CC1: 'Comment on egusphere-2025-2124', Nima Zafarmomen

This is a carefully done study and the findings are of considerable interest. And the submission is worth of publication. Following are some minor comments:

1. The paper presents a novel multivariate data assimilation (DA) framework for integrating cosmic-ray neutron sensor (CRNS) soil moisture (SM) and groundwater level (GWL) data into the Terrestrial System Modeling Platform (TSMP). The approach is innovative in its use of a weakly coupled DA scheme to independently update saturated and unsaturated zones, addressing limitations of fully coupled DA systems. However, the manuscript could strengthen its claim of novelty by explicitly comparing the proposed method to existing multivariate DA frameworks in other coupled models (e.g., CATHY, Flux-PIHM, MIKE-SHE, and SWAT-MODLFOW) beyond the brief mentions in the introduction and discussion. For example, "Assimilation of Sentinel-Based Leaf Area Index for Modeling Surface-Ground Water Interactions in Irrigation Districts" used the integrated model fully coupled DA systems and you can cite it to make a stronge fundation for you research. Moreover, the introduction effectively highlights the importance of SM and GWL in terrestrial hydrology and the role of DA in reducing model uncertainties. However, it could better contextualize the study by discussing recent advancements in CRNS technology and its adoption in DA frameworks. For instance, referencing studies like Bogena et al. (2022) or Schrön et al. (2017) earlier in the introduction would clarify why CRNS is a superior choice compared to traditional in-situ or RS-based SM data.

Response: We thank the reviewer for these constructive comments and for recognizing the value of our study. We have expanded the introduction to provide a more explicit overview of existing multivariate DA approaches implemented in coupled hydrological models, including CATHY, Flux-PIHM, and MIKE-SHE. Reference to related multivariate DA framework in SWAT-MODFLOW has also been added to better introduce our approach within existing studies. In the revised manuscript, the introduction now includes the following text reviewing existing multivariate DA studies (lines 88-103):

"Previous studies have applied multivariate EnKF within coupled models like CATHY and Flux-PIHM to jointly assimilate multiple observations, including SM, groundwater, discharge, and land surface fluxes, demonstrating improved estimates of hydrologic states and parameters (Camporese et al., 2009a; Shi et al., 2014; Botto et al., 2018; Shi et al., 2015). Despite being tested primarily on small experimental catchments, these multivariate DA frameworks remain computationally intensive and may involve trade-offs among variables. Some parameters can only be identified under specific hydrological conditions, particularly in strongly nonlinear problems involving the unsaturated zones. To overcome these challenges, some studies have explored alternative multivariate DA strategies within coupled models. Using MIKE-SHE, Zhang et al. (2016) highlighted the importance of spatial and variable-based localization in jointly assimilating SM and groundwater head. Yet, its unsaturated flow is still modeled in one dimension, limiting full system representation. More recently, Zafarmomen et al. (2024) demonstrated that a multivariate particle filter framework assimilating Sentinel-based leaf area index (LAI) and streamflow in a coupled SWAT-MODFLOW model improved estimates of vegetation and hydrologic states. However, the loosely coupled model, in which surface and groundwater components interact via data exchange, may not fully capture integrated dynamics of saturated and unsaturated zones."

Additionally, the discussion section has been extended to compare our proposed weakly coupled multivariate DA framework with these previous studies, highlighting the novel aspects and strengths of our method. The revised text reads as follows (lines 694-703):

"In multivariate DA, previous studies have shown that challenges persist despite methodological advances. Shi et al. (2015) combined model states and global calibration coefficients into a high-dimensional joint vector, requiring covariance relaxation, conditional covariance inflation, and quality control to prevent filter divergence and ensure physical plausibility. Zhang et al. (2016) employed distance and variable localization to control spurious correlations in joint SM and groundwater head assimilation, but this approach relies on manually defined rules and may lose physically meaningful cross-variable information. Botto et al. (2018) applied normalization to measurement error covariance matrices and addressed simulated data anomalies and innovation vectors to prevent ill-conditioning of the Kalman gain. While these measures ensure numerical stability, they require careful manual scaling of each variable."

We have also revised the introduction to better highlight recent advancements in CRNS technology and its integration into data assimilation frameworks, citing relevant studies (e.g., Schrön et al., 2017; Bogena et al., 2022). These revisions clarify why CRNS provides superior soil moisture observations compared to conventional in-situ and RS-based measurements and explain why CRNS was chosen as the data source in our assimilation framework. This revised text has been added in the manuscript (lines 64-76) and is detailed below:

"As an alternative, Cosmic-Ray Neutron Sensors (CRNS) (Zreda et al., 2008) provide reliable, non-invasive SM estimates at the field scale (~18 ha), with deeper penetration (~80 cm) and reduced bias compared to RS products (Zreda et al., 2012; Köhli et al., 2015; Bogena et al., 2022). Recent advances in CRNS techniques, including improved footprint characterization and revised calibration strategies, have substantially enhanced its robustness (Franz et al., 2013; Köhli et al., 2015; Schrön et al., 2017). As a result, CRNS data have been adopted in diverse applications such as hydrology, snow and vegetation monitoring, and land surface modeling (Fersch et al., 2020; Dimitrova-Petrova et al., 2021; Bogena et al., 2022). With the establishment of long-term monitoring networks, CRNS data have also been increasingly integrated into DA frameworks (Baatz et al., 2017; Cooper et al., 2021; Patil et al., 2021). By bridging the scale gap between point measurements and model grids, CRNS serves an effective data source in DA frameworks, thereby reducing model uncertainties and enhancing the reliability of terrestrial hydrology simulations (Shuttleworth et al., 2013; Han et al., 2015; Baatz et al., 2017; Mwangi et al., 2020)."

2. The description of the Rur catchment and data sources (Section 2.1 and 2.3) is thorough, but the rationale for selecting specific CRNS sites and GWL wells is not fully explained. For example, why were only 78 out of 616 wells used for DA, and how was the median GWL selection criterion determined? A

brief justification of these choices would enhance transparency.

Response: We thank the reviewer for highlighting the need to clarify our data selection criteria. To ensure the reliability and representativeness of groundwater level (GWL) observations for assimilation, we applied multiple selection criteria to wells across the study area. Selected wells were required to have GWL observations at depths of 0-20 m within the unconfined upper aquifer, provide at least monthly records during the assimilation period, and should not be located in persistently saturated or river-adjacent grid cells. In addition, when multiple wells were located within a single model grid cell, the well with the median GWL was selected as representative. From a groundwater modeling and parameterization perspective, this ensures that the assimilated observation reflects typical conditions within the grid cell and provides a stable and representative input for data assimilation, while wells with consistently higher or lower GWL may represent extreme or unrepresentative conditions and could introduce biases if used. The median GWL is therefore a robust choice for assimilating state variables and model parameters. Following these criteria, 78 wells were selected for data assimilation, and the remaining wells were reserved for independent validation. A brief explanation of these selection criteria has been added to Section 2.3.3 (Field Measurements of Soil Moisture, Groundwater, and Evapotranspiration) in the revised manuscript (lines 213-225) to clarify our data selection criteria.

"Groundwater table depth data for assimilation and independent validation were obtained from the Geoportal NRW platform (www.geoportal.nrw, accessed May 2, 2025). Given the weak hydraulic connectivity between the RZSM and the deep confined aquifer, this study focused on assimilating data from the unconfined upper aquifer. Wells selected exhibited observation depths between 0 to 20 meters and supplied records with at least monthly observations. In total, 616 wells met these criteria during the 2016-2018 period (Fig. 1). Due to the 500 m model resolution and the spatial clustering of observation wells near rivers, multiple wells were often located within a single grid cell or within river cells. To ensure representative observations for assimilation, the median GWL was chosen among multiple wells within a grid cell to minimize potential biases from unusually high or low groundwater levels. Additionally, grid cells adjacent to stream networks were excluded from the assimilation process, as persistent saturation in these areas caused large discrepancies with observed values. Accordingly, wells situated in river grid cells were excluded from the assimilation. Following these screening procedures, 78 wells were selected for DA, while the remaining 465 wells were reserved for independent validation."

3. The results section provides a comprehensive analysis of ubRMSE, RMSE, and correlation coefficients across multiple experiments. However, the focus on ubRMSE as the primary metric is not fully justified. While ubRMSE accounts for bias, a discussion of why it is prioritized over RMSE or other metrics (e.g., mean absolute error) would clarify its relevance.

Response: In this study, three performance metrics, ubRMSE, RMSE, and R were calculated. ubRMSE is highlighted in the manuscript because it is commonly used in the remote sensing DA literature, which facilitates comparison with existing studies. Focusing on a single metric in the main text also helps avoid redundancy. RMSE and R are also reported in Supplementary Tables to provide a comprehensive *assessment of model performance. Section 3.3 (Model Performance Assessment, lines 380-382) has been revised to clarify this motivation.*

"Among these, ubRMSE was emphasized in our analysis because it is widely applied in DA research and facilitates comparison with previous studies. To avoid redundancy, detailed results for RMSE and R are presented in the Supplementary Tables to ensure a comprehensive evaluation of model performance."

4. The discussion compares the proposed method to Hung et al. (2022) and Zhang et al. (2016), but it could be expanded to include other multivariate DA studies (e.g., Botto et al., 2018; Shi et al., 2015) to highlight how the weakly coupled approach addresses their limitations. For instance, how does the proposed method mitigate the issue of spurious correlations noted in Zhang et al. (2016)?

Response: We thank the reviewer for this valuable suggestion. We have expanded discussion to include Botto et al. (2018) and Shi et al. (2015) to highlight limitations of previous multivariate DA, which can propagate observation errors and generate spurious correlations, as noted by Zhang et al. (2016). In contrast, our weakly coupled DA scheme updates variables sequentially, applying variable-specific spatial localization to restrict cross-variable influence to physically meaningful scales. This approach reduces spurious correlations and maintains physically consistent interactions. The revised manuscript now includes this extended discussion (5.1 Benefits and Challenges of the New Multivariate Data Assimilation Framework, lines 694-718).

"In multivariate DA, previous studies have shown that challenges persist despite methodological advances. Shi et al. (2015) combined model states and global calibration coefficients into a high-dimensional joint vector, requiring covariance relaxation, conditional covariance inflation, and quality control to prevent filter divergence and ensure physical plausibility. Zhang et al. (2016) employed distance and variable localization to control spurious correlations in joint SM and groundwater head assimilation, but this approach relies on manually defined rules and may lose physically meaningful cross-variable information. Botto et al. (2018) applied normalization to measurement error covariance matrices and addressed simulated data anomalies and innovation vectors to prevent ill-conditioning of the Kalman gain. While these measures ensure numerical stability, they require careful manual scaling of each variable.

In contrast, the weakly coupled DA scheme adopted in this study updates states and parameters sequentially, with each variable employing its own spatial localization and independent updates. This allows saturated zone pressure to be updated using GWL observations, while SM estimates in the unsaturated zone are adjusted based on CRNS-derived measurements. The use of variable-specific localization parameters further improves the representation of their distinct spatial characteristics, reduces the influence of spatially distant uncertainties, and limits unphysical information propagation. Importantly, this framework achieves these benefits without requiring extensive manual tuning or high-dimensional corrective procedures, which are often needed in traditional multivariate DA approaches. Additionally, asynchronous assimilation enables different update intervals for each variable: SM, which varies rapidly, is typically updated daily, whereas groundwater, with slower dynamics, is updated weekly.

This approach allows coupled models to better accommodate the differing timescales of fast-evolving and slowly changing processes and to assimilate multiple variables from diverse data inputs. These characteristics enhance the robustness and reliability of the assimilation framework in real-world catchments, where observations are spatially heterogeneous and hydrological processes operate across multiple timescales."

5.Terms like "weakly coupled DA" and "fully coupled DA" are used consistently but may confuse readers unfamiliar with DA jargon.

Response: We thank the reviewer for this helpful comment. To improve clarity for readers unfamiliar with data assimilation terminology, we have added explicit definitions and explanations of the terms "weakly coupled DA" and "fully coupled DA" in the section 2.4 (Localized Ensemble Kalman Filter for Data Assimilation). The revised manuscript now includes the following explanations to clarify these terms (lines 295-308):

"Earlier research by Zhang et al. (2018) showed that in TSMP, assimilating SM and/or GWL enables updates to all relevant subsurface states via DA. In this fully coupled DA configuration of Zhang et al. (2018), cross-variable covariances ensured that observations of one variable (e.g., SM) could directly adjust others (e.g., GWL). Later, Hung et al. (2022) applied GWL assimilation restricted to the saturated zones and demonstrated that this approach outperformed the fully coupled strategy of Zhang et al. (2018). In this study, we develop a new weakly coupled DA scheme that introduces separate update restrictions for each observation type: GWL observations are used to update only saturated cells, while SM observations are used to update only unsaturated zones. This design minimizes potential spurious cross-variable correlations and enhances the robustness of multivariate assimilation. Additionally, updates are applied asynchronously to account for the different temporal dynamics of the variables: SM, which changes more rapidly, is typically updated daily, whereas groundwater, with slower dynamics, is updated weekly. Furthermore, unlike previous DA studies of TSMP, which generally used the same localization radius for joint GWL and SM assimilation, our approach applies different localization radii for the two variables, accounting for their distinct spatial correlation characteristics."

New references added in the revised manuscript:

Bayat, B., Camacho, F., Nickeson, J., Cosh, M., Bolten, J., Vereecken, H., and Montzka, C.: Toward operational validation systems for global satellite-based terrestrial essential climate variables, International Journal of Applied Earth Observation and Geoinformation, 95, 102240, 10.1016/j.jag.2020.102240, 2021.

Cooper, E., Blyth, E., Cooper, H., Ellis, R., Pinnington, E., and Dadson, S. J.: Using data assimilation to optimize pedotransfer functions using field-scale in situ soil moisture observations, Hydrology and Earth System Sciences, 25, 2445-2458, 10.5194/hess-25-2445-2021, 2021.

Dimitrova-Petrova, K., Rosolem, R., Soulsby, C., Wilkinson, M. E., Lilly, A., and Geris, J.: Combining static and portable Cosmic ray neutron sensor data to assess catchment scale heterogeneity in soil water storage and their integrated role in catchment runoff response, Journal of Hydrology, 601, 126659, 10.1016/j.jhydrol.2021.126659, 2021.

Fersch, B., Francke, T., Heistermann, M., Schrön, M., Döpper, V., Jakobi, J., Baroni, G., Blume, T., Bogena, H., Budach, C., Gränzig, T., Förster, M., Güntner, A., Hendricks Franssen, H. J., Kasner, M., Köhli, M., Kleinschmit, B., Kunstmann, H., Patil, A., Rasche, D., Scheiffele, L., Schmidt, U., Szulc-Seyfried, S., Weimar, J., Zacharias, S., Zreda, M., Heber, B., Kiese, R., Mares, V., Mollenhauer, H., Völksch, I., and Oswald, S.: A dense network of cosmic-ray neutron sensors for soil moisture observation in a highly instrumented pre-Alpine headwater catchment in Germany, Earth Syst. Sci. Data, 12, 2289-2309, 10.5194/essd-12-2289-2020, 2020.

Franz, T. E., Zreda, M., Rosolem, R., and Ferre, T. P. A.: A universal calibration function for determination of soil moisture with cosmic-ray neutrons, Hydrology and Earth System Sciences, 17, 453-460, 10.5194/hess-17-453-2013, 2013.

Patil, A., Fersch, B., Hendricks Franssen, H.-J., and Kunstmann, H.: Assimilation of Cosmogenic Neutron Counts for Improved Soil Moisture Prediction in a Distributed Land Surface Model, Frontiers in Water, 3, 10.3389/frwa.2021.729592, 2021.

Xue, Y., Houser, P. R., Maggioni, V., Mei, Y., Kumar, S. V., and Yoon, Y.: Evaluation of High Mountain Asia - Land Data Assimilation System (Version 1) From 2003 to 2016, Part I: A Hyper - Resolution Terrestrial Modeling System, Journal of Geophysical Research: Atmospheres, 126, 10.1029/2020jd034131, 2021.

Zafarmomen, N., Alizadeh, H., Bayat, M., Ehtiat, M., and Moradkhani, H.: Assimilation of Sentinel-Based Leaf Area Index for Modeling Surface - Ground Water Interactions in Irrigation Districts, Water Resources Research, 60, 10.1029/2023wr036080, 2024.