008). CLM calculates the transfer of energy, momentum and carbon between subsurface, vegetation and the atmosphere. In CLM, the subsurface is represented with ten soil layers of variable thickness with a total extent of 3 m. Soil water and soil temperature dynamics are calculated only in a vertical direction, i.e. ~~the~~[there](#) is no lateral exchange between grid cells. Snow accumulation is represented with up to ~~5~~[five](#) snow layers on top of the soil layer. Vegetation is
185 parametrized with up to 16 plant functional types (PFT's) which provide the plant physiological parameters that are used to calculate the contribution of vegetation to radiative transfer, land surface fluxes and carbon dynamics. CLM provides prognostic variables for the subsurface (soil moisture, soil temperature, groundwater storage), surface water routing, land surface fluxes (evaporation from ground and vegetation, transpiration from vegetation, sensible heat fluxes from ground and vege-
190 tation), radiative transfer (adsorption/transmittance of solar radiation, adsorption/emission of short wave radiation) and carbon fluxes.

The subsurface part of TerrSysMP consists of the variably-saturated finite-difference groundwater model ParFlow (Ashby and Falgout, 1996; Jones and Woodward, 2001; Kollet and Maxwell, 2006; Maxwell, 2013). ParFlow solves the 3-D-Richards equation and includes a surface water routing
195 scheme which is based on the kinematic wave approximation of overland flow which couples subsurface and overland flow in an integrated fashion (Kollet and Maxwell, 2006). The system of partial differential equations is solved with a Newton–Krylow method (Jones and Woodward, 2001). Additionally, ParFlow provides a terrain-following grid transform with variable vertical discretization (Maxwell, 2013) which allows [it](#) to solve groundwater problems with high topographic gradients.

200 The coupling of the three component models of TerrSysMP is accomplished with the coupling software OASIS-MCT (Valcke, 2013; Valcke et al., 2013; Gasper et al., 2014). The OASIS-MCT

coupler is a library that provides a generic interface to exchange information between two models. OASIS-MCT routines are called during the initialisation stage of each component model to define the model variables that should be exchanged between the component models and to establish the parallel communication between the coupled models. The exchange of variables then takes place during the runtime of the models by calling OASIS-MCT routines at explicitly defined time intervals. During this exchange of data between models, it is also possible to define interpolation and scaling operations for the respective variables. The coupled models within TerrSysMP are run in a multiple program multiple data (MPMD) fashion, that is, the different program executables are started independently in the same parallel environment and share the same global communicator (MPI_COMM_WORLD) which. This global communicator is utilized by the OASIS-MCT library functions to establish the data transfer between the different component models. Note that the data assimilation framework for TerrSysMP presented in this study does not follow this MPMD program execution mode any more (see Sect. 4).

The data that are exchanged in TerrSysMP via OASIS-MCT are schematically shown in Fig. 1. ParFlow provides CLM with its calculated subsurface pressure (ψ) and saturation (S_w) values for the first 10 subsurface layers and in return CLM provides the upper boundary condition for ParFlow which consists of the recharge values (q_{inf}) which are calculated based on the land surface fluxes of CLM (precipitation, interception, total evaporation, total transpiration). In the land surface – atmosphere part of TerrSysMP, CLM provides land surface fluxes (sensible heat flux SH and latent heat flux LH), outgoing long wave radiation (LW \uparrow), momentum flux (τ) and albedo (α) as a lower boundary condition to COSMO-DE. In turn, COSMO-DE provides forcing data to CLM including air pressure (P), air temperature (T), wind velocity (U), incoming short wave (SW) and long wave (LW \downarrow) radiation, specific humidity (Q_v) and precipitation (R).

The advantages of this integrated modelling approach with TerrSysMP are two-fold:

1. The coupling of the different component models improves the physical representation especially at the interfaces of the different geoscientific compartments. For example, ParFlow replaces the simplified soil hydrology (1-D only) and surface water routing (uncoupled) schemes in CLM by a fully integrated 3-D variably-saturated surface–subsurface flow model. In COSMO the simplified land surface scheme TERRA is replaced with the more sophisticated land surface scheme of CLM, for example, concerning the representation of vegetation.
2. This modelling approach allows for an integrated view on of the terrestrial water, energy and carbon cycles because the dynamic feedbacks of the different geoscientific compartments are explicitly taken into account.

Another important point that is noteworthy is that TerrSysMP is designed in a modular fashion, that is, interesting feature of TerrSysMP is its modularity: apart from the fully coupled system (ParFlow, CLM and COSMO-DE) it is also possible to compile and run only the land surface –

subsurface part (CLM and ParFlow) or the land surface – atmosphere part (CLM and COSMO-DE) or each of the component models individually. Regarding the parallel performance, TerrSysMP has
240 already ~~proved a high scalability~~ shown to be highly scalable on the massively parallel supercom-
puting environment ~~JUQUEEN~~ JUQUEEN (Gasper et al., 2014).

3 Parallel Data Assimilation Framework (PDAF)

The Parallel Data Assimilation Framework (PDAF) library (Nerger and Hiller, 2013) provides a generic framework for applying data assimilation with any kind of geoscientific model. PDAF
245 provides parallel algorithms of already well established data assimilation methods like the Ensemble Kalman Filter (Evensen, 1994; Burgers et al., 1998) or the Local Ensemble Transform Kalman Filter (Hunt et al., 2007). Furthermore, PDAF provides the user with generic routines to interface the model with the data assimilation algorithms and it includes methods for establishing the parallel communication for the model and the data assimilation algorithms. ~~If the model source code is~~
250 ~~not available and the model is only present as a single executable, the model is integrated forward by system calls from within PDAF. If the model source code is available, the coupling routines for PDAF can be included in the model source code.~~The data transfer (coupling) between the model and the data assimilation module can be handled in two ways:

- offline coupling: data exchange via the input/output files of the model
- 255 – online coupling: data exchange via main memory

The first method ~~is more ad-hoc (offline coupling) is more ad hoc~~ and also applicable when the source code of the model is not available ~~and the model is integrated through system calls.~~ In this case, the user needs to take care of the execution of the model forward runs to the next assimilation cycle. An additional executable containing calls to PDAF routines is then used to perform the data assimilation. Within this executable, PDAF reads the state vector from the model output files, performs the assimilation and writes out the assimilation results in the form of input files for the next model integration. One drawback is that this coupling method produces ~~more~~ a lot of I/O overhead because a huge amount of files has to be read and written at each assimilation step. Another drawback of the offline coupling is that the model needs to be re-initialised after each assimilation
260 step. ~~The~~ In the second variant (online coupling), PDAF is directly integrated into the model source code. This enables a direct data transfer between the model and the data assimilation algorithms of PDAF via main memory. Additionally, the model only needs to be initialised once because the model integration is only paused for the data assimilation with PDAF within the time stepping loop of the model. This coupling variant is significantly faster in terms of CPU-time but requires more
270 programming effort and the availability of the model source code.

The model coupling for both coupling variants (offline and online) is defined by the user through the aforementioned generic interface routines that are provided by PDAF. These routines include:

- Definition of the state vector for PDAF which has to be provided by the model either from the model output files or via exchange in main memory.
- 275 – Definition of the measurement vector and the corresponding measurement uncertainties and error covariances (usually via observation files).
- Rules how the updated state vector is transferred back to the model.
- Pre- and post-processing routines for, e.g., printing out diagnostic information on the assimilation process

280 These interface routines partly depend on the filter algorithm that is used for data assimilation. For example, local filter variants like LETKF need special routines to infer the position of each element of the state vector in the model domain in order to perform the localization ~~which is not needed by global filter algorithms like EnKF~~. Also the definition of the error covariance matrix can vary depending on the application and several interface routines are provided by PDAF to construct this

285 matrix.

At the very beginning of the initialisation phase of the model, a PDAF routine needs to be called that establishes the parallel communication within the model and the data assimilation algorithms. This is especially important for fully parallel models like the ones in TerrSysMP. In this phase, PDAF creates three parallel communicators: The model communicator, the coupling communicator

290 and the filter communicator. The general layout of these communicators is depicted in Fig. 2 for a model setup with 3 ensemble members and 4 processors per model realisation. The model communicator is created for each ensemble member separately and in case of a parallel model it is equal to the models' internal communicator (i.e., a replacement of `MPI_COMM_WORLD`). The filter communicator is used to perform the filter algorithms which are only applied on the processors of the first

295 ensemble member (marked in red colour in Fig. 2) while the other processors remain idle during the filter update. Within the filter communicator, the processors exchange information about the simulation results at observation points and global ensemble statistics (ensemble mean and variance). The coupling communicator is the communicator for exchanging data between the processors in the filter communicator and the remaining ensemble members before and after the assimilation step. As

300 noted by the arrows in Fig. 2, this data exchange is according to the processor ranks in the model communicator, i.e., the data exchange only takes place for each subdomain of the model and not on a global level. A global vector of model states is never used in this scheme.

4 TerrSysMP-PDAF

This section describes the implementation and usage of the data assimilation system for TerrSysMP

305 which is referred to as TerrSysMP-PDAF in the following.

4.1 Technical implementation

In order to establish a data assimilation system for the land surface–subsurface part of TerrSysMP (CLM and ParFlow) with the data assimilation framework PDAF, an interface between the model and the data assimilation framework was created. As the forward model is already computationally
310 very demanding and the source code of the model is readily available, we decided to follow the online coupling approach (data exchange via main memory and not running the model as a single executable) in order to avoid frequent re-initialisations of the model and a significant overhead in I/O operations which both degrade the performance of the constructed data assimilation system for TerrSysMP. In order to accomplish this, several changes in the source code and the building script
315 of TerrSysMP had to be undertaken: First, the main program sections of the two component models were split into separate callable routines for initialising, advancing and finalizing the respective model. With these routines the models were packed into (pseudo-)libraries making them callable from within the main program section of TerrSysMP-PDAF. This step was undertaken to keep all the necessary model data in main memory and thus avoid a frequent re-initialisation of the model
320 which e.g., would be present if TerrSysMP was called as a binary program. ~~Secondly~~Second, several changes in OASIS-MCT were necessary to allow the propagation of all ensemble members at once. One problem that arose here was that OASIS-MCT implicitly used the global communicator `MPI_COMM_WORLD` to establish the exchange of state and flux variables between the component models of TerrSysMP. As only one `MPI_COMM_WORLD` can be present within a MPI job
325 this prevented the ensemble propagation. Therefore, this implicit declaration of the data exchange communicator was replaced in several OASIS-MCT routines and the data exchange communicator was replaced with the model communicator that is provided by PDAF. ~~Thirdly~~Third, several CLM and OASIS-MCT output files have a fixed naming convention. In order to avoid an overwriting of these files by the different ensemble members it was necessary to rename these output files. This
330 was done by adding the realisation number of the respective ensemble member to these file names. With these changes in the model source code (and building procedure) it was possible to combine the model libraries for CLM and ParFlow (including OASIS-MCT) with the data assimilation libraries provided by PDAF in one main program. Figure 3 sketches the different components of the TerrSysMP-PDAF framework. The TerrSysMP-PDAF driver (i.e., the main program) controls the
335 whole framework. This includes the initialisation and finalisation of MPI, TerrSysMP and PDAF as well as the time stepping control for the model forward integration and the data assimilation. The TerrSysMP wrapper is used to interface the driver program with the individual model libraries (`lib-clm` and `libparflow` coupled via OASIS-MCT). The PDAF user(-defined) functions are specifically adapted to TerrSysMP and the desired assimilation scheme (EnKF in this case) and include e.g.,
340 the definition of the state vector, the observation vector and the observation error covariance matrix. These data are either provided by the model directly (e.g., state vector) or are read from files or command line options (e.g., observations and observation errors). The PDAF core functions provide the

algorithms for different filtering methods. This part of PDAF is not modified for the implementation of TerrSysMP-PDAF because the input for the PDAF core functions (e.g., state vector, observation
345 vector, observation error covariance matrix) is already provided by the PDAF user functions.

The TerrSysMP-PDAF driver program proceeds in the following steps:

1. Initialisation of MPI
2. Initialisation of the parallel communication by PDAF
3. Model initialisation for CLM and ParFlow
- 350 4. Initialisation of data structures in PDAF (state vector, measurement vector, etc.)
5. Time loop over measurement time steps:
 - a. Advance CLM and ParFlow to the next assimilation time step
 - b. Filter step by PDAF
 - c. Update of the relevant model variables in CLM and ParFlow
- 355 6. Finalization of PDAF, CLM and ParFlow

In steps 1 and 2, the global MPI communicator as well as the PDAF communicators (see Sect. 3 and Fig. 2) are initialised. In step 3, all processors first read a common input file which holds information about specific settings for the data assimilation run. This includes the number of processors for CLM and ParFlow for each model realisation, the number of ensemble members, time stepping
360 information, specification of the observation data and the model variables that should be updated as well as settings for the model output. Then, within each realisation (model communicator) each processor is assigned either to CLM or ParFlow depending on the processor rank within the model communicator. An example of this model assignment is given in Fig. 4. The first processors within a model communicator are always assigned to CLM and the rest to ParFlow summing up to the total
365 number of processors for each model realisation. Afterwards, each of the component models is initialised with the initialisation function of the corresponding model library (see above). In this step also the model communicators of the respective model realisation are handed over to OASIS-MCT. For the model initialisation, each realisation of CLM and ParFlow reads a different model-specific input file (see Sect. 4.2) which holds information about the specific initial conditions, forcings or pa-
370 rameters of the corresponding realisation. Furthermore, in this step some data structures which hold the model-specific state vector are created. In step 4, the data structures for the data assimilation in PDAF are created. This, for example, includes the size of the state and measurement vector, the matrices for model and measurement covariances, etc. After the initialisation phase of TerrSysMP-PDAF (steps 1 to 4) the time loop over the assimilation cycles takes place. Note that this loop only
375 refers to the updating cycles and that CLM and ~~Parflow~~ ParFlow can run at a smaller time step, i.e.,

the updating cycle is a multiple of the model time steps. For each assimilation cycle, first TerrSysMP is advanced to the next observation time in step 5a. At the end of this step the data structure holding the state vector for the respective model component is filled with the corresponding model variable. The model variables that form the state vector are described further below. Next, in step 5b, the data assimilation algorithm in PDAF is called. In this step the model state vectors are collected on the filter communicator with the help of the coupling communicator (see Fig. 2). Then the observation data are read from netCDF files which hold the ~~observation data~~measurement values, the corresponding measurement errors and information on their spatial location. ~~Currently, the observations are clipped to the nearest grid cell in the model domain~~The spatial location of observations has to be provided in the form of model grid cell indices, i.e. the user needs to determine the grid cells which match the observation locations. The grid cell indices provided in the observation files are then handed over to PDAF which will use these indices to extract the simulation results at observation locations from the state vector. Note that by using grid cell indices, no interpolation or other kind of measurement operation is performed because the observations are simply clipped to the nearest model grid cell.

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The measurement covariance matrix in the current implementation is always diagonal (i.e., the measurement errors for the different observations are uncorrelated) and the measurement error can be different for the individual observations. Afterwards, the filter update is performed. The choice of the data assimilation algorithm for TerrSysMP is currently restricted to the Ensemble Kalman Filter. After the filtering step, the updated state vector is transferred back to the corresponding model variables in step 5c and TerrSysMP-PDAF proceeds to the next assimilation cycle. When all assimilation cycles are finished, the data structures of the individual components of TerrSysMP-PDAF are deallocated in step 6 and the program is shut down.

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Time stepping for the TerrSysMP component models as well as in the data assimilation loop is static, i.e., there is a constant time step for the model integration of TerrSysMP and a constant frequency for the assimilation steps which is a multiple of the TerrSysMP time step.

As TerrSysMP is designed in a modular fashion, the same approach was also chosen for the data assimilation system for the land surface–subsurface part of TerrSysMP. That is, the data assimilation system can run only with ~~Parflow~~ParFlow, only with CLM or for CLM and ~~Parflow~~ ParFlow coupled with OASIS-MCT. In case of using a single model of TerrSysMP, the aforementioned changes of OASIS-MCT communicators for allowing an ensemble propagation are not applicable any more. Instead, the model communicator of PDAF is directly transferred to the internal model communicators of CLM or ParFlow respectively.

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~~Currently, data assimilation with TerrSysMP-PDAF mainly focuses on the update of model variables in ParFlow with EnKF.~~ In the coupled (ParFlow + CLM) and uncoupled (~~Parflow~~ ParFlow standalone) TerrSysMP configuration, measurements of pressure or soil moisture can be assimilated in ParFlow. ~~In the first case,~~ The assimilation of both measurement types involves an update of pressure values in ParFlow because this is ParFlow's prognostic variable and soil moisture (or

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saturation) is a derived quantity which is not directly used as a state variable for the next time step. For the assimilation of pressure data, simulated pressure values in ParFlow are directly modified by the pressure measurements. In the second case, the state vector is constructed with the observations. For the assimilation of soil moisture data, two options are implemented in TerrSysMP-PDAF to update pressure values with soil moisture observations: (1) The state vector consists of soil moisture and pressure values of ParFlow. In this case, pressure values in ParFlow are indirectly corrected with the incoming soil moisture measurements through the correlations between soil moisture and pressure. This is necessary, because the prognostic variable in ParFlow is pressure and soil moisture (or saturation) is a derived quantity which is not directly used as a state variable for (2) The state vector solely contains soil moisture values and the updated soil moisture values are transformed back to pressure values via the 'inverse' van Genuchten function before the next time step. Additionally, besides the state update, it is also possible to include permeability values or Mannings coefficients of ParFlow in the state vector (both log-transformed) and thus to correct these model parameters with incoming pressure or soil moisture measurements. In case the data assimilation framework is only applied with the CLM component, the state vector is constructed with the soil moisture provided by CLM which can be corrected with incoming soil moisture measurements.

4.2 Installing and running TerrSysMP-PDAF

TerrSysMP-PDAF can be seen as an add-on to a regular TerrSysMP installation. A patch script is provided that applies the necessary code changes in OASIS-MCT, ParFlow and the build script of TerrSysMP (see Sect. 4.1). All other routines (e.g., initialisation of parallel communication with PDAF, user specified routines to create the state vector for PDAF, wrapper functions for TerrSysMP, etc.) are additional components on top of a regular TerrSysMP installation. In order to run TerrSysMP-PDAF, the user needs to provide separate model input files for CLM and/or ParFlow for each single ensemble member which follow a certain naming convention (`<< problemname_XXXXX >>`) where XXXXX is the number of the realisation preceded by zeros. In each of these input files the user can specify a different input for initial conditions, forcing terms or parameters, which are used to approximate the variability of the model prediction in the data assimilation framework. These files have the same structure as the standard model input files for ParFlow and CLM except for the special naming convention. Additionally, an input file for the control of the data assimilation has to be provided which includes information on the number of model realisations, the number of processors that are used for each model component, the timing information, information on the desired updating scheme (e.g., kind of observation data and additional parameter update) and settings for the output profile of TerrSysMP-PDAF.

5 Illustrative example

In order to illustrate the TerrSysMP-PDAF framework and investigate its scaling properties, we provide a simple synthetic data assimilation exercise (twin experiment) in the following section. This example deals with the assimilation of soil moisture data into a virtual catchment which is set up for the land surface–subsurface part of TerrSysMP (CLM + ParFlow). A synthetic reference run with predefined subsurface parameters (spatially distributed field of saturated hydraulic conductivity K_s) provides virtual measurement data of soil moisture content for several observation locations. The ensemble for the data assimilation experiment consists of different realisations for spatially-distributed saturated hydraulic conductivity and different precipitation rates. The synthetic soil moisture observation data are used to jointly update soil water content and saturated hydraulic conductivity with EnKF on a daily basis.

5.1 ~~Experimental~~ Experimental setup

The domain of the virtual catchment has a horizontal extension of $5000\text{ m} \times 5000\text{ m}$ and is discretized into 200×200 grid cells with a grid cell size of $25\text{ m} \times 25\text{ m}$ (see Fig. 5). The subsurface domain (modelled with ParFlow) has a vertical extension of 13 m which is discretized into 20 cells with variable thickness. The uppermost ten subsurface layers in ParFlow have an exponentially increasing profile with depth which corresponds to the soil layer thicknesses in CLM. These ten layers sum up to a total thickness of 3 m . Note that for these ten layers, pressure, saturation and land surface fluxes are exchanged between CLM and ParFlow (see Sect. 2). The ten remaining subsurface layers have a constant thickness of 1 m . The topography of the model domain is flat which means that there is no topographically driven overland flow within the domain. The porosity is set to a value of $0.4\text{ m}^3\text{ m}^{-3}$ and the specific storage to $1 \times 10^{-4}\text{ m}^{-1}$ and both are spatially constant throughout the subsurface domain. Variably saturated flow was ~~parameterized~~ parametrized with the van Genuchten model (van Genuchten, 1980). The van Genuchten parameters α and n were both set to a spatially constant value of 2.0 m^{-1} and 2.0 respectively.

The land surface is covered by three vegetation types (i.e., plant functional types) in this example: deciduous forest, crop and grassland (see Fig. 5). The meteorological forcings (Fig. 6) are taken from reanalysis data of the German Weather Service (DWD) for the year 2013 for a grid cell close to Juelich (Germany) and the assigned meteorological forcings are spatially homogeneous within the virtual catchment. The boundary conditions for the subsurface domain are no flow in the southern, eastern and western faces and a constant head boundary condition (water table depth of -3 m) at the northern face. The initial groundwater table in all simulations is linearly decreasing from -2 m at the southern boundary to -3 m at the northern boundary.

For the data assimilation experiments a synthetic reference run was created with the model mentioned above. The synthetic reference field of $\log_{10}(K_s)$ was generated with two dimensional un-

conditioned sequential Gaussian simulation using the gstat package (Pebesma, 2004) in the statistical software R (R Core Team, 2015). A spherical variogram with a nugget of $0.0 \log_{10}(\text{m h}^{-1})$, a sill of $0.1 \log_{10}(\text{m}^2 \text{h}^{-2})$ and a range of 70 model grid cells (1750 m) was used for the simulations. A constant value of $-3 \log_{10}(\text{m h}^{-1})$ was added to the generated $\log_{10}(K_s)$ -field and the final
485 field was assigned to each model layer. The synthetic reference simulation was run for six months (January–June 2013, 181 days) with an hourly time step for both ParFlow and CLM. Observation data (soil water content) from this reference run are collected at 16 observation points (Fig. 5) which are evenly distributed over the whole virtual catchment. Observations are taken at different depths ranging from the uppermost model layer (-1 cm) in the south to the sixth model layer (-65 cm)
490 in the north. [Additionally, four verification points are defined to assess the effect of soil moisture assimilation in between the observation points.](#)

For the data assimilation experiment, an ensemble of 128 realisations of subsurface parameters ($\log_{10}(K_s)$) and meteorological forcings was created. The $\log_{10}(K_s)$ -fields were also generated with unconditioned sequential Gaussian simulation with the same geostatistical parameters as for
495 the reference field. Only the sill value was increased to $0.2 \log_{10}(\text{m}^2 \text{h}^{-2})$. The ensemble of meteorological forcings was generated by perturbing precipitation rates from the DWD reanalysis data with multiplicative noise sampled from a uniform distribution $U(0.5, 1.5)$. For each realisation, daily perturbation factors were sampled from the uniform distribution and the hourly precipitation values were multiplied with the corresponding perturbation factor. The daily perturbation factors were ran-
500 domly sampled, i.e., no temporal correlation was considered.

First, the ensemble was used to perform an open-loop simulation (i.e., no observation data are assimilated) for the whole simulation period (January–June 2013). This simulation serves as a spinup and benchmark for the following data assimilation run. Data assimilation was performed for the second half of the simulation period (April–June 2013) after the ensemble was spun-up for the first
505 three months (January–March). Observation data from the reference run (soil moisture content) were assimilated on a daily basis for all 16 observation points. The measurement error for all observations was set to $0.02 \text{ m}^3 \text{ m}^{-3}$ and measurement errors were assumed to be spatially uncorrelated. The measurement data were used to jointly update the pressure and $\log_{10}(K_s)$ fields in ParFlow [with an augmented state vector approach](#), resulting in 1.6 million unknowns for the data assimilation
510 problem.

5.2 Scaling behaviour of TerrSysMP-PDAF

In order to check the computational efficiency of TerrSysMP-PDAF in a high-performance computational environment, we performed a weak scaling study on the supercomputer JUQUEEN located at Forschungszentrum Jülich (Germany). JUQUEEN consists of 28 672 IBM BlueGene/Q compute
515 nodes with a total of 458 752 processors and 448 TB main memory. Each compute node consists of 17 cores (16 for computation, 1 for operating system services) running at 1.6 GHz and 16 GB main

memory. The compute nodes allow for simultaneous multithreading (SMT) up to a factor of four which means that up to 64 processes can run on one node. JUQUEEN uses a static memory mapping to processors, so one processor can utilise a maximum of 1 GB main memory (256 MB in case of
520 four-way SMT). The whole system reaches a Linpack performance of 5.0 Petaflops. More details on the system architecture of JUQUEEN can be found in Gasper et al. (2014).

In a weak scaling study, which is typically performed for such kinds of systems, the workload per processor is held constant and the problem size linearly increases with the number of processors. As we are not interested in the scaling properties of TerrSysMP itself, which have been described in
525 detail by Gasper et al. (2014), we keep the number of processors for each model realisation constant and increase the number of model realisations along with the number of processors. For the scaling study, the synthetic model setup described in Sect. 5.1 is used but only the first 20 assimilation time steps (1 April–20 April 2013) are calculated. For each model realisation 128 processors were used which keeps the workload per processor constant. The partitioning of processors for one realisation
530 was 96 for ParFlow and 32 for CLM which was found to be the most optimal ratio for both models in terms of simulation time and computational efficiency. Furthermore, preliminary tests suggested that using 32 processors per node (two-way SMT) on JUQUEEN was the best compromise between execution time and memory requirements of ParFlow and CLM. For the weak scaling study, the number of realisations was increased from 8 to 256 and the corresponding number of proces-
535 sors ranged from 1024 to 32 768. Between each step of the scaling the number of realisations and processors was doubled (see Table 1 for information on all investigated scaling steps). The lowest number of realisations (processors) was set to 8 (1024) because this is the lowest possible job size on JUQUEEN given our chosen setup (128 processors per model realisation, 32 ranks per compute node). The scaling behaviour can be ~~accessed~~-assessed by calculating parallel efficiency E for weak
540 scaling:

$$E(n_p) = \frac{T_{1024}}{T(n_p)} \quad (1)$$

where $E(n_p)$ is the parallel efficiency of n_p processors, T_{1024} is the execution time with 1024 processors and $T(n_p)$ is the execution time with n_p processors. The timing information for the weak scaling study was acquired by instrumenting TerrSysMP-PDAF with the parallel performance
545 tool Scalasca (Geimer et al., 2010) (version 2.2.1). Note that no special optimisation (such as critical path analysis) was performed to acquire the timing information with Scalasca.

A specific problem that occurs for ~~accessing~~-assessing the parallel performance of ensemble methods like the EnKF in TerrSysMP-PDAF is that the simulation times for different ensemble members varies according to the assigned forcings and parameter sets. This, of course, can introduce some
550 load balance issues because the filtering step introduces an effective barrier for the parallel computation. This implicit barrier causes the processors, for which the computation of the specific realisation is already finished for the current time step, to wait until the computation of the remaining model

realisations is finished before they can proceed to the filtering step. This is typically not the case when parallel performance is measured for a deterministic model (as for example in Kollet et al., 555 2010; Gasper et al., 2014). In this case, the same model setup is extended spatially for keeping a fixed workload per processor, meaning that the internal model processes during the calculation stay the same when the weak scaling behaviour is ~~accessed~~ assessed by simultaneously increasing the domain size and the number of processors.

Therefore, the scalability of TerrSysMP-PDAF was first tested with a homogeneous ensemble 560 where all ensemble members are identical to the reference run that was used to generate the observation data. This means that for all ensemble members the reference $\log_{10}(K_s)$ -field and the deterministic (unperturbed) forcings were used. As a result, there is no variability in the ensemble for this setup. Although this idealised setup is not meaningful from a methodological perspective (as all ensemble members are identical) this will provide information about the scaling of TerrSysMP 565 in a pure technical sense and helps to gain insight into the computational limits for performing data assimilation with TerrSysMP in a massively parallel environment. In a second step, the scaling was investigated for the heterogeneous ensemble that is described in Sect. 5.1. For this setup, also the load imbalance caused by variable forcing and parameter sets is taken into account in the scaling results. Note that results from this scaling setup heavily depend on the chosen uncertainty descrip- 570 tion and the model dynamics of the chosen assimilation time period. Furthermore, the settings of the solver and the time stepping that is used to solve the transient variably saturated groundwater flow equations in ParFlow influence the scaling behaviour in this case. Therefore, results from this study are only meant to provide an example on how the scaling could look like for a typical application of TerrSysMP-PDAF for a coupled land surface–subsurface environment. In this study, no attempt 575 was made to optimise the time stepping and solver settings of ParFlow in order to decrease load imbalance issues.

Aside from the above mentioned effect of ensemble heterogeneities, another important issue that influences the parallel performance of data assimilation algorithms are the input/output (I/O) settings of the model code. Compared to a deterministic model run, the I/O operations multiply with the 580 number of realisations in a data assimilation run. This can create a certain bottle neck for the code performance when large amounts of output data are written to disk simultaneously. Usually, in data assimilation applications the model output is restricted to the most important variables and mostly include the assimilated state variable and possibly other state variables or parameters that are jointly updated with measurement data or provide diagnostic information on the model performance. In 585 some cases, detailed information on the distribution of certain variables is required which means that output files from all ensemble members are needed for this variable. In other cases, knowledge on the statistics (e.g., mean and standard deviation) of a certain variable is sufficient. As ensemble output might be of importance for the parallel efficiency we also compared three scenarios with a varying degree of model output:

- 590 – No model output
- Mean and standard deviation of simulated pressure and updated $\log_{10}(K_s)$ -fields are calculated during model execution and are written to file by the filter communicator
 - Output files for simulated pressure and updated $\log_{10}(K_s)$ -fields are written for all ensemble members

595 These three I/O scenarios were compared for the idealised test case (homogeneous ensemble) as well as the test case with a heterogeneous ensemble. This gives a total of six scaling scenarios. For each of these scenarios, the parallel efficiency was calculated with Eq. (1) separately meaning that the parallel efficiency is always normalised to the respective simulation with 1024 processors (T_{1024}).

Figure 7 shows the scaling behaviour and timing information for the ideal (homogeneous ensemble) and non-ideal (heterogeneous ensemble) scaling runs. The parallel efficiency for the ideal test case stays very high (> 0.8) for all output scenarios within the investigated range of resources. The scenarios with model output show a slight reduction of parallel efficiency for a higher amount of processors (> 8192). From the absolute timing information one can see that the scenario with full ensemble output requires systematically more time than the scenarios with no model output and statistical output only. The scenario with statistical output requires approximately the same simulation
605 time as the no I/O scenario for a lower number of processors but then levels off for higher processor numbers (> 8192).

The parallel efficiency with the more realistic setting (heterogeneous ensemble) in Fig. 7 generally shows a stronger and faster decrease with increasing resource allocation. The differences to the
610 ideal test case are in the order of 10–20% which is mainly caused by the load imbalance within the heterogeneous ensemble. Nevertheless, the parallel efficiency for the heterogeneous setup is still around 0.6 for the largest tested processor allocation. From the timing information in Fig. 7 one can see that the scenario with full ensemble output requires more CPU-time than the other scenarios for a lower number of processors. For a higher resource allocation, the differences between
615 the I/O scenarios tend to vanish which is a significant difference to the idealised test case. This behaviour is probably related to the load imbalance within the ensemble which leads to a certain time delay in the writing of output files. On the contrary, in the idealised test case all ensemble members finish the model forward integration at approximately the same time which means that all ensemble members tend to write output files synchronously. Note that for the heterogeneous case,
620 an offline coupling between TerrSysMP and PDAF would also lead to a certain time overhead due to I/O operations because the writing and reading of restart files after the assimilation step would also occur simultaneously before the next model integration.

~~A more~~ More detailed information on the timing of individual components of TerrSysMP-PDAF for the idealised scenario can be found in Fig. 8. Here, the total execution time is categorised in four
625 components: model initialisation, model integration, data assimilation and model shut-down. These

categories sum up to the total execution time and are normalised to the total amount of processors that are used for the respective simulation. From the absolute values of the different model components it can be seen that by far most of the time is dedicated to the model integration. The computation time for model initialisation and the assimilation step have a similar order of magnitude but also exhibit some differences with respect to the I/O scenarios. The finalisation step only consumes a negligible part of the simulation time. In the initialisation phase, there is a significant increase of computation time for all three I/O scenarios when the number of processors exceeds 8192. This increase is related to the fact that many common input files are shared among the different realisations. The access to these shared input files on the storage system can be a bottleneck especially for a higher number of processors. Furthermore, the initialisation and setup of the parallel communication through OASIS leads to a certain communication overhead when moving to a higher number of processors. During the model integration and the assimilation step, the scenario with the complete ensemble output again shows a significant deviation compared to the no I/O scenario. The reason is that in both phases the ensemble output is written to disk. At the end of the model integration the output files for the state variable (pressure) are written and at the end of the assimilation phase the same is done for the updated parameter fields (K_s). For the scenario with statistics output a slightly different pattern can be observed. The run times for this scenario are similar to the no I/O scenario for lower processor number (up to 8192) for both the model integration and the assimilation step. When the number of processors is further increased, the calculation of ensemble statistics leads to a certain overhead which degrades the performance compared to the no I/O scenario. Also in this case the ensemble statistics are calculated and printed out at the end of the model integration (pressure fields) and at the end of the assimilation phase (updated K_s). In the finalisation phase there is also a certain offset for the scenario with full ensemble output but the required computation time is in general very low compared to the other parts of the program.

The scaling results for the idealised setup are in general very good as the parallel efficiency stays above >0.8 even for a large amount of processors. This is an indication that the coupling between TerrSysMP and PDAF is working very well in a technical sense. Furthermore, the results show that the filter algorithms implemented in PDAF scale well to an even higher number of processors than reported before in Nerger and Hiller (2013). The bottleneck of the parallel performance is mainly the initialisation phase (reading operations and setup of OASIS communication) and the output operations. Here, parallel I/O concepts could help to further improve the parallel performance of TerrSysMP-PDAF. [The scaling results for the more realistic heterogeneous ensemble are also promising for the application of TerrSysMP-PDAF for more complex land surface-subsurface data assimilation problems. Generally, for any given model setup, the scaling behaviour of the data assimilation problem will particularly depend on the numerical robustness of the deterministic forward model towards ensemble perturbations. Critical situations with respect to convergence could occur, e.g., for strong heterogeneities in the subsurface parameterization \(e.g.,](#)

hydraulic conductivities) or for the coupling of overland and subsurface flow. For the latter case, especially the computationally demanding onset and offset of overland flow at particular grid cells (e.g., due to heavy rainfall or recession events) can have a negative influence on the scaling behaviour of the deterministic forward model (Kollet and Maxwell, 2006; Osei-Kuffuor et al., 2014). If only a subset of realisations is affected by such convergence problems, also the scalability of the ensemble propagation might be influenced negatively. Therefore, it is important to configure the deterministic forward model well with respect to numerical stability and execution time. This can be achieved, e.g., through the correct choice of solver parameters, an adequate spatio-temporal discretization of the problem and a proper choice of model parameters and ensemble perturbations.

5.3 Data assimilation results

Figure 9 shows time series of simulated soil water content at four ~~observation points~~ verification points (see Fig. 5) along the south-north direction for both the open-loop (upper row) and the assimilation run (lower row). Results for the open-loop simulations already show that the temporal dynamics of the reference run are well represented by the ensemble and that the changes in soil moisture very much depend on the dynamics of the meteorological forcing data. Assimilation of soil moisture data leads to a reduction of the ensemble spread and a reduction of the ~~bias-mismatch~~ between the ensemble mean of forecasted soil moisture and the reference values. ~~Figure 10 additionally compares~~ Additionally the absolute average error (AAE) of soil moisture content θ ~~for is used to assess the model performance of~~ the open-loop and the assimilation run:

$$\text{AAE}_\theta = \frac{1}{N_t} \sum_i^{N_t} |\bar{\theta}_i^{\text{sim}} - \theta_i^{\text{ref}}| \quad (2)$$

where $\bar{\theta}^{\text{sim}}$ is the ensemble mean of simulated soil moisture, θ^{ref} is the reference soil moisture content and N_t is the number of assimilation time steps. AAE $_\theta$ averaged over the uppermost ten model layers reduced from 0.0135 m³ m⁻³ (open-loop simulation) to 0.0096 m³ m⁻³ (assimilation experiment) through the assimilation of soil moisture data (the ten lower model layers were excluded from this calculation because they are constantly saturated during the whole simulation period). In Fig. 10 AAE $_\theta$ is shown for one specific model layer at -65 cm depth. It can be seen from Fig. 10 that AAE $_\theta$ is reduced in large parts of the model domain which means that data assimilation was not only effective at the observation locations but also significantly improved the model performance in the surrounding grid cells. Several spots in the model domain, e.g., at the southern boundary and in the north-east show less improvement which may be related to the assigned boundary conditions and the fact that the distance to observation points is larger at the model boundaries which reduces the correlation between observation points and those grid cells.

~~The errors of~~ The effect of soil moisture assimilation on land surface fluxes (latent and sensible heat flux) ~~were also analysed and their spatial pattern is very similar~~ was also analysed for this setup. The total AAE values (averaged over all grid cells and time steps) in the open-loop run were

1.003 Wm^{-2} for sensible heat flux and 1.212 Wm^{-2} for latent heat flux. The spatial pattern of errors in land surface fluxes is closely related to those of AAE_θ in Fig. 10. However, the absolute magnitude of AAE. In principal, the calculation of land surface fluxes within TerrSysMP can be affected by: (1) plant physiological parameters (2) meteorological forcings that affect stomatal conductance and (3) the availability of water in the subsurface. In the chosen setup neither plant physiological parameters nor meteorological forcings (with the exception of precipitation) were perturbed, so the variability of land surface fluxes is relatively low and lies around 0.2–4.4 for latent heat flux and 0.2–3.4 for sensible heat flux (both for mainly influenced by the availability of water in the rooting zone. The relatively low errors in the open-loop simulation). The improvements made by assimilating indicate that the variability of soil moisture content are relatively limited for only had a limited effect on land surface fluxes which is related to the shallow ground water table in the simulations guaranteeing that actual evapotranspiration is equal to potential evapotranspiration in the chosen setup and that most of the model domain is not affected by water limitation. With the assimilation of soil moisture contents, the total AAE values of sensible (latent) heat fluxes were reduced to 0.730 (0.876) Wm^{-2} respectively which is a relative improvement of about 27%. Nevertheless, the absolute magnitude of land surface flux errors and the improvements by data assimilation are relatively low due to the fact that the system was not affected by water limitation throughout the simulation period.

In the presented data assimilation experiment, soil moisture data from the reference run are also used to simultaneously update the $\log_{10}(K_s)$ -fields of the ensemble. In Fig. 11 the reference field of $\log_{10}(K_s)$ is compared with the average $\log_{10}(K_s)$ -field of the initial ensemble and the average $\log_{10}(K_s)$ -field after the assimilation period. It becomes obvious that the correction of $\log_{10}(K_s)$ values through the assimilation of soil moisture observations leads to a significant improvement of the estimated average $\log_{10}(K_s)$ -field. Compared to the initial estimate of $\log_{10}(K_s)$, the updated average $\log_{10}(K_s)$ -field includes the main structural features of the reference field, e.g., the higher $\log_{10}(K_s)$ values in the eastern part and the lower values in the western part. Again, as for AAE_θ , the improvement is less pronounced at the model boundaries especially in the southern part. This can again be related to the lower observation density at the model borders.

5.4 Applicability at hyper-resolution

The problem size of the TerrSysMP model used for the scaling study and the verification example in the previous two subsections is very close to typical state-of-the-art applications of integrated land surface–subsurface models at the catchment scale. However, integrated modelling is also continuously moving forward towards higher model resolutions (e.g., Maxwell et al., 2015) which was identified as one of the forthcoming challenges in earth system modelling (e.g., Wood et al., 2011; Bierkens et al., 2014). Therefore, it was also tested whether the TerrSysMP-PDAF data assimilation framework is also applicable for models with a much bigger problem size.

For this purpose, the problem size of the forward model was increased by a factor of 25 by increasing the horizontal model resolution to 5 m (1000×1000 grid cells) leading to 20 Mio. grid cells
735 for the subsurface part of TerrSysMP.

The model input for the synthetic reference and the ensemble was re-gridded to this higher model resolution. The $\log_{10}(K_s)$ -fields for the synthetic reference and the individual ensemble members were additionally perturbed with small-scale noise which was introduced to resemble a certain sub-scale variability within the original 25 m grid cells. The small-scale perturbation fields were generated with the Parallel Gaussian simulation algorithm implemented in ParFlow with a horizontal correlation length of 20 m and a standard deviation of 0.2 log units. The reference $\log_{10}(K_s)$ -fields for the 25 m- and 5 m-resolution models are shown in Figs. 11 and 12 respectively. ~~Note that the scale in both figures is different and covers the respective range of the $\log_{10}(K_s)$ -values which is a bit higher for the 5-resolution model due to the additional small-scale perturbation.~~ The setup for
740 the data assimilation experiment for the high-resolution model was identical to the 25 m-resolution case, i.e., 90 days of model spinup and daily assimilation of 16 soil moisture observations for 91 days with a joint state-parameter estimation.

The simulations for the 5 m-resolution model were run using 4 complete racks (65 536 physical cores with 2-way SMT) on JUQUEEN to solve the data assimilation problem for 40 Mio. unknowns.
750 The simulation time for the assimilation period (91 days) with this configuration was about 4.5 h. Figure 12 shows the initial and updated ensemble mean of $\log_{10}(K_s)$ for the 5 m-resolution model. As for the 25 m-resolution model, the main features of the reference field, e.g., the high conductivity parts in the eastern part of the model domain, were retrieved through the update of $\log_{10}(K_s)$ -values with soil moisture data. However, the updated $\log_{10}(K_s)$ -patterns do not match exactly which can
755 be explained by the different support range of observations for the two model resolutions and the additional sub-scale variability added in the 5 m-resolution model.

Of course, the model setup that was used here is relatively simple in terms of model dynamics compared to typical real-world applications of integrated earth system models. Topography, heterogeneous land surface parameters and spatially distributed meteorological forcings usually lead to
760 a much more complex model behaviour which also leads to far longer simulation times compared to the model setup used in this study. This will make data assimilation with high-resolution integrated models for real-world applications very challenging with respect to the amount of necessary computational resources. Nevertheless, these simulations with a relatively simple high-resolution model setup show that the TerrSysMP-PDAF framework is technically able to cope with data assimilation
765 problems where the problem size of the forward model is in the range of tens of millions grid cells. Such problem sizes will become more common especially in the context of integrated hydrological modelling on the catchment scale (e.g., to better resolve small scale variabilities in hydraulic parameters) as well as for large-scale applications in order to improve hydrological and meteorological forecasts on the basin and the continental scale.

770 6 Conclusions and outlook

In this paper, we presented a modular high-performance data assimilation framework for the land surface–subsurface part of the integrated terrestrial system modelling platform TerrSysMP. In TerrSysMP, land surface processes are modelled with CLM 3.5 and subsurface processes with ParFlow where both models are coupled via the exchange of states and fluxes with the coupling software OASIS-MCT. The data assimilation system for this model was established with the Parallel Data Assimilation Framework (PDAF) which provides a suite of efficient and scalable data assimilation algorithms. The coupling between TerrSysMP and PDAF is done in a fully integrated fashion meaning that the model ensemble as well as the infrastructure for data assimilation is only initialised once and the data assimilation system is continuously integrated forward in time without the need of system calls to the model or re-initialisation of any of the system components. The data exchange between TerrSysMP and PDAF is done completely via main memory which avoids the need for a frequent reading and writing of model restart files. TerrSysMP as well as PDAF are fully parallelized and the data exchange between the two components makes effective use of the domain decomposition in the models. This significantly reduces the memory requirements of the system because the global state(-parameter) vector does not need to be stored completely in any part of the filter algorithm. In addition to the parallelism in the model integration (provided by the component models of TerrSysMP) and in the filtering step (provided by PDAF) also the ensemble propagation is running fully parallel. The data assimilation system for TerrSysMP is designed in a modular fashion, i.e., assimilation can either run with the coupled land surface–subsurface model (ParFlow + CLM coupled via OASIS-MCT) or with one of the standalone models (~~Parflow~~ ParFlow or CLM). This provides the user with some flexibility regarding the model choice because for certain modelling purposes the use of a single compartment model (subsurface or land surface) may be sufficient in the context of data assimilation whereas in other situations a fully coupled approach may be more adequate. Currently, pressure and soil moisture data can be assimilated in ParFlow. These data are used in ParFlow for a state update of the 3-D pressure field but they can also be used for a joint update of saturated hydraulic conductivities or Mannings coefficients. If the assimilation system is only running with CLM, soil moisture data can be assimilated directly into CLM.

In this study we also provide a scaling study on the massively parallel environment JUQUEEN which shows that the assimilation system runs efficiently and scales well even for a high amount of processors (32 768). These results are promising for the application of the data assimilation system for large scale applications or high-resolution models which require a huge amount of computational resources and therefore also benefit from an efficient implementation of the ensemble propagation and the filtering step. Additional tests with a high-resolution model setup where 20 Mio. states and 20 Mio. parameters were updated simultaneously (as compared to 0.8 Mio. states and 0.8 Mio. parameters in the scaling study) revealed that the infrastructure of the proposed TerrSysMP-PDAF framework is well suited for such large problem sizes. Results from the scaling study also showed

that the output strategy (ensemble output vs. statistical output) as well as load balancing issues between the different ensemble members can have a certain influence on the parallel efficiency which should be carefully taken into consideration when data assimilation is performed with a large amount
810 of computational resources.

In further work we plan to include also the atmospheric compartment model of TerrSysMP (COSMO-DE) in the assimilation system. This will allow us to investigate the effect of data assimilation in a fully coupled system from the subsurface to the atmosphere. It is also planned to extend the data assimilation system to make full use of the functionality of PDAF with respect to filter variants and assimilation options (e.g., localization and smoothing). Furthermore, the data assimilation system will be extended with additional measurement operators for soil moisture assimilation including measurement operators for active and passive radar remote sensing data and cosmic ray sensors.
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Code availability

820 The source code of TerrSysMP-PDAF ~~will be made available on the HPSC-TerrSys website () for academic and non-commercial use~~ is added as a supplement to this article.

Author contributions. G. He and W. Kurtz developed the model code. H.-J. Hendricks Franssen, S. J. Kollet and W. Kurtz designed the simulation experiments and W. Kurtz carried them out. R. M. Maxwell and S. J. Kollet provided consultancy for the ParFlow and TerrSysMP model code. W. Kurtz prepared the manuscript with
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Table 1. Number of processors, compute nodes and realisation used in the weak scaling study for TerrSysMP-PDAF on JUQUEEN. Each realisation was computed with a constant number of processors for ParFlow (96) and CLM (32).

# processors	# compute nodes ^a	# realisations
1024	32	8
2048	64	16
4096	128	32
8192	256	64
16 384	512	128
32 768	1024	256

^a A compute node on JUQUEEN consists of 16 + 1 physical cores but allows for simultaneous multithreading up to a factor of four. For the weak scaling study 32 ranks per compute node were used for simulations.

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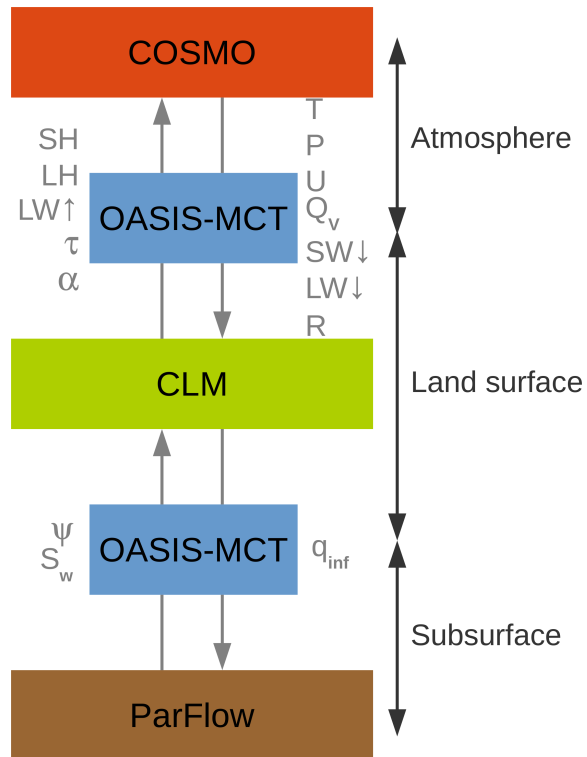


Figure 1. Coupling of the TerrSysMP component models ParFlow (subsurface), CLM (land surface) and COSMO-DE (atmosphere) by OASIS-MCT. The exchanged fluxes and state variables are: ψ (subsurface pressure), S_w (subsurface saturation), q_{inf} (net infiltration flux), SH (sensible heat flux), LH (latent heat flux), $LW \uparrow$ (outgoing long wave radiation), τ (momentum flux), α (albedo), P (air pressure), T (air temperature), U (wind velocity), $SW \downarrow$ (incoming short wave radiation), $LW \downarrow$ (incoming long wave radiation), Q_v (specific humidity) and R (precipitation).

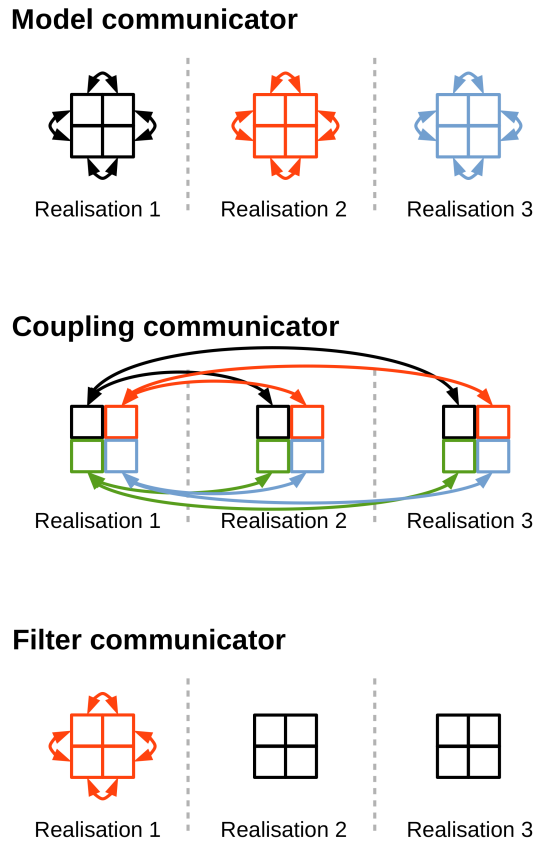


Figure 2. Communicators in PDAF for a parallel setup with 3 ensemble members and 4 processors per ensemble member. Colours indicate the membership of the respective processors and arrows exemplify the parallel communication between the different processors.

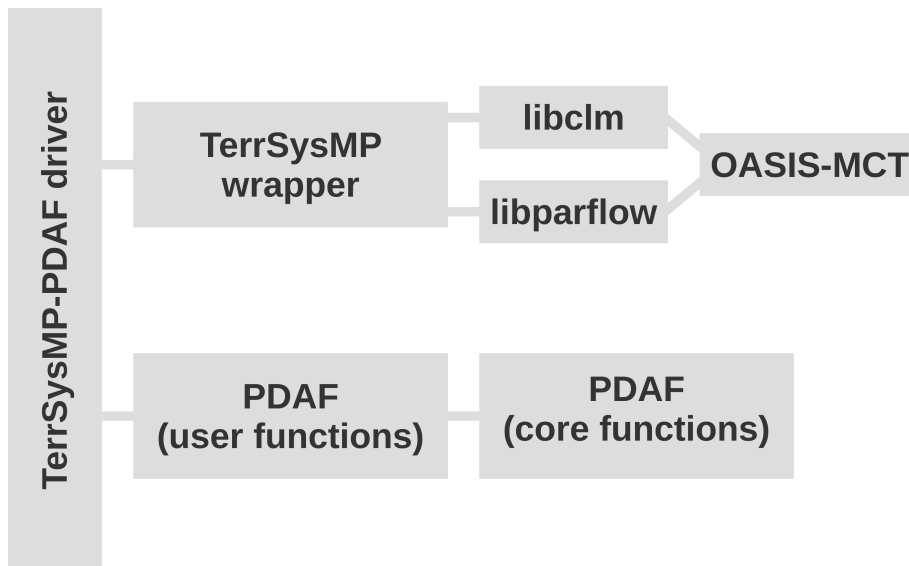


Figure 3. Components of TerrSysMP-PDAF.

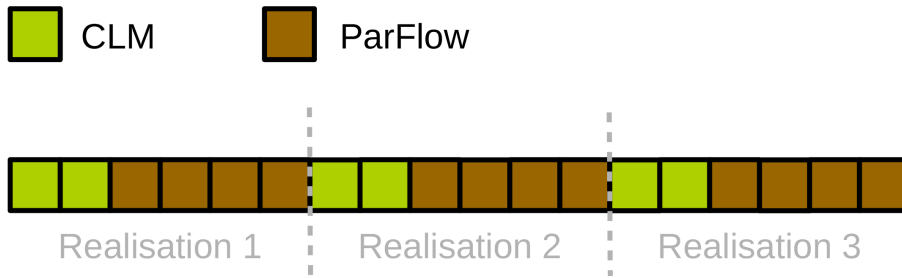


Figure 4. Example of the processor layout of TerrSysMP-PDAF for three model realisations where each realisation is simulated with two processors for CLM and four processors for ParFlow.

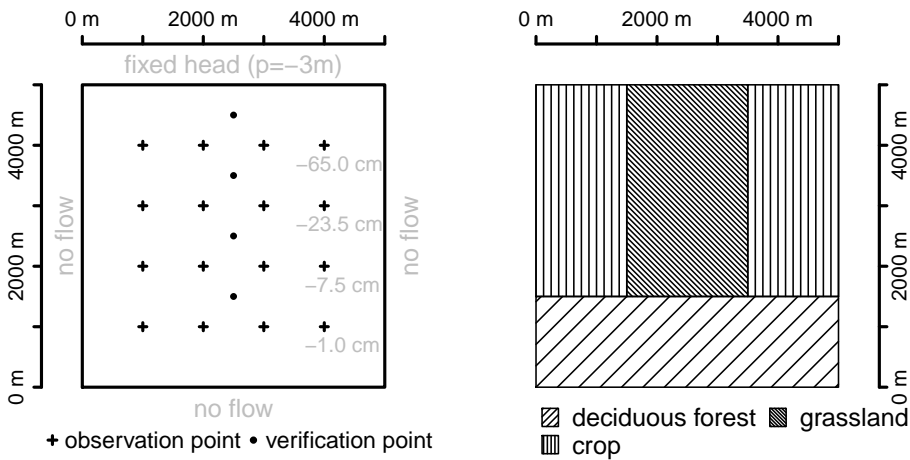


Figure 5. Synthetic setup for the twin experiment. **Crosses-mark** [The left hand figure shows boundary conditions of the subsurface model \(ParFlow\) and the location of observation points \(crosses\) and verification \(filled circles\) points.](#) **Grey** numbers indicate the depth of observation **points and verification nodes** which are constant in W-E-direction. [The right hand figure shows the spatial distribution of plant functional types used in the land surface model \(CLM\).](#)

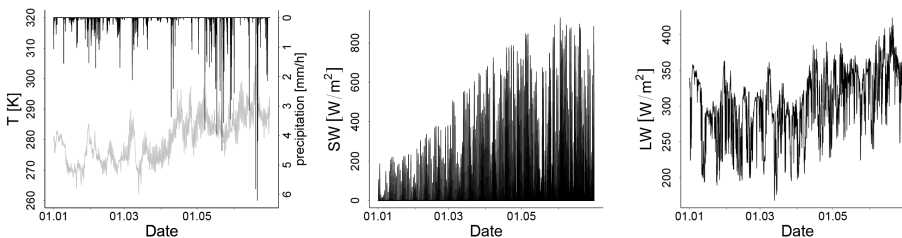


Figure 6. Hourly meteorological forcings for twin experiment from 1 January to 30 June 2013. Left panel shows 2 m air temperature and precipitation, middle panel shows incoming short wave radiation and right panel shows incoming long wave radiation.

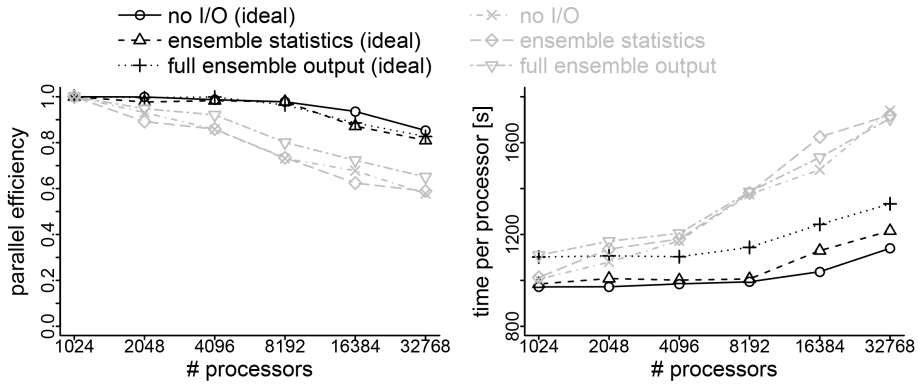


Figure 7. Scaling behaviour (left) and timing information (right) for TerrSysMP-PDAF for a weak scaling test on JUQUEEN. Black lines show results for an idealized test case (identical ensemble members) and grey lines show results for a heterogeneous ensemble. The number of ensemble members is increased from 8 to 256. Each ensemble member used 32 processors for CLM and 96 processors for ParFlow.

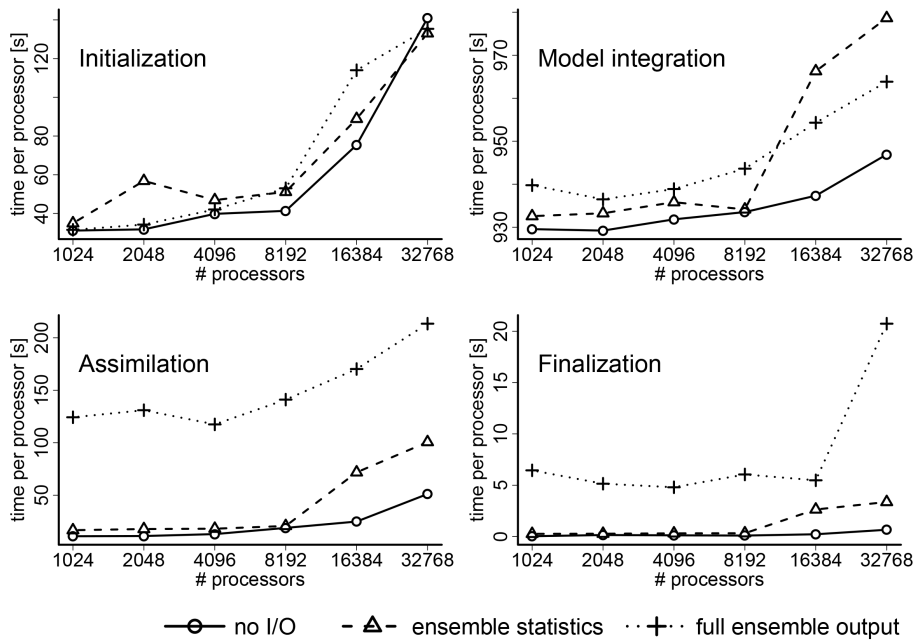


Figure 8. Timing information for individual components of TerrSysMP-PDAF for three I/O scenarios for the ideal test case.

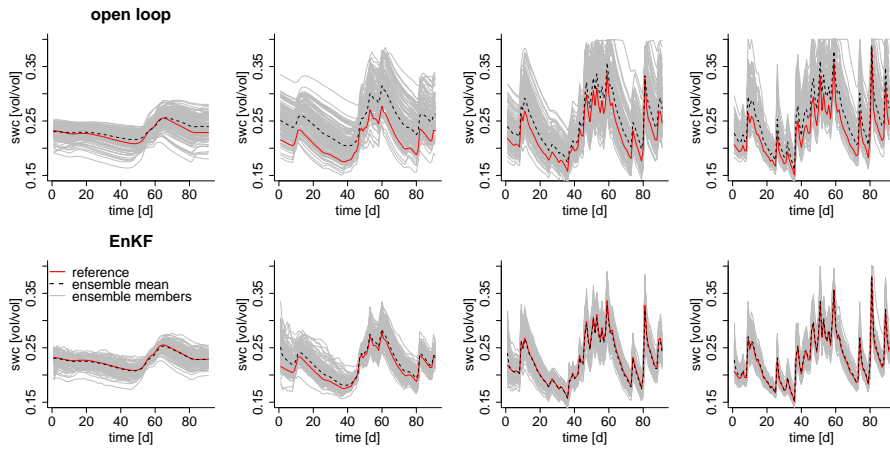


Figure 9. Simulated soil water content at the four observation-verification nodes (second column ($x = 2000$)) in Fig. 5 (from north to south) for April–June 2013 (91 days). Upper row shows results for open-loop simulations and lower row for assimilation.

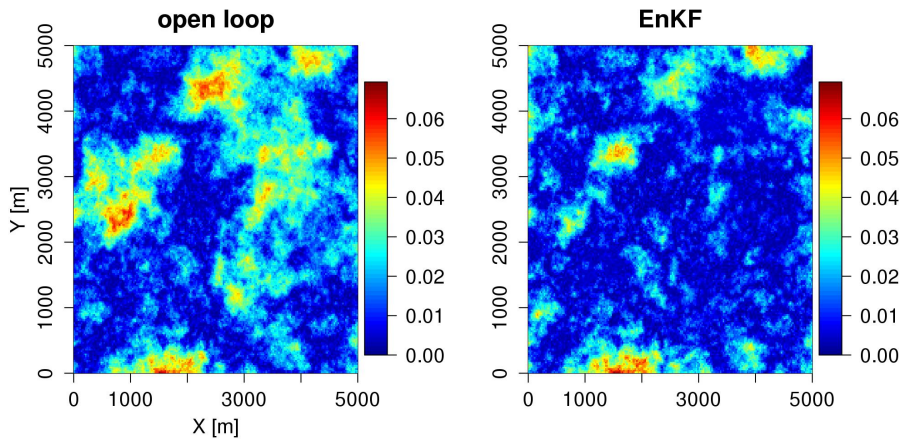


Figure 10. Absolute average error of soil water content AAE_{θ} for open-loop (left) and assimilation (right) at a depth of -65 cm from April–June 2013.

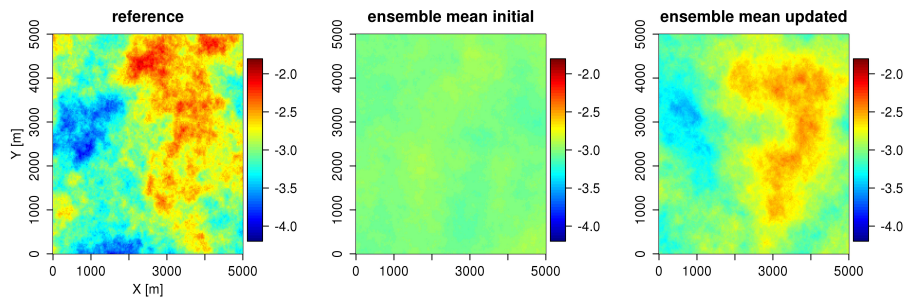


Figure 11. Log-transformed saturated hydraulic conductivity fields of the reference (left), the initial ensemble mean (middle) and the updated ensemble mean at the end of the assimilation period (right).

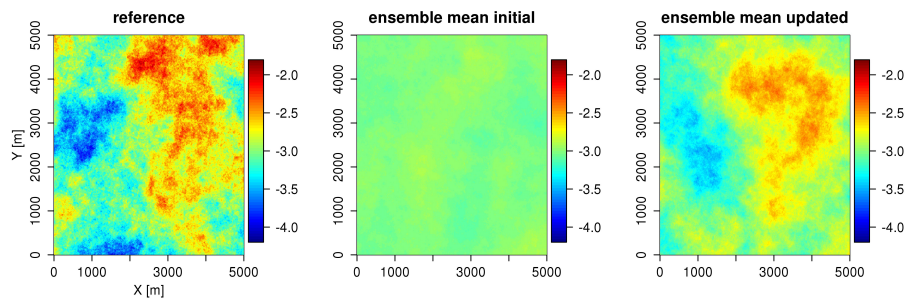


Figure 12. Log-transformed saturated hydraulic conductivity fields of the reference (left), the initial ensemble mean (middle) and the updated ensemble mean at the end of the assimilation period (right) for the 5 m-resolution model.