

Responses to Reviewers

Response to review comments on manuscript originally entitled "*Assimilation of near-surface cosmic-ray neutrons improves summertime soil moisture profile estimates at three distinct biomes in the USA*" by Rosolem et al. submitted to Hydrology and Earth System Sciences.

To Editor and All Reviewers

We would like to propose a new title to the manuscript, as follows:

"Translating above-ground cosmic-ray neutron intensity to high-frequency soil moisture profile at sub-kilometer scale"

After carefully revisiting the manuscript and while incorporating the changes and suggestions made by the reviewers, we believe this title is much stronger related to the objectives proposed in this study because:

- (1) Our ultimate goal is to evaluate how effectively the information from the aboveground measured neutrons originated from cosmic-rays can constrain soil moisture profile (as stated in the last paragraph of the Introduction);
- (2) Although the simulations are conducted in column-mode experiments using a land surface model, the inherent spatial heterogeneity observed within the same footprint of a cosmic-ray neutron sensor is successfully emulated by accounting for spatial variability of key soil properties obtained from field samples, hence the words "sub-kilometer scale"; and
- (3) In an OSSE, it is likely and somewhat expected that the assimilation of such information will improve soil moisture estimates given the small number of a priori assumptions in the method (this is extensively discussed in this manuscript). Because of the novelty of such technology, OSSEs are of paramount importance for understanding the mechanisms of this combined framework. It identifies potential benefits and limitations for a wide range of applications. We, however, found that the title could potentially be misinterpreted as coming only from real experiments.

We hope the Editor and all Reviewers accept our proposed change in order to enhance the clarity and information in the manuscript for the rest of the scientific community.

Reviewer #1

[1] The authors try to demonstrate the merits of assimilating cosmic-ray neutron measurements in a land surface model. The trial of this kind is very innovative, since the integrated soil moisture profile signal can be used to update soil moisture states at different layers simultaneously. The only limitation is that other factors that may affect cosmic-ray neutron measurements cannot be explored with the current OSSE. This limits the application of the approach developed in the manuscript. It is understandable though to keep that part of discussion in other works. Therefore, it is suggested to accept this manuscript with minor revision.

Response: We first would like to thank the reviewer for carefully reviewing the manuscript and for his/her positive feedback on our study. Indeed, the experiments undertaken in this study do not account for other sources of hydrogen except for lattice water (included in the COSMIC parameterization) and soil moisture itself. The focus of our study is to evaluate the benefits and limitations when using the cosmic-ray soil moisture technology with hydrometeorological models to assess the soil moisture signal solely, as we expect the cosmic-ray soil moisture community to continue to develop approaches which will better isolate the soil moisture signal from other sources of hydrogen (e.g., Franz et al., 2013; Hawdon et al. 2014). This has been emphasized in the original manuscript (P19/L25-P20/L11).

Franz, T. E., M. Zreda, R. Rosolem, and T. P. A. Ferré (2013), *A universal calibration function for determination of soil moisture with cosmic-ray neutrons*, *Hydrol. Earth Syst. Sci.*, 17(2), 453–460, doi:10.5194/hess-17-453-2013.

Hawdon, A., D. McJannet, and J. Wallace (2014), *Calibration and correction procedures for cosmic-ray neutron soil moisture probes located across Australia*, *Water Resour. Res.*, n/a–n/a, doi:10.1002/2013WR015138.

[2] The major concerns appeared when trying to understand the data assimilation procedure and the experimental setup. It is suggested to make these two parts more explicitly, which will help readers to understand the points easier. For the detailed comments, please check the attached PDF.

Response: We thank the reviewer for providing a PDF copy of the manuscript with annotated comments. The response to all comments made in the PDF are shown below. Please, notice that the reviewer's comments refer to the page/line numbers in the original PDF file sent by Reviewer #1 (available at <http://www.hydrol-earth-syst-sci-discuss.net/11/C1951/2014/hessd-11-C1951-2014-supplement.pdf>). However, the page/line numbers mentioned in our responses are associated with the new version of the manuscript submitted.

[3] P5517/L23: not exactly true. It says about 5cm.

Response: This is a good point made by the reviewer. The text was changed appropriately (P3/L2-3).

[4] P5523/L14: There is a need to add a flow chart here to indicate the whole data assimilation procedure. It is for the convenience of readers.

Response: The reviewer made a good suggestion which will help clarify the data assimilation and state update procedures used in this study. We have added a schematic diagram of the DART framework as Figure 2 in the new version of the manuscript. Reference to Figure 2 is made at the end of sub-section 2.4 (P8/L4-5).

[5] P5524/L1: Experimental Setup - For the sake of convenience, it is illustrative to add a table (or, add few columns in Table 1) describing the experimental setup for each studied location? In the current manuscript, it is difficult to perceive which set of soil moisture simulation being used to generate synthetic observation or which set of soil moisture data being used to generate uniformly-distributed soil moisture values, and which set of meteorological forcing being perturbed and used for which site and so on. It would be convenient as well if you list out which set of data are 'true' and so on. A table with the information mentioned above will help readers to know exactly your experimental setup. And will help better the reader to understand the points of your research.

Response: This is a good point made by the reviewer. We have added a few sentences (P8/L20-23) in the Experimental Setup section (Section 3) and included a new figure (Figure 3) to better clarify this information to readers.

[6] P5525/L6: The saturated hydraulic conductivity is straightforwardly linked to soil porosity, so does saturated soil diffusivity and other relevant parameters. It is needed to explain if they are physically consistent or not. It is suggested to put all the parameter value in a table for clarification.

Response: This is an interesting point raised by the reviewer. We introduced small perturbations (within $\pm 10\%$ range from the nominal value) to some of the Noah model parameters in order to emulate effective properties at the sensor scale which are similar but not necessarily captured in the look-up table values traditionally available for land surface modeling. Although such relationships among soil properties are of great importance, the strict validity of them should not constitute a major issue in our synthetic observation study for the following reasons: (1) the percent variation of each parameter with respect to its original value is small and based on the uncertainty values obtained in the field from gravimetric samples, and (2) those relationships have been usually studied at scales which are not necessarily the same as the cosmic-ray sensor support volume, so we cannot ensure such relationships are scale-independent (this is the main motivation for introducing the idea of effective parameter values as traditionally employed in optimization approaches in hydrological models and more recently in land surface models). We have included a list of parameter values for each site as supplemental material and added a sentence in the main text (P9/L26-27)

[7] P5525/L17: Do you mean by using the original parameter set and the meteorological forcing without being disturbed, you run a 10 year spin-up? From when to when for this 10yr spin up?

Response: Following the reviewer's suggestions, we hope that the new changes made in this version of the manuscript (including additional information in Table 1 and Figure 3, along with some additional text in P9/L30-32, P10/L1, and P10/L13-14) is more clear with respect to the experimental setup. The spin-up period is now shown in Table 1 and the spin-up strategy shown in Figure 3.

[8] P5525/L22: Is it from spin-up period?

Response: Please, notice that this sentence no longer appears in the manuscript due to changes made in response to reviewer's comment [7].

[9] P5528/L5: An Equation may help to explain this concept more clearly. Please add one.

Response: Both comments [9] and [10] made by the reviewer indicated a potential lack of clarity in our original manuscript. We have made major changes to section 4.1 (P11/L29-P13/L16). We hope the revised paragraphs are now more clear and thank the reviewer for raising these issues.

[10] P5528/L7: Why the total spread is the sum of the ensemble variance plus the observational error variance? I assumed you referred the spread as the ensemble spread, which is the rms - difference between ensemble members and ensemble mean. Could you clarify what do you mean here by your definition of spread? The combination of instrument error and representativeness error should represents the total observation error. Do you mean the total spread should equal to the total observation error in your case?

Response: Please, refer to the response in the previous item [9].

[11] P5528/L19: what do you mean by 'damping'? could you explain a bit more from DA perspective and physics perspective?

Response: We thank the reviewer for raising this point. We believe the 'damping' effect observed for the 'No DA' case, which we discussed in this sentence (P12/L16-18), which refers to the results shown in Figure 5 (in the new version of the manuscript), is due to the fact that at the Kendall site, rainfall ceases in the pre-monsoon period allowing for soil moisture to stabilize towards a similar "preferred" state over a

short period of time. This is analogous to spin-up or warm-up procedures where giving a initial state as “first guess”, a model predicting soil moisture dynamics will tend to find its “preferred” conditions after some simulation time. This happens when all perturbations come from initial condition since the soil dynamics used in the model are practically the same for each ensemble member. Here, the spread is mainly driven by perturbations in IC (and meteorological forcing, arguably rainfall), and as soon as the impact on IC decays in time (spin-up), then the spread becomes very low. However, our statistical analyses indicate the OSSE was successful and no issues with spread were observed (see new Figure 5, and modified text on P11/L29-P13/L16). We had originally included a sentence describing this analogy to help the readers understand the mechanism that is probably taking place in this case, but the reviewer is welcome to suggest another way to make this statement more clear to readers.

[12] P5528/L23: could you explain more on this point. It seems the ensemble collapse?

Response: Please, refer to the response in the previous item [11].

Reviewer #2

[1] Section 3.1, Was the initial condition perturbed at each assimilation step or only the at the beginning of the time period? The model parameter are usually perturbed in the land data assimilation, otherwise the spread of model ensemble members could not be kept enough (e.g. the soil moisture ensembles during the dry period). What is the variance for the initial condition perturbation? It has large impacts on the assimilation results. One major issue is that the soil moisture ensemble spread in case of DA-2-day will decrease rapidly during the forward run compared with the DA 1-hour, than it decreases the performance of DA 2-day assimilation due to the small model uncertainty.

Response: Based on both reviewers’ comments, we recognize that Section 3 (Experiment Setup) in our original manuscript was not very clear. With respect to subsection 3.1, as pointed out by reviewer #2, we have slightly modified the paragraph in subsection 3.1 and include Figure 3. We hope these will help clarify the experimental setup used in this study. The initial soil moisture conditions were first perturbed at the beginning of any assimilation condition (including the ‘no DA’ simulations). Following updates in soil moisture profiles occur as part of the assimilation procedure. Notice, as mentioned in P8/L16-20, that we assume no prior knowledge about soil moisture states at the beginning of our assimilation experiment, and hence used the Latin Hypercube Random Sampling method which generates initial soil moisture conditions following a near uniform distribution between minimum and maximum allowed soil moisture values. The average soil moisture variance at each soil layer in the model is approximately $0.02 \text{ m}^3 \text{ m}^{-3}$ which is consistent with typical uncertainty levels found for cosmic-ray sensors and traditional point-scale methods. Our statistical analyses indicate the OSSE was successful and no issues with spread were observed (see new Figure 5, and modified text on P11/L29-P13/L16).

[2] Section 3.2, the perturbed forcing and model parameters were used to generate the synthetic observations, but there is only one ensemble in this parallel run. How were these perturbations applied for this single run?

Response: We thank the reviewer for raising this point as it appears the original manuscript was not clear on the description of the experimental setup (please refer to previous item for new changes to this section). For each site, we generate a total of 41 ensemble members having different (perturbed) meteorological conditions whose characteristics are described in Table 2. Of those 41 members, 40 members were used directly to force the Noah model during the data assimilation experiments (including the ‘no DA’ simulations). The remaining forcing (member #41) was used in a single (offline) simulation in which some model parameters were also perturbed (as described in section 3.2 and summarized in

Figure 3). These parameters were identified as most influential using a simple sensitivity analysis approach as described on P9/L4-32. The reason we used perturbed parameters was to emulate the lack of true information about soil properties at the measurement scale of the cosmic-ray sensor (hence, we use spatial variability of dry soil bulk density as a proxy for parameter variability). The reason we use perturbed meteorological forcing (rather than the original forcing) was in recognition that additional uncertainties due to measured meteorological conditions are inherent in hydrometeorology, and that it is unlikely we record the true meteorological variables, but rather expect to measure something “close enough” to the true conditions.

[3] How was the state vector defined in EAKF? Because the sensor depth of the COSMOS will change between 10 cm and 70 cm. In $y-H(x)$, how was the observation y related to the model x ? Was the first layer of NOAH used always?

Response: This is an important point made by the reviewer which we believe was caused by a possible misunderstanding related to the original manuscript. This also relates to some of the subsequent points made by the reviewer. A detailed description of the Ensemble Adjustment Kalman Filter is given in subsection 2.4 and was summarized based on the original work by Anderson (2001). The key equations are the ones used in the assimilation step (equation 4) and in the updating step (equation 5). It is important to understand that the quantity assimilated is not soil moisture but the actual neutron counts typically measured by those cosmic-ray sensors (hence the original title of the manuscript). This is explicitly stated in our objectives (see P3/L29-P4/L4). The conversion of simulated soil moisture profile (i.e., including contribution from all layers) to equivalent neutron counts (i.e., the quantity used in the assimilation) is done through the use of the COSMIC operator (as described in subsection 2.3). The updating step allows for observation increments (in terms of neutron counts) to be linearly regressed onto each state-vector component (i.e., soil moisture from individual layers), following equation 5.

Anderson, J. L.: An ensemble adjustment Kalman filter for data assimilation, Mon. Wea. Rev., 129(12), 2884–2903, 2001.

[4] Were the instantaneous observations assimilation both in the hourly and daily assimilation? In the daily assimilation, how accurate can be for this one instantaneous observation because of the large variations of neutron counts in hourly step? And the soil moisture could not change so rapidly. Is it reasonable to use instantaneous observation for soil moisture assimilation?

Response: This is an interesting point made by the reviewer. Yes, instantaneous observations of neutron counts were used in all assimilation experiments throughout the manuscript. This was the main motivation of the manuscript whose goal is to better understand how observations of neutron counts can or cannot be used to properly constrain soil moisture profiles simulated by a model. In addition, the reason for assessing the impact of different retrieval frequencies was to make a better link to the use with remote sensing products which are widely employed by hydrometeorological community.

[5] Is it worth assimilating the soil moisture in hourly step? Why should we assimilate the soil moisture so frequently?

Response: Please, refer to the response in item [3]. Soil moisture was not assimilated in this study but rather neutron count. According to our results, the successful assimilation of hourly neutron counts indicated an improvement in the dynamics of soil moisture profiles at much deeper soils in comparison to a lower-frequency assimilation experiment. This is one of the main findings from this study presented in the Results (section 4; more specifically subsections 4.2 and 4.3) and discussed in section 5 (Summary and Conclusions; more specifically on P18/L15-P19/L10).

[6] In this OSSE, the openloop run is quite close to the truth. Generally the model simulation will not obtain such good openloop run due to the uncertainty of forcing, parameters and model physics. It is better to show a case with large model error. If the model behaves like this, what is the value of data assimilation? Is it still necessary?

Response: We thank the reviewer for this comment. We explicitly recognize that results from OSSE will tend to be more optimistic in comparison to assimilation of real neutron count observations. This is why the analysis of RMSE and spread was introduced in section 4.1 in order to clearly identify advantages and disadvantages of the approach at distinct sites and with different retrieval frequencies. Please, refer to discussion paragraphs from P11/L29 to P13/L16, and Figure 5 in this new version of the manuscript. Examining a case with larger model error would generally make the impacts of the assimilation appear more advantageous compared to the openloop. The OSSE can only identify the potential for improvements given assumptions about the model. Subsequent work with real assimilation is needed to quantify the actual impact of the observations.

[7] And where the model bias came from? Because the same perturbations were used for all layers, but the deep layers were more biased.

Response: Please, refer to items [1] and [2] above for information on experimental setup. Observations (in terms of neutron counts) were generated from a single (offline) simulation with slightly perturbed parameters based on uncertainty of *in situ* soil properties (i.e., dry soil bulk density). In terms of synthetic observation no significant biases were found at the three sites and hence the data assimilation was performed under the zero-mean random error assumption. The model bias the reviewer is probably referring is due to (1) the mean initial conditions from the prior ensemble just before the beginning of the assimilation experiments which tend to be located in the mid-point between minimum and maximum soil moisture at each site given the Latin Hypercube Random Sampling strategy (this approach was used because we assumed lack of any prior information about soil moisture at the beginning of our assimilation experiment); and (2) the fact that the synthetic observations were generated with the Noah model with slightly perturbed parameters. For assimilation cases where there is no or low rainfall conditions, little information is added to the model from observations and the soil moisture dynamics simulated in the model is closely related to its default parameters which will never be the same as the parameters used for generating the synthetic observations.

[8] The validations of assimilation results are not enough. The soil moisture can be easily improved with the assimilation of soil moisture information. I suggest to add some discussion of the surface fluxes. Moreover, the surface fluxes could be influenced under the dry condition.

Response: This is an interesting point raised by the reviewer. We agree that the evaluation of soil moisture improvements due to direct soil moisture assimilation can be limited, but we would like to emphasize that this is not the case for this study (please refer to item [3]). Here, we are evaluating how the information obtained from aboveground cosmic-ray neutrons can influence not only a single layer in the model but also the entire profile, and how this information is translated at distinct sites (i.e., under different meteorological forcing conditions) as well as under distinct retrieval frequencies. We believe both objectives merit the publication of the manuscript to HESS because it expands the initial and arguably limited results published in our previous article (Shuttleworth et al. 2013) because this previous paper focused only on the integrated soil moisture rather than assessing impact on soil moisture profiles. Our preliminary results indicated that when the Noah model was successfully calibrated against real neutron counts from each site (hence, better constraint on soil moisture dynamics), the surface energy fluxes were not improved appropriately (in some cases, even deteriorated). Although we recognize that

such analyses are important, we believe this would shift the focus of the current paper (which is to address the capabilities of cosmic-ray neutrons to soil moisture profiles). Moreover, efforts to improve the Noah model have recently been in place (e.g., the development of Noah-MP; Niu et al., 2011; Yang et al., 2011). Arguably, the Noah-MP contains additional features not present in the Noah model but to change the land surface model at this stage would be unfeasible for the publication of the manuscript. In the near future, we will aim for the assimilation of actual cosmic-ray neutrons to be used in hydrometeorological applications as stated in P20/L18-22.

Niu, G.-Y. et al. (2011), The community Noah land surface model with multiparameterization options (Noah-MP): 1. Model description and evaluation with local-scale measurements, J. Geophys. Res., 116(D12), D12109, doi:10.1029/2010JD015139.

Shuttleworth, J., Rosolem, R., Zreda, M. and Franz, T.: The COsmic-ray Soil Moisture Interaction Code (COSMIC) for use in data assimilation, Hydrol. Earth Syst. Sci., 17(8), 3205–3217, doi:10.5194/hess-17-3205-2013, 2013.

Yang, Z.-L. et al. (2011), The community Noah land surface model with multiparameterization options (Noah-MP): 2. Evaluation over global river basins, J. Geophys. Res., 116(D12), D12110, doi:10.1029/2010JD015140.

1 **Suggested New Title: Translating above-ground cosmic-ray neutron intensity to**
2 **high-frequency soil moisture profile at sub-kilometer scale**

3 *Original/Previous Title: Assimilation of near-surface cosmic-ray neutrons improves*
4 *summertime soil moisture profile estimates at three distinct biomes in the USA*

5
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16
17 **Abstract**

18 Aboveground cosmic-ray neutron measurements provide an opportunity to infer soil
19 moisture at the sub-kilometer scale. Initial efforts to assimilate those measurements
20 have shown promise. This study expands such analysis by investigating (1) how the
21 information from aboveground cosmic-ray neutrons can constrain the soil moisture at
22 distinct depths simulated by a land surface model, and (2) how changes in data
23 availability (in terms of retrieval frequency) impact the dynamics of simulated soil
24 moisture profiles. We employ ensemble data assimilation techniques in a 'nearly-
25 identical twin' experiment applied at semi-arid shrubland, rainfed agricultural field, and
26 mixed forest biomes in the USA. The performance of the Noah land surface model is
27 compared without and with assimilation of observations at hourly intervals and every 2
28 days. Synthetic observations of aboveground cosmic-ray neutrons better constrain the
29 soil moisture simulated by Noah in root zone soil layers (0-100 cm) despite the limited
30 measurement depth of the sensor (estimated to be 12-20 cm). The ability of Noah to

Rafael Rosolem 9/8/14 4:03 PM

Comment [1]: Authors comment to Editor and both Reviewers

1 reproduce a 'true' soil moisture profile is remarkably good regardless of the frequency of
2 observations at the semi-arid site. However, soil moisture profiles are better constrained
3 when assimilating synthetic cosmic-ray neutrons observations hourly rather than every 2
4 days at the cropland and mixed forest sites. This indicates potential benefits for
5 hydrometeorological modeling when soil moisture measurements are available at
6 relatively high frequency. Moreover, differences in summertime meteorological forcing
7 between the semi-arid site and the other two sites may indicate a possible controlling
8 factor to soil moisture dynamics in addition to differences in soil and vegetation
9 properties.

10 **1 Introduction**

11 The water stored in soils controls the hydrometeorology of a region by partitioning the
12 rainfall into surface runoff and infiltration. In addition, soil water controls the amount of
13 available energy used for water vapor exchanges with the atmosphere as opposed to
14 sensible or ground heat exchange. Soil moisture can also potentially impact
15 biogeochemical interactions between land and atmosphere. With the increased
16 frequency of relevant hydrometeorological events (Coumou and Rahmstorf, 2012;
17 Dokken, 2012) such as floods and droughts and consequences to the ecosystem, a
18 more accurate representation of the soil water is needed for improved weather and
19 climate predictions and for better practices in agriculture and water resources planning
20 (Koster et al., 2004; Seneviratne, 2012).

21 In weather and climate models the exchanges of water, heat, and momentum between
22 land and atmosphere are simulated by so-called land surface models (LSMs). Such
23 models have evolved over the last few decades (Best et al., 2011; Bonan et al., 2002;
24 Clark et al., 2011; Niu et al., 2011; Oleson et al., 2008; Pitman, 2003; SELLERS et al.,
25 1997; Yang et al., 2011) in part due to comparison studies using flux tower
26 measurements (e.g., (Baker et al., 2008; 2003; Rosolem et al., 2012a; 2012b; Sakaguchi
27 et al., 2011; SELLERS et al., 1989; Wang et al., 2010), such as the Ameriflux network
28 (BALDOCCHI, 2003). However, until recently soil moisture measurements at spatial
29 scales comparable to the horizontal footprint of flux towers and grid sizes employed in
30 LSMs (Wood et al., 2011) had been difficult and costly (Robinson et al., 2008).

31 Traditional point-scale soil moisture measurements are usually available at high
32 frequency (e.g., hourly) but suffer from having a small support volume (a few tens of
33 cm). On the other hand, large-scale soil moisture measurements are available globally

1 through satellite remote sensing (Brown et al., 2013; Entekhabi et al., 2010; Kerr et al.,
2 2010), but have low-frequency retrievals (1-3 days) and shallow penetration depths (1-5
3 centimeters). This potentially limits knowledge of the root zone soil moisture that
4 provides the link between land and atmosphere via evapotranspiration (Seneviratne et
5 al., 2010).

Rafael Rosolem 9/8/14 4:52 PM
Comment [2]: Response [3] to Reviewer
#1

6 Recent innovative technology provides an opportunity to estimate soil moisture at scales
7 comparable to flux tower footprints using cosmic rays (Zreda et al., 2008). The
8 measurement relies on the natural production of fast (low-energy) neutrons in the soil
9 from high-energy neutrons created by cosmic rays. This process is strongly controlled by
10 the much higher absorbing/moderating power of hydrogen atoms relative to other
11 chemical elements (see Figure 5 in (Zreda et al., 2012)). Therefore, when soil is
12 relatively wet with high hydrogen content, fewer fast neutrons reach the surface than
13 when the soil is dry with low hydrogen content. The cosmic-ray sensor measures the
14 neutron intensity (referred to as moderated neutrons count over a given period of time,
15 usually an hour) which is consequently related to the soil water content. The horizontal
16 effective measurement area is near-constant and approximately 300 m in radius at sea
17 level under a dry atmosphere (Desilets and Zreda, 2013), while the effective
18 measurement depth varies approximately from 10 to 70 cm depending on the total soil
19 water (i.e., pore plus chemically bound "lattice" water, as discussed in (Franz et al.,
20 2012a)), see Figure 1. This new technology is being investigated around the globe in
21 newly established networks such as the COsmic-ray Soil Moisture Observing System in
22 the USA (COSMOS; <http://cosmos.hwr.arizona.edu>) (Zreda et al., 2012), the Australian
23 National Cosmic Ray Soil Moisture Monitoring Facility (CosmOz;
24 <http://www.ermt.csiro.au/html/cosmoz.html>) (Hawdon et al., 2014), the German
25 Terrestrial Environmental Observatories (TERENO; [http://teodoor.icg.kfa-
26 juelich.de/overview-en](http://teodoor.icg.kfa-
26 juelich.de/overview-en)) (Zacharias et al., 2011), and most recently in Africa
27 (<http://cosmos.hwr.arizona.edu/Probes/africa.php>) and the UK (COSMOS-UK;
28 <http://www.ceh.ac.uk/cosmos>).

29 Initial efforts to assimilate near-surface cosmic-ray neutrons into hydrometeorological
30 models have shown promising results (Shuttleworth et al., 2013), Han et al., 2014) but
31 focused mainly on the signal associated with the integrated, depth-weighted soil
32 moisture estimates. The present study expands the application of the cosmic-ray soil
33 moisture using ensemble data assimilation techniques. The objectives here are:

- 1 i. to determine how effectively the information from aboveground cosmic-ray neutrons is
- 2 propagated to individual soil moisture layers in a land surface model;
- 3 ii. to assess the benefits/limitations of high-frequency retrieval offered by this new
- 4 technology.

5 Analyses are carried out for the summer period (May through September 2012) at three
6 distinct biomes in the USA using synthetic observations of neutron intensity obtained
7 from the LSM.

8

9 **2 Data and methods**

10 **2.1 Sites description**

11 Site selection was made based on the availability of meteorological forcing data from the
12 Ameriflux network (<http://ameriflux.lbl.gov>), and to include characteristic differences in
13 site-to-site climatology, land cover and soil types, as summarized in Table 1. The soil
14 and vegetation types at each site were assigned the following classifications obtained
15 from the Ameriflux database. The Kendall site located in the Walnut Gulch Experimental
16 Watershed is a semi-arid grassland comprising mainly C4 grasses with a few scattered
17 shrubs with a dominant growing season in response to the summer rains (Scott et al.,
18 2010). The Nebraska site located at the University of Nebraska Agricultural Research
19 and Development Center is a rainfed agricultural field characterized by maize-soybean
20 rotation with growth period (planting to harvest) from May to October (VERMA et al.,
21 2005). The Park Falls/WLEF tower located in the Park Falls Ranger District of the
22 Chequamegon National Forest is characterized by a managed landscape where logging
23 activities such as thinning and clear-cuts are concentrated in the upland region (DAVIS
24 et al., 2003). The growing seasons are typically short and the winters long and cold
25 (Mackay et al., 2002). Soil moisture availability controls summer evapotranspiration at
26 the Kendall and Nebraska sites and to a lesser extent at the Park Falls (Teuling et al.,
27 2009).

28 In order to produce a continuous set of hourly meteorological forcing data for each site
29 for the period of interest (May through September 2012), the following data gap filling
30 rules were applied following (Rosolem et al., 2010):

- 31 i. If the gap was less than 3 hours, it was filled by linear interpolation.

Rafael Rosolem 9/8/14 5:01 PM

Comment [3]: Response [3] to Reviewer #2

- 1 ii. If the gap was greater than 3 hours, the missing hours were replaced by values for the
- 2 same hours averaged over the previous and subsequent 15 days.
- 3 iii. If any additional gap filling was needed, the missing data were replaced by the
- 4 average value for the specific hour calculated in the monthly mean diurnal cycle.

5

6 **2.2 Noah Land Surface Model**

7 The Noah used operationally at the National Centers for Environmental Prediction
8 (NCEP) for coupled weather and climate modeling (Ek, 2003) was adopted in this study.
9 This LSM is also used in the NASA Land Information System (LIS) (Kumar et al., 2008),
10 and in the Global (Rodell et al., 2004) and North American (Mitchell, 2004) Land Data
11 Assimilation Systems (GLDAS and NLDAS, respectively).

12 The model contains four soil layers that extend two meters below the surface;
13 specifically, a 10-cm thick surface layer, a 30-cm thick root zone layer, a 60-cm thick
14 deep root zone layer, and a 1-m thick sub-root zone layer. The present study focuses on
15 the first three layers of the model where roots are prescribed to be present (0 to 1 m total
16 depth). Soil moisture parameterization is based on the one-dimensional Richards
17 equation (Chen et al., 1996; Ek, 2003). Soil and vegetation parameters were defined
18 from look-up tables and the Noah simulation run at hourly time steps at each selected
19 site. A full description of Noah can be found in (Chen and Dudhia, 2001) and in (Ek,
20 2003) and the model is available from the Research Applications Laboratory at the
21 National Center for Atmospheric Research (RAL/NCAR) at
22 <http://www.ral.ucar.edu/research/land/technology/lsm.php>.

23

24 **2.3 Cosmic-ray Soil Moisture Interaction Code (COSMIC)**

25 In this study the COsmic-ray Soil Moisture Interaction Code (Shuttleworth et al., 2013) is
26 the forward observational operator used in data assimilation. COSMIC is characterized
27 by a simple, physically-based parameterization of belowground processes relevant for
28 soil moisture estimates using cosmic-ray sensors which includes (1) the degradation of
29 the incoming high-energy neutron flux with soil depth, (2) the production of fast neutrons
30 at given depth in the soil, and (3) the loss of the resulting fast neutrons before they reach
31 the soil surface. Despite its simplicity, COSMIC is robust and much more efficient than
32 the traditional Monte Carlo neutron particle model commonly employed in cosmic-ray

1 soil moisture applications (Franz et al., 2012b; 2013b; Rosolem et al., 2013). Here, the
2 COSMIC is used to convert soil moisture profiles derived from the Noah into an
3 equivalent neutron intensity as seen by a cosmic-ray sensor. The code has been
4 developed as part of the COSMOS network and is available at
5 <http://cosmos.hwr.arizona.edu/Software/cosmic.html>.

6

7 **2.4 Ensemble data assimilation**

8 Data assimilation combines the information from observations and model predictions in
9 order to estimate the state of a physical system while recognizing both have some
10 degree of uncertainty. Given the complexity of geophysical models in general, ensemble
11 data assimilation techniques were originally developed to decrease the computational
12 cost of the nonlinear filtering problem patterned after the Kalman filter (Kalman, 1960;
13 Kalman and Bucy, 1961) by using a sample of model-state vectors to compute their
14 statistical moments (i.e., mean and covariance) (Evensen, 1994; 2003; Houtekamer and
15 Mitchell, 1998). In the hydrometeorological community interest in ensemble data
16 assimilation methods is growing rapidly for flood forecasting (Clark et al., 2008) and soil
17 moisture applications (e.g., (Draper et al., 2012; Kumar et al., 2012; Li et al., 2012).

18 The ensemble data assimilation method used in this study is an approximation to a
19 general filtering algorithm developed using Bayes Theorem (Wikle and Berliner, 2007),
20 and the method is described in detail by (Anderson, 2003) and (Anderson, 2009). The
21 probability distribution of a model state is approximated by an N -member sample of M -
22 dimensional state vectors (\mathbf{x}_i ; $i = 1, 2, \dots, N$), where N is the ensemble size (in this study,
23 $N = 40$) and each \mathbf{x}_i is an M vector (e.g., soil moisture at each model layer). Because the
24 error distributions for observations taken at different times are usually assumed
25 independent in geophysical applications, each available observation can be assimilated
26 sequentially. Hence, for simplicity, the assimilation of a single scalar observation, y , is
27 used here. The Bayes Theorem is as follows:

$$28 \quad p(\mathbf{x} | \mathbf{Y}, y) = p(y | \mathbf{x}) p(\mathbf{x} | \mathbf{Y}) / \eta \quad (1)$$

29 where \mathbf{x} is the model state variable, \mathbf{Y} is the set of all observations that have already
30 been assimilated which does not include the new observation, y , available at the current
31 time, and η refers to a normalization factor. The ensemble assimilation procedure is
32 summarized below:

1 (1) Each ensemble member is advanced from the time of the most recently used
2 observation to a time sufficiently close to the time of the next available observation using
3 the Noah.

4 (2) A prior ensemble estimate of y is created by applying the forward operator h (in this
5 case, COSMIC) to each sample of the prior state.

6 (3) An updated ensemble estimate of y conditioned on the new observation is computed
7 from the prior ensemble estimate of y and the observed value, y_o , using Eq. (1). In this
8 study, the Ensemble Adjustment Kalman Filter (EAKF) (Anderson, 2001) is used.

9 In order to account for uncertainty in the model, the prior ensemble estimate of y is
10 approximated as $Normal(\bar{y}_p, \sigma_p^2)$ where \bar{y}_p and σ_p^2 are the sample mean and variance
11 computed from the model ensemble while the uncertainty in the observation, y_o , is
12 defined as σ_o^2 . Given the nature of the cosmic-ray sensor and the large number of counts
13 per integration time (i.e., hourly), the assumption of observation uncertainty to be
14 normally distributed (with $\sigma_o^2 = y_o$) is appropriate. The product of $Normal(\bar{y}_p, \sigma_p^2)$ and
15 $Normal(y_o, \sigma_o^2)$ in Eq. (1) is computed resulting in a Gaussian updated distribution for y ,
16 $Normal(\bar{y}_u, \sigma_u^2)$ with an updated variance (σ_u^2) and mean (\bar{y}_u) defined as:

$$17 \sigma_u^2 = \left[(\sigma_p^2)^{-1} + (\sigma_o^2)^{-1} \right]^{-1} \quad (2)$$

18 and

$$19 \bar{y}_u = \sigma_u^2 \left[(\sigma_p^2)^{-1} \bar{y}_p + (\sigma_o^2)^{-1} y_o \right] \quad (3)$$

20 respectively. In the EAKF, the prior ensemble distribution of y is then shifted and linearly
21 contracted to create an updated ensemble with sample statistics as in Eqs. (2) and (3).
22 Observation increments are computed as

$$23 \Delta y_i = \sqrt{\sigma_u^2 / \sigma_p^2} (y_{p,i} - \bar{y}_p) + \bar{y}_u - y_{p,i} ; i = 1, 2, \dots, N \quad (4)$$

24 where the subscript i refers to ensemble member.

25 (4) Increments to the prior ensemble of each state-vector element ($x_{j,i}$, where j refers to
26 an element of the state vector, while i refers to an ensemble member) are computed by
27 linearly regressing the observation increments (Δy_i) onto each state-vector component
28 independently using the prior joint sample statistics, so that:

1 $\Delta x_{j,i} = (\sigma_{p,j}/\sigma_p^2)\Delta y_i ; j = 1,2, \dots, M ; i = 1,2, \dots, N$ (5)

2 The Noah, the COSMIC operator and COSMOS observations have all been
3 implemented into the Data Assimilation Research Testbed (DART) framework (Anderson
4 et al., 2009). Figure 2 shows a schematic diagram of the assimilation and state update
5 procedures used in this study. DART is an open-source community facility that provides
6 software tools for ensemble data assimilation research in geosciences. The modularity
7 of DART makes the interface to new models and observations straightforward and clean.
8 The DART code is available at <http://www.image.ucar.edu/DAReS/DART>.

Rafael Rosolem 9/8/14 4:52 PM
Comment [4]: Response [4] to Reviewer #1

9

10 3 Experimental setup

11 3.1 Perturbed meteorological forcing and initial conditions

12 In order to ensure appropriate ensemble spread throughout the assimilation procedure,
13 time series of cross-correlated perturbation fields were generated for all meteorological
14 forcing inputs from Noah and applied to each individual ensemble member (total of 40
15 members), similar to the approach used by (Shuttleworth et al., 2013), see Table 2 for
16 more details. In all cases, the Latin Hypercube Random Sampling method (McKay et al.,
17 1979) was used to generate uniformly-distributed soil moisture values (for each model
18 layer) varying between minimum and saturated soil water contents in the model. We
19 therefore assume no information about the soil moisture profiles prior to the initial
20 simulation time step (i.e., 01 May 2012). All remaining model states were obtained from
21 the previous timestep (30 April 2012 at 23Z) from a spin-up simulation with four repeated
22 cycles (spin-up periods shown in Table 1) using the original meteorological forcing data
23 (i.e., unperturbed) and original model parameters (Figure 3).

Rafael Rosolem 9/8/14 5:00 PM
Comment [5]: Response [1] to Reviewer #2

24

25 3.2 Synthetic observations

26 We employ the use of synthetic observations in this study in order to better assess the
27 advantages and limitations of this novel cosmic-ray technology. The approach allows a
28 direct comparison between simulated and 'true' soil moisture states at the three sites
29 where no additional soil moisture observations are available at the same spatial scale
30 measured by the cosmic-ray sensors. The use of synthetic observations in data
31 assimilation studies targeted to satellite remote sensing soil moisture missions continues

Rafael Rosolem 9/8/14 4:53 PM
Comment [6]: Response [5] to Reviewer #1

1 to show great importance for advancing our understanding of regional
2 hydrometeorological modeling (Kumar et al., 2012; Nearing et al., 2012; Reichle et al.,
3 2008).

4 For each studied location, synthetic neutron intensity observations (referred in the rest of
5 the article simply as “observations”) are generated directly from the Noah in combination
6 with the COSMIC. An additional set of perturbed meteorological forcing (not from the
7 original pool of ensemble members) is generated following the same procedure
8 described in the previous section. Additionally, ten Noah parameters originally identified
9 as influential using a simple “One-At-Time” sensitivity analysis approach (not shown) are
10 perturbed within $\pm 10\%$ range from their default values to generate a single parameter
11 set (for each location) used in Noah for the synthetic output generation in a “nearly-
12 identical twin experiment”. The idea is to emulate some unexpected (or unidentifiable)
13 variability observed in soil moisture due to small spatial-scale heterogeneities (Crow et
14 al., 2012; Famiglietti et al., 2008; Western and Blöschl, 1999) through changes in key
15 parameter values in the Noah model. Identified parameters include *fxexp* (bare soil
16 evaporation exponent), *refdk* (reference value for saturated hydraulic conductivity),
17 *refkdt* (reference value for surface infiltration parameter), *bb* (Clapp and Hornberger “b”
18 parameter), *refsmc* (soil moisture threshold for onset of some transpiration stress),
19 *drysmc* (top layer soil moisture threshold at which direct evaporation from soil ceases),
20 *wltsmc* (soil moisture wilting point), *satdk* (saturated hydraulic conductivity), *satdw*
21 (saturated soil diffusivity), and *rs* (minimum stomatal resistance). Soil porosity was not
22 included and hence the default values were used for each site. We use the coefficient of
23 variation from the *in situ* dry soil bulk density collected within the cosmic-ray footprint at
24 all three sites combined as a proxy for the perturbation magnitude (i.e., $\pm 10\%$) applied to
25 parameter variations to account for uncertainty due to spatial heterogeneity embedded in
26 the single-point simulation (please refer to the supplemental table for detailed description
27 of Noah parameter values). Such perturbations applied both to the meteorological
28 forcing and to above-mentioned parameters produce slightly different soil moisture
29 dynamics (and hence ‘true’ neutron counts) when compared to COSMIC-derived neutron
30 counts when forced with Noah with the original parameter set (not shown). For each site,
31 the spin-up corresponds to the period shown in Table 1, repeated for four times (i.e., four
32 cycles).

Rafael Rosolem 9/8/14 4:54 PM
Comment [7]: Response [6] to Reviewer #1

Rafael Rosolem 9/8/14 4:57 PM
Comment [8]: Response [7] to Reviewer #1

Rafael Rosolem 9/8/14 5:01 PM
Comment [9]: Response [2] to Reviewer #2

Rafael Rosolem 9/8/14 4:57 PM
Comment [10]: Response [7] to Reviewer #1

1 After the spin-up period, the simulated soil moisture at each soil layer from May through
2 September 2012 was then used as input data for the COSMIC to generate a 'true'
3 equivalent neutron intensity time series (counts per hour). This 'true' neutron intensity is
4 finally perturbed following a probability distribution associated with the uncertainty
5 observed in the actual cosmic-ray sensors as described by (Zreda et al., 2008)
6 ($\sigma_{N_{counts}}^2 = N_{counts}$; where N_{counts} is the neutron intensity), and a time-series of hourly
7 synthetic observations is produced for each site. In addition, a subset from the hourly
8 time-series is produced assuming observations are available every other day (for
9 simplicity, defined always at noon GMT). The 2-day frequency was selected because it
10 is similar to the temporal resolution likely to be achieved by the most recent satellite
11 remote sensing soil moisture missions (Brown et al., 2013; Entekhabi et al., 2010; Kerr
12 et al., 2010). In order to avoid undesired instabilities at the beginning of the simulation,
13 no observation is assimilated during the first 24 hours. A schematic diagram of the
14 experimental setup is shown in Figure 3.

Rafael Rosolem 9/8/14 4:58 PM
Comment [11]: Response #7 to Reviewer #1

15 We use these observations in our experiments to evaluate the ability of Noah to
16 reproduce the synthetically observed neutron intensity and consequently to analyze the
17 updated soil moisture profile against the 'true' soil moisture state. Notice that the neutron
18 intensity time-series produced in this study are not rescaled to correspond to the location
19 of the original COSMOS probe site in the San Pedro, as discussed by (Zreda et al.,
20 2012). This is because we want to preserve the site-specific count statistics to better
21 describe measurement uncertainty (lower count rates, on average, will tend to be more
22 uncertain compared to locations where count rates are relatively high). Moreover, there
23 are no systematic biases between observed and simulated neutron counts (not shown),
24 and data assimilation is performed with zero-mean random errors only (Dee, 2005).
25 Observing System Simulation Experiments (OSSE) such as those proposed in this study
26 allow us to accurately isolate the signal in the neutron measurements that comes directly
27 from the soil moisture (through the COSMIC) for more rigorous analyses. Model
28 structural deficiencies, which could potentially result in systematic biases, are therefore
29 not accounted for, and observation uncertainties not related to soil moisture (e.g.,
30 atmospheric water vapor, changes in biomass) do not impact the simulations. In
31 addition, independent observations of soil moisture profiles representing similar
32 horizontal effective measurement area are generally not available.

33

1 **4 Results**

2 **4.1 Assimilation of neutron counts**

3 For all analyzed sites, the assimilation of summertime neutron observations in Noah
4 improves the dynamics relative to the true neutron count time-series in comparison with
5 the no Data Assimilation case (i.e., 'no DA') (Figure 4). The ensemble mean of the prior
6 distribution is used for all ensemble simulations throughout this study. As discussed in
7 Section 1, the higher the neutron counts at a specific location, the lower the integrated
8 soil moisture is expected to be. Rainfall events are therefore associated with sharp
9 decreases in the neutron counts following by a relatively slower dry-down period.
10 Noticeably, the Kendall site (Figure 4a) is characterized by an initial long period with very
11 low or no rain (pre-monsoon) until early-July, followed by more frequent rainfall events
12 (monsoon) between July and early-September. Both the Nebraska and Park Falls sites
13 (Figure 4b and 4c, respectively) show the opposite rainfall pattern with an initial period
14 with frequent rainfall (slightly more frequent at Park Falls) until about mid-June/early-
15 July, followed by a relatively dry period for about 1-2 months (slightly longer at Park
16 Falls). Notice that 2012 was one of the driest years on record for the Midwestern USA
17 (Blunden and Arndt, 2013).

18 Both assimilation cases (i.e., with hourly-available observations – 'DA 1-hour' shown as
19 the red line; and with observations available once every 2 days – 'DA 2-day' shown as
20 green circles) suggest superior performance compared with the case without
21 assimilation (light blue line) (Table 3). Overall, the 'DA 1-hour' case approaches more
22 rapidly to the true neutron counts and also exhibits a tendency for relatively smaller
23 differences when compared to the 'DA 2-day' case. Notably, at the onset of the monsoon
24 at Kendall (i.e., early-July), the low frequency assimilation case does not reproduce the
25 high-frequency dynamics as well as the 'DA 1-hour' case (Figure 4a). At the Nebraska
26 and Park Falls sites (Figures 4b and 4c), there is not much improvement in Noah-
27 derived neutron counts from the 'DA 2-day' relative to the 'no DA' in periods where little
28 or no rainfall occurs.

29 The use of synthetic observations ensures that the neutron signal from the measurement
30 comes from direct contribution of soil moisture dynamics solely, and that any model
31 structural deficiency does not impact the results. Hence, a potential limitation of an
32 OSSE is that the results can be very optimistic in comparison to a data assimilation
33 experiment using real observations. For instance, when comparing against real

1 observations, one would like the RMSE (which represents the accuracy of the ensemble
2 mean state relative to the observations) to be comparable to the total spread (which
3 contains both the ensemble spread and observational error signals). In that case, the
4 RMSE is defined as the square root of the average squared difference between the
5 model estimates and the observations while the total spread is defined as $\sqrt{\sigma_p^2 + \sigma_o^2}$
6 where $(\sigma_p^2 + \sigma_o^2)$ represents the total variance (i.e., the sum of the ensemble variance,
7 σ_p^2 , plus the observational error variance, σ_o^2). In our case, however, one way to test the
8 success of an OSSE is to compare the RMSE computed with respect to the 'true'
9 observations with the ensemble spread (σ_p) directly because the variance of the 'true'
10 observations (σ_o^2) is by definition zero.

11 Figure 5 shows the comparison between the RMSE (black circles) and spread (red
12 diamonds) for all analyzed cases at all sites. Overall, the magnitudes for the spread
13 compare well with the ones for RMSE suggesting that this is a successful assimilation
14 experiment. Notice that these two quantities tend to be closest to each other for the 'DA
15 1-hour' case (right column) and the largest differences are seen for the 'No DA' case (left
16 column). The rapid reduction in total spread at the Kendall site with time for the 'No DA'
17 case is due to the fact that soil moisture presents a strong 'damping' signal, especially in
18 the first few months when little rainfall occurs (May-July). This is fundamentally the same
19 behavior observed when models are 'spun-up' or 'warmed-up' for a selected period of
20 time prior to their final analysis simulation. Consequently, individual ensemble members
21 move towards a preferred state. Notice that this behavior is not clearly observed at the
22 Nebraska and Park Falls site where rainfall occurs continuously in the first months (May-
23 July). In comparison to the 'No DA' case, RMSE for both assimilation cases are reduced,
24 with the lowest RMSE values found for the 'DA -1hour' case.

25 As expected, the time at which rainfall occurs appears to control the characteristics of
26 both statistical quantities. We therefore identified two patterns that emerged in Figure 5.
27 The first pattern is associated with a rapid increase in both RMSE and spread during
28 large rainfall events (rapid reduction in neutron counts as shown in Figure 4). These are
29 more clearly observed for the 'DA 2-day' cases (middle-column) at Kendall (mid-May,
30 early-July, mid-August, and early-September) and at Nebraska (mid-July, late-August,
31 and mid-September). These peaks are substantially reduced when observations of
32 neutron counts are assimilated at higher frequency (i.e., 'DA 1-hour' as shown in the

Rafael Rosolem 9/8/14 4:59 PM
Comment [12]: Response [11] to
Reviewer #1

1 right column). No large rainfall event was identified at the Park Falls site (Figure 4).
2 Consequently, this pattern was not observed in Figure 5.

3 The second pattern relates to the overall timing of the summer rainfall. At the Kendall
4 site, once the monsoon period begins (early-July), the assimilation of observations
5 successfully constrains the model which produces consistent equivalent neutron counts
6 (Figures 5b and 5c). In other words, rainfall pulses provide “new information” to the
7 assimilation system. For the two other sites (Nebraska and Park Falls), an active rainfall
8 period lasts until early-July and is then followed by a period of low or no rainfall
9 (arguably, no substantial “information” to the assimilation system). In this case, we
10 observe a tendency for lower spread values in comparison to RMSE at both sites for the
11 ‘DA 2-day’ case. This tendency disappears when high-frequency observations are
12 assimilated (i.e., ‘DA 1-hour’) at the Park Falls site. For the Nebraska site, although still
13 present, the tendency is reduced for the ‘DA 1-hour’. These results highlight the quality
14 of the OSSE carried out in this study as well as the distinct performance of the
15 assimilation system due to different timing in rainfall events occurred at all three
16 Ameriflux sites.

17 Finally, the results summarized in Table 3 show better overall performance for ‘DA 1-
18 hour’ compared to ‘DA 2-day’, with both cases being almost always superior to the ‘No
19 DA’ case. In almost all cases, computed statistics with respect to the true counts are
20 better than those computed with the synthetic observations. This is expected because
21 an additional degree of randomness is introduced in the synthetic observations (i.e., light
22 gray circles in Figure 4). The degree of improvement compares well with the results from
23 (Shuttleworth et al., 2013).

24 25 **4.2 Impact of near-surface cosmic-ray neutrons on simulated soil moisture** 26 **profiles**

27 In the case of cosmic-ray sensors, the dynamics of equivalent neutron counts observed
28 can be assumed to be a proxy for integrated, depth-weighted variation of soil moisture at
29 sub-kilometer scales, as shown in (Shuttleworth et al., 2013). Here, we expand this
30 analysis by assessing how well all root zone layers in the Noah (prescribed as the first
31 one meter of soil in the model) are simulated with and without the assimilation of
32 observed neutron counts. The effective sensor depth computed from the synthetic

Rafael Rosolem 9/8/14 5:02 PM
Comment [13]: Response [9] to Reviewer #1
Responses [1] and [6] to Reviewer #2

1 observations at all three sites varies on average from ~12 cm during the wet period to
2 ~20 cm in the dry months. This corresponds to the entire surface (first) soil layer of Noah
3 with an additional contribution from the second soil layer in the model (10-40 cm layer).
4 Overall results are summarized in Table 4, and presented for each site in Figures 6, 7,
5 and 8.

6 In those figures, the left column is related to the first soil layer, and the right column is
7 related to the deepest layer analyzed. The top row corresponds to the actual soil
8 moisture simulated by Noah for the three cases (i.e., 'no DA', 'DA 2-day', and 'DA 1-
9 hour') in comparison to the true soil moisture state (same color-coding as before). The
10 middle row shows the difference between the Noah-derived and true soil moisture. We
11 selected an "uncertainty range" of $\pm 0.02 \text{ m}^3 \text{ m}^{-3}$ as our target for comparison which is
12 similar to the accuracy found in more traditional point-scale measurements (TOPP et al.,
13 1980) and also comparable to the accuracy of cosmic-ray sensors (Franz et al., 2012a;
14 Rosolem et al., 2013). Note that the target accuracy from satellite remote sensing
15 products is twice as big, as discussed by (Brown et al., 2013; Entekhabi et al., 2010;
16 Kerr et al., 2010). The bottom row corresponds to a simple convergence criterion based
17 on the results from the middle row. For each hourly time step, we check whether the
18 difference with respect to the true soil moisture is within the "uncertainty range". If it is
19 within this range, the value is added to the current number of counts, and the percentage
20 convergence is taken with respect to the total number of points analyzed at that given
21 time. As an example, if the first point found within the "uncertainty range" is located in
22 position 50 of the time array, its convergence is computed as 2% (i.e., 1/50). If the next
23 time step is also within this range, its convergence is computed as ~3.9% (i.e., 2/51),
24 and so on. With this simple metric we can determine not only the overall percentage of
25 hours when the difference was within this uncertainty range (obtained at the end of the
26 simulation) but also how the convergence evolves as the simulation period progresses.

27 At the Kendall site, the results suggest overall improved performance of Noah for all soil
28 layers (including those beyond the sensor effective depth) when observed neutron
29 counts are assimilated regardless of the availability of observations (Figure 6a-f).
30 Differences between 'DA 1-hour' and 'DA 2-day' cases are larger at deeper soil layers
31 with 'DA 1-hour' showing superior performance. For the 'no DA' case, only the soil
32 moisture at the first layer in the model is within the uncertainty range for the majority of
33 the simulated period. The soil moisture for the 'DA 2-day' case compares relatively well

1 with the true soil moisture at the first two layers but estimated soil moisture in the third
2 layer is almost always outside of the uncertainty range. The 'DA 1-hour' case, however,
3 shows a remarkable response to neutron count and effectively simulates the soil
4 moisture dynamics at all Noah soil layers (basic statistics are calculated and presented
5 in Table 4).

6 The convergence calculated for the Kendall site suggests that, overall, soil moisture is
7 constrained more effectively when observations of cosmic-ray neutrons are assimilated
8 into Noah (Figure 6g-i). For the first soil layer, total convergence levels are high in all
9 cases and little difference is observed between the two DA cases. The benefit of
10 assimilating observed neutron counts is more clear in the results for the second layer,
11 with no substantial differences between the high- and low-frequency assimilation
12 strategies. However, the impact of higher retrieval frequency becomes evident in the
13 third soil layer in which soil moisture is only successfully constrained in the 'DA 1-hour'
14 case.

15 The results from the Nebraska and Park Falls sites are comparable and they show
16 superior performance of Noah when assimilating neutron counts at high-frequency
17 (Figures 7a-f and 8a-f). Surprisingly, for the first two soil layers in Noah the dynamics of
18 soil moisture obtained from the ensemble average for 'DA 2-day' is similar to the model
19 behavior for the 'no DA' case. In addition, 'no DA' soil moisture at the deepest analyzed
20 layer at the Nebraska site follows the true soil moisture states quite well. This is likely
21 related to the fact that the initial conditions randomly obtained in the model were already
22 similar to the true soil moisture state (in terms of ensemble averages) for the 'no DA'
23 case, although the overall magnitude of the spread is much larger compared to
24 assimilation cases (Table 4). At Park Falls, the results from the deepest soil layer
25 analyzed show superior performance of 'DA 1-hour' while 'no DA' and 'DA 2-day' have
26 similar dynamics especially after late-June.

27 The convergence criterion computed for the first two soil layers in Noah at the Nebraska
28 and Park Falls sites (Figures 7g-h and 8g-h) are slightly different from the results
29 discussed for the Kendall site (Figure 6g-h). First, the percentage of points within the
30 uncertainty range at these two sites is greater than the percent values obtained at
31 Kendall (compare for instance, 'DA 1-hour' case across all sites). There is a much
32 sharper increase in the convergence criterion with time at these two sites as opposed to
33 the pattern observed for Kendall. However, unlike the Kendall site where the patterns of

1 both DA cases were somewhat similar, it is much more clear for both the Nebraska and
2 Park Falls cases that the 'DA 1-hour' is able to update soil moisture much more rapidly
3 than the 'DA 2-day' when compared to the response to the 'no DA' case. As mentioned
4 previously, the convergence results for the 'no DA' case at the third soil layer in the
5 model are likely to be related to the initial conditions from the ensemble mean being
6 already to close to the true states (Figures 6i and 7i).

7 **4.3 Impact of retrieval frequency on simulated soil moisture dynamics**

8 The previous sub-section reports the improved ability of Noah to estimate soil moisture
9 profiles when assimilating cosmic-ray neutron counts measured aboveground, and
10 included some initial comparison between assimilation frequencies ('DA 1-hour' and 'DA
11 2-day'). In this section we compare the "average" performance of Noah for continuous
12 periods of 2 days after the cosmic-ray neutron measurement is assimilated into the
13 model throughout the simulation period. The aim is to evaluate Noah performance within
14 individual time windows when neutron measurements are assimilated every 2 days,
15 every hour, or not assimilated. In this study, the RMSE of soil moisture is calculated with
16 respect to the true state for a fixed time-window of 2 days applied throughout the entire
17 simulation period. For comparison, the results discussed in the previous section were
18 based on actual model simulations at hourly timescales. The results are presented in
19 Figure 9 with top, middle, and bottom rows corresponding, respectively to the Kendall,
20 Nebraska, and Park Falls sites, with left and right columns corresponding to the
21 shallowest and deepest Noah soil layers analyzed in this study (same color-coding as
22 shown in previous figures).

23 The first noticeable result from Figure 9 is that the average performance of Noah (i.e.,
24 using the 2-day time windows) when trying to simulate true soil moisture profiles is best
25 when neutron measurements are assimilated at hourly timescales (i.e., 'DA 1-hour') at
26 all sites. At the Kendall site, which is characterized by a long dry period followed by the
27 monsoon onset early in July, the performance of Noah for the 'DA 2-day' case is similar
28 to that obtained with 'DA 1-hour' at the first two layers of the model (Figure 9a-b), and
29 slightly worse at the deepest layer (Figure 9c). Surprisingly, a different pattern emerges
30 from both the Nebraska and Park Falls sites where an initial period of frequent rainfall is
31 followed by a relatively long dry period which also starts in July (Figure 9d-i). In those
32 cases, the performance of 'DA 2-day' is not improved substantially in comparison to 'no
33 DA', and a noticeable increase in RMSE is observed in both cases right after rainfall

1 ceases in July. Unlike the 'DA 1-hour' case, the 'DA 2-day' case allows for Noah to freely
2 advance in time for the rest of the 2-day period once it has assimilated the neutron count
3 measurement, and because the true simulation was generated with a different set of
4 parameters than the cases analyzed here, model simulations in the 'DA 2-day' case are
5 unable to represent the dynamics of dry-down appropriately due to different soil
6 properties. The lack of rainfall in this case, reduces the potential magnitude for soil
7 moisture updates (i.e., 'model innovation'), and hence the dynamics of the model are
8 little improved. The results shown here suggest the performance of summertime cosmic-
9 ray neutron data assimilation may be slightly dependent on climatological conditions
10 (i.e., meteorological forcing), and the period during which rainfall occurs in the summer,
11 while also depending on model uncertainties due to lack of representativeness of key
12 soil and vegetation properties at the scale of interest (here, accounted for by the fact that
13 true soil moisture is generated from a model simulation obtained with slightly perturbed
14 parameter values).

15

16 **5 Summary and conclusions**

17 The use of cosmic-ray neutron sensors for soil moisture monitoring has been fast
18 growing because the technique provides root-zone soil moisture estimates at
19 unprecedented spatial scales and at high temporal resolution. This paper evaluates the
20 ability of a land surface model to translate the information obtained from cosmic-ray
21 neutrons observed aboveground into soil moisture estimates for individual soil layers. A
22 "nearly-identical twin experiment" approach is adopted in which observations of cosmic-
23 ray neutrons were generated from the land surface model with a slightly different model
24 configuration (perturbed key soil and vegetation parameters). Below we discuss the
25 implications and summarize the main findings of this work.

26 *How effectively is the information from aboveground cosmic-ray neutrons translated to*
27 *individual soil moisture layers in the model?*

28 When assimilating neutron counts at high frequency, the performance of the land
29 surface model is remarkably improved in comparison with the soil moisture profiles
30 simulated without data assimilation. This finding is observed for all three biomes with
31 degree of improvement varying slightly from site-to-site. Of importance, we found that
32 water in the soil is better estimated at depths well below the effective sensor depth and

1 encompassing the entire rooting zone in the model. Therefore, the high observational
2 frequency of the cosmic-ray sensors can potentially introduce additional benefits relative
3 to assimilating local/regional soil moisture observations from satellite remote sensing
4 products available at coarser temporal resolution. However, care must be taken when
5 accounting for measurement uncertainty by removing any potential signal in the
6 measurement from other sources of hydrogen (atmospheric water vapor, water in
7 biomass), hence isolating or maximizing the soil moisture information content in the
8 measurement. Another important aspect is to ensure sufficient ensemble spread from
9 the model to avoid, for instance, filter divergence (over-confidence in the model), or
10 alternatively directly inserting observations with little or no model influence (over-
11 confidence in the observations) (Anderson, 2007; Hamill et al., 2001; Houtekamer and
12 Mitchell, 1998).

13 *How does frequency of available observations of cosmic-ray neutrons influence model*
14 *performance?*

15 We use the RMSE calculated for every 2-day time-window as a metric for model
16 performance. At the Kendall site, 'DA 1-hour' and 'DA 2-day' showed good agreement
17 for soil moisture in the first two layers of the model (0-10 and 10-40 cm). However, the
18 benefits of high-frequency retrievals in the case of cosmic-ray neutron observations is
19 also observed for the third soil layer in Noah (40-100 cm), where 'DA 1-hour' is much
20 superior to 'DA 2-day'. Particularly to the Noah, the distribution of roots is directly
21 proportional to the thickness of each soil layer. Therefore, the third layer of the model
22 plays a significant role in determining evapotranspiration rates at the surface.
23 Summertime is characterized by an initial relatively dry period which lasts for about 2
24 months followed by the monsoon.

25 Unlike the results at Kendall, the comparison between 'DA 1-hour' and 'DA 2-day' for
26 Nebraska and Park Falls suggest that the performance of Noah for the 'DA 1-hour' case
27 is always superior to that from 'DA 2-day' in all soil layers analyzed. Surprisingly, the
28 model performance for the 'DA 2-day' case is not much different from simulations made
29 without assimilating cosmic-ray neutron counts (i.e., 'no DA' case). A distinct
30 characteristic from both the Nebraska and Park Falls sites in comparison to Kendall is
31 the overall dynamics of soil water in the summertime. At Nebraska and Park Falls, a
32 relatively wet period with frequent rainfall is observed at the beginning of the
33 summertime period, lasting for about 2 months, and followed by a relatively dry period

1 with low or no rainfall. Overall, the benefits of assimilating neutron measurements at
2 relatively higher frequency are more clearly observed at the Nebraska and Park Falls
3 sites relative to the semi-arid Kendall. This could indicate that the assimilation
4 performance of summertime cosmic-ray measurements at high temporal resolution may
5 depend not only on heterogeneity of soil properties (accounted for by slightly perturbing
6 model parameter from true soil moisture states) but also slightly on meteorological
7 forcing and its climatology (namely, rainfall). Also, these findings suggest an important
8 role of high-frequency measurements to better constrain soil moisture states simulated
9 by hydrometeorological models when applied to drought monitoring given that the
10 summer of 2012 was one of the driest on record in the Midwestern USA region.

11 Due to the characteristics of the sensor, the integration time used to compute neutron
12 intensity should potentially be longer than one hour at some locations. In practice, this is
13 done to reduce the uncertainty in the measurement and consequently ensure an
14 accurate estimate of soil moisture. For instance, neutron count rates integrated over the
15 entire day were used in a humid forest ecosystem located in western of Germany
16 because hourly count rates were too low for accurate soil moisture measurements
17 (Bogena et al., 2013). The results presented in our study show that care must be taken
18 when integrating the cosmic-ray measurements over a longer-period while combining
19 with models, suggesting a potential trade-off between individual sensor accuracy and
20 successful representation of soil moisture profile dynamics. This could imply in an
21 'optimal range' for integration of neutron counts for a specific site location but the
22 investigation is beyond the scope of this study. For example, our initial preliminary
23 analysis indicated little difference between the 'DA 2-day' case with another assimilation
24 case where neutron measurements were assimilated daily.

25 This study focused on the analysis using synthetic observations mainly because (1)
26 there is a lack of independent soil moisture observations corresponding to similar
27 effective horizontal area measured by the cosmic-ray sensor, and (2) the neutron
28 intensity signal is entirely derived from soil moisture dynamics, which allows us to focus
29 on the key aspects of the neutron-soil moisture interactions. Neither the COSMIC
30 operator nor the Noah have explicitly dealt with additional sources of hydrogen (Franz et
31 al., 2013a) other than the lattice water (explicitly described by a parameter in COSMIC;
32 see (Shuttleworth et al., 2013)). Typical sources include surface water (Franz et al.,
33 2012a), atmospheric water vapor (Rosolem et al., 2013), biomass (Franz et al., 2013b),

Rafael Rosolem 9/8/14 5:02 PM

Comment [14]: Response [5] to Reviewer #2

1 and litter layer, carbohydrates of soil organic matter and belowground biomass (Bogena
2 et al., 2013). For instance, changes in biomass over time may become important
3 especially at the Nebraska (cropland) site. However, as with any OSSE, there are some
4 limitations in our approach because the uncertainties due to the above-mentioned
5 sources of hydrogen are not introduced in the measurements. Furthermore, any
6 potential structural deficiency in Noah when simulating soil moisture is ignored in this
7 OSSE, hence model adjustments to remove or reduce systematic biases (Draper et al.,
8 2011; Kumar et al., 2012; Yilmaz and Crow, 2013) need not be applied. As a
9 consequence, the results from the OSSE are likely to indicate better agreement relative
10 to those obtained from assimilation of real neutron measurements. The assimilation of
11 actual cosmic-ray neutron measurements will be investigated in the near future.

12 Finally, these results can also give some additional insights into applications of data
13 assimilation to satellite remote sensing products whose measurements are provided
14 globally at coarser temporal resolution. However, it is not the intention of the present
15 study to directly compare the value of the cosmic-ray observations with more traditional
16 satellite remote sensing products, especially because their horizontal effective
17 measurement areas are quite different (Robinson et al., 2008) and hence are likely to be
18 influenced differently by distinct factors (see Figure 1 in (Crow et al., 2012)). Such
19 analyses are beyond the scope of this study but we encourage the use of cosmic-ray
20 sensors in combination with satellite remote sensing products for hydrometeorological
21 applications because the information content from each measurement can be strongly
22 linked to their individual dynamics.

23

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Rafael Rosolem 9/8/14 4:52 PM

Comment [15]: Response [1] to Reviewer #1

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Comment [16]: Response [8] to Reviewer #2

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- 3

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- 19

1 Table 1. Site information obtained from Ameriflux database (<http://ameriflux.lbl.gov>).
 2 MAT = Mean Annual Temperature, and MAP = Mean Annual Precipitation. Notice the
 3 analyzed period in this study is a subset of the available data from each site and it is
 4 defined from 2012-05-01_00Z* to 2012-09-30_23Z*.

Site	Latitude	Longitude	Land cover	Soil type	MAT (°C)	MAP (cm)	Spin-up period (one cycle)
Kendall	31° 74'N	109° 94'W	Grasslands	Loam	16	41	2010-01-01_00Z to 2012-12-31_23Z
Nebraska	41° 10'N	96° 26'W	Croplands	Silty Clay Loam	10	78	2011-01-01_00Z to 2012-12-31_23Z
Park Falls	45° 56'N	90° 16'W	Mixed forest	Sandy Loam	4	82	2011-01-01_00Z to 2012-12-31_23Z

Rafael Rosolem 9/8/14 10:50 PM
 Comment [17]: Response [7] to Reviewer #1

5 * Date/time format as follows YYYY-MM-DD_HH, where YYYY is the year, MM is the
 6 month, DD is the day of the month, and HH is the hour in GMT.

Rafael Rosolem 9/8/14 10:55 PM
 Comment [18]: Response [7] to Reviewer #1

Rafael Rosolem 9/8/14 10:50 PM
 Comment [19]: Response [7] to Reviewer #1

1 Table 2. Perturbation magnitudes of meteorological inputs used by Noah for individual
 2 ensemble members in this study. The perturbation distribution is either *log-Normal* (i.e.,
 3 multiplying the reference variable) or *Normal* (i.e., adding to or subtracting from a
 4 reference value). Values within parentheses correspond respectively to mean and
 5 standard deviation. Notice, vegetation greenness fraction has been added to the list
 6 given its strong sensitivity in Noah (Miller et al., 2006). The adopted magnitude values
 7 follow standard procedures described in the literature, including (Dunne and Entekhabi,
 8 2005; Kumar et al., 2012; Margulis et al., 2002; Reichle and Koster, 2004; Reichle et al.,
 9 2008; 2007; 2002; Sabater et al., 2007; Walker and Houser, 2004; Zhang et al., 2010;
 10 Zhou et al., 2006).

Noah Forcing	Perturbation Magnitude
Wind Speed (m s^{-1})	<i>log-Normal</i> (1,0.3)
Air temperature (K)	<i>Normal</i> (0,5)
Relative Humidity (fraction)	<i>log-Normal</i> (1,0.2)
Surface Pressure (Pa)	<i>Normal</i> (0,10)
Incoming Shortwave Radiation (W m^{-2})	<i>log-Normal</i> (1,0.3)
Incoming Longwave Radiation (W m^{-2})	<i>Normal</i> (0,50)
Precipitation rate ($\text{kg m}^{-2} \text{s}^{-1}$)	<i>log-Normal</i> (1,0.5)
Vegetation greenness fraction (-)	<i>Normal</i> (0,0.05)

11

12

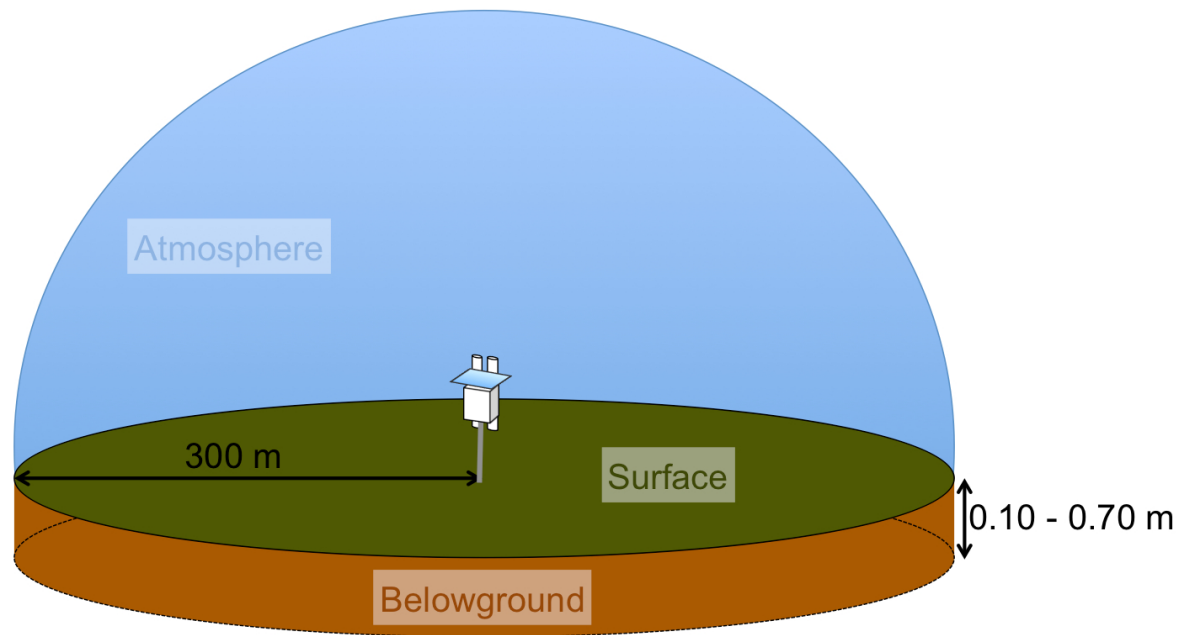
- 1 Table 3. Summary of statistics computed for Noah for assimilation of synthetic neutron
- 2 intensity measurements in counts per hour (cph). Metrics are computed with respect to
- 3 both true counts and synthetic observations, respectively 'w.r.t. True' and 'w.r.t. Obs'.
- 4 The ensemble mean of the prior distribution is used for all ensemble simulations.

Site	Simulation	Mean Bias		RMSE		Total Spread	R ²	
		w.r.t. Obs	w.r.t. True	w.r.t. Obs	w.r.t. True		w.r.t. Obs	w.r.t. True
Kendall	no DA	-89	-90	119	109	96	0.89	0.94
	DA 2-day	-9	-13	63	60	57	0.91	0.92
	DA 1-hour	0	-1	63	60	50	0.91	0.92
Nebraska	no DA	-15	-14	49	32	51	0.90	0.97
	DA 2-day	-13	-15	45	28	40	0.89	0.97
	DA 1-hour	-8	-8	38	12	37	0.93	1.00
Park Falls	no DA	-8	-8	30	15	36	0.82	0.98
	DA 2-day	-6	-8	27	14	27	0.81	0.96
	DA 1-hour	-2	-2	25	3	26	0.84	1.00

5

1 Table 4. Summary of statistics computed for Noah for assimilation of synthetic neutron intensity measurements for all sites. All
 2 metrics are calculated only when individual layer convergence is above 40% for the case 'DA 1-hour' (see bottom panel of Figures 6,
 3 7, and 8), and with respect to the true soil moisture state. The ensemble mean of the prior distribution is used for all ensemble
 4 simulations. Numerical values are rounded to the first three decimal points.

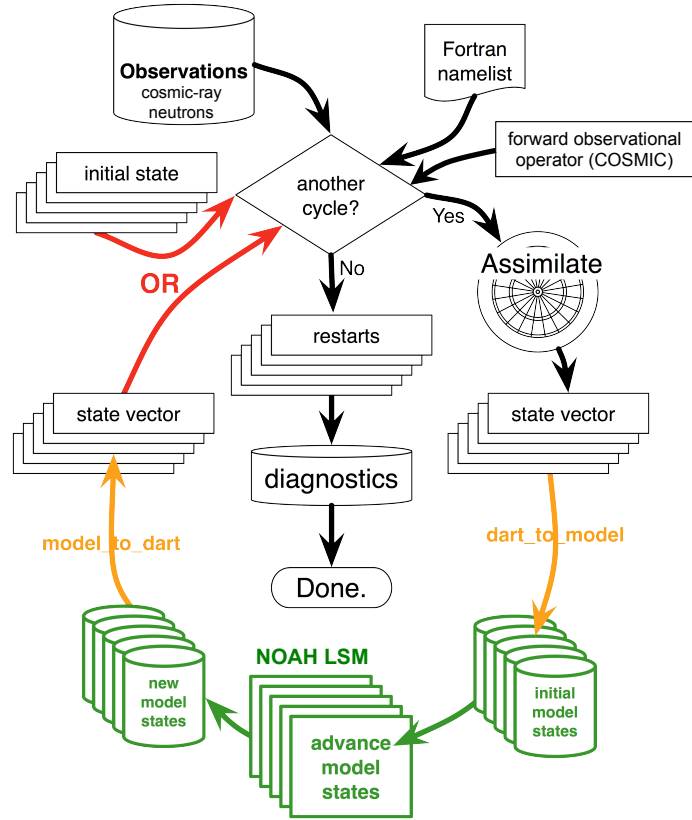
Noah Soil Moisture (m ³ m ⁻³)	Mean Bias			RMSE			Spread			R ²		
	No DA	DA 2-day	DA 1-hour	No DA	DA 2-day	DA 1-hour	No DA	DA 2-day	DA 1-hour	No DA	DA 2-day	DA 1-hour
Kendall												
θ ₁ (0 – 10 cm)	0.009	-0.003	-0.003	0.011	0.006	0.005	0.019	0.007	0.003	0.988	0.990	1.000
θ ₂ (10 – 40 cm)	0.037	0.009	0.006	0.042	0.011	0.007	0.033	0.012	0.006	0.907	0.981	0.995
θ ₃ (40 – 100 cm)	0.071	0.030	0.009	0.072	0.033	0.012	0.051	0.032	0.015	0.906	0.872	0.989
Nebraska												
θ ₁ (0 – 10 cm)	0.004	0.005	0.001	0.010	0.009	0.004	0.016	0.008	0.003	0.978	0.987	0.996
θ ₂ (10 – 40 cm)	0.007	0.011	0.006	0.017	0.013	0.007	0.022	0.009	0.003	0.962	0.987	0.998
θ ₃ (40 – 100 cm)	0.012	0.012	0.009	0.012	0.012	0.009	0.038	0.018	0.007	0.999	0.998	0.993
Park Falls												
θ ₁ (0 – 10 cm)	0.005	0.007	0.001	0.009	0.009	0.003	0.018	0.008	0.003	0.984	0.985	0.996
θ ₂ (10 – 40 cm)	0.006	0.008	0.002	0.010	0.010	0.004	0.022	0.009	0.003	0.986	0.987	0.997
θ ₃ (40 – 100 cm)	0.007	0.013	0.005	0.011	0.015	0.007	0.031	0.013	0.005	0.974	0.980	0.990



1

2 Figure 1. Schematic representation of the effective measurement volume for the cosmic-ray soil moisture sensor. The effective depth
3 depicted in the figure refers to the overall range in the sensor (Zreda et al., 2008). Notice the effective depth estimated for the
4 synthetic experiments in this study varies approximately between 12 and 20 cm (refer to text).

5

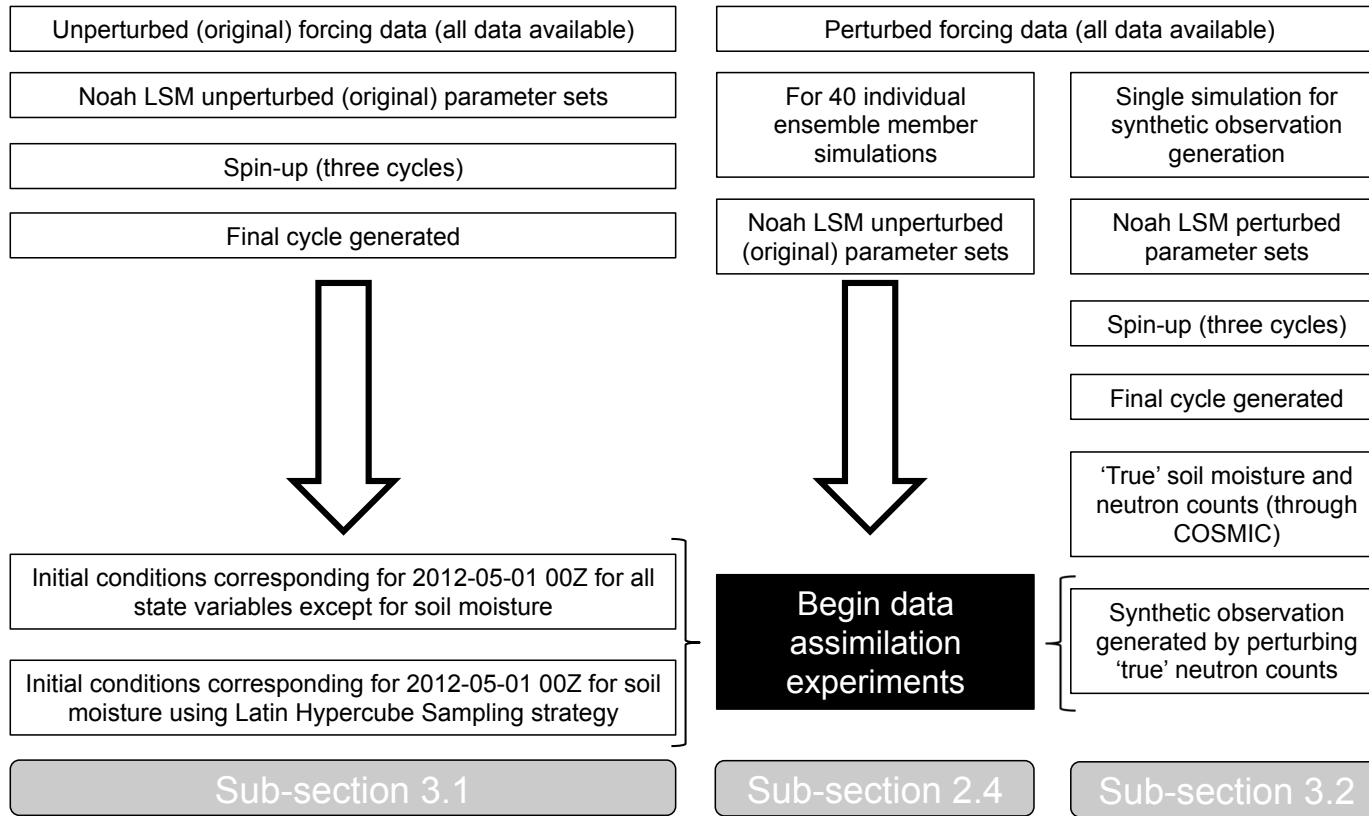


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2 Figure 2. Schematic representation of the data assimilation and state update procedures in the Data Assimilation Research Testbed

3 (DART) used in this study. Adapted from original DART diagram available at <http://www.image.ucar.edu/DARes/DART>.

Rafael Rosolem 9/8/14 10:48 PM
Comment [20]: Response [4] to Reviewer #1



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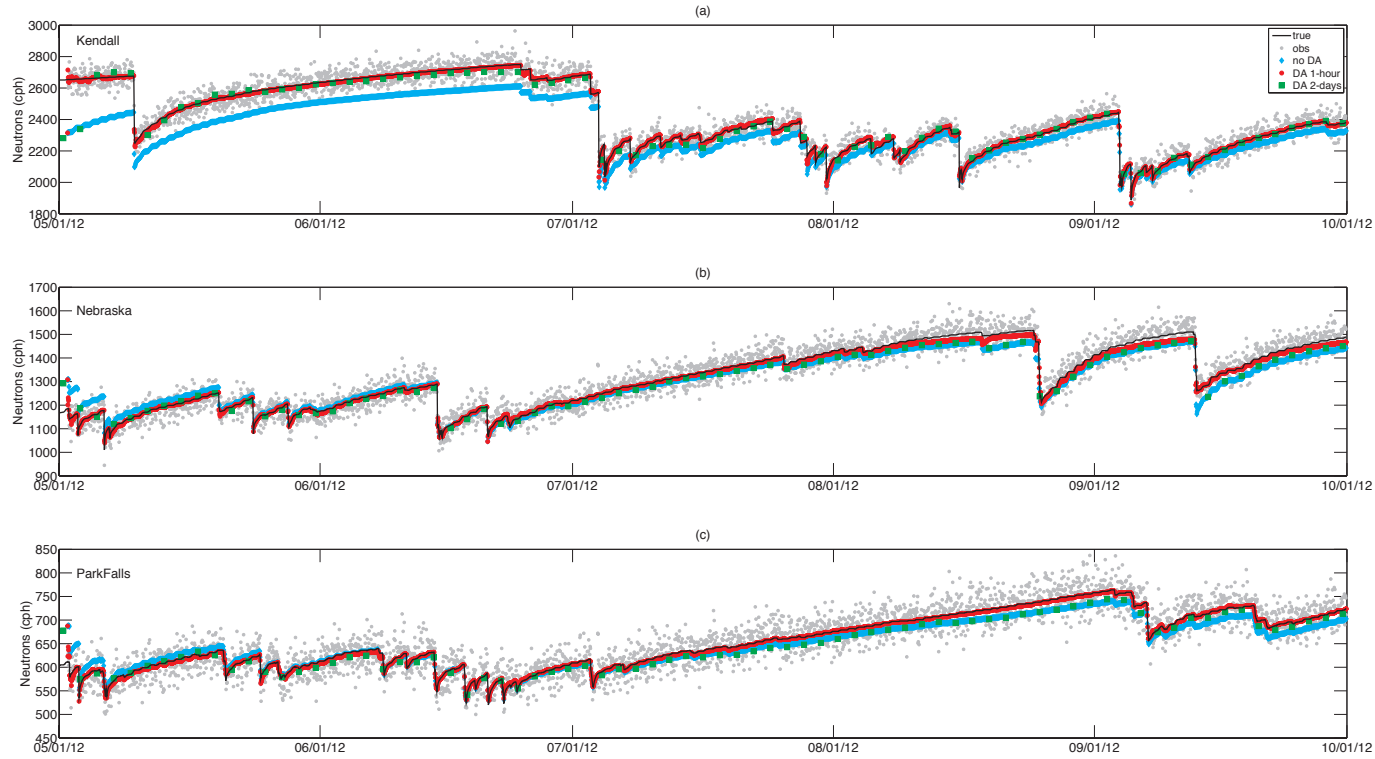
2 Figure 3. Experimental setup used in this study for data assimilation of synthetic observations of cosmic-ray neutrons.

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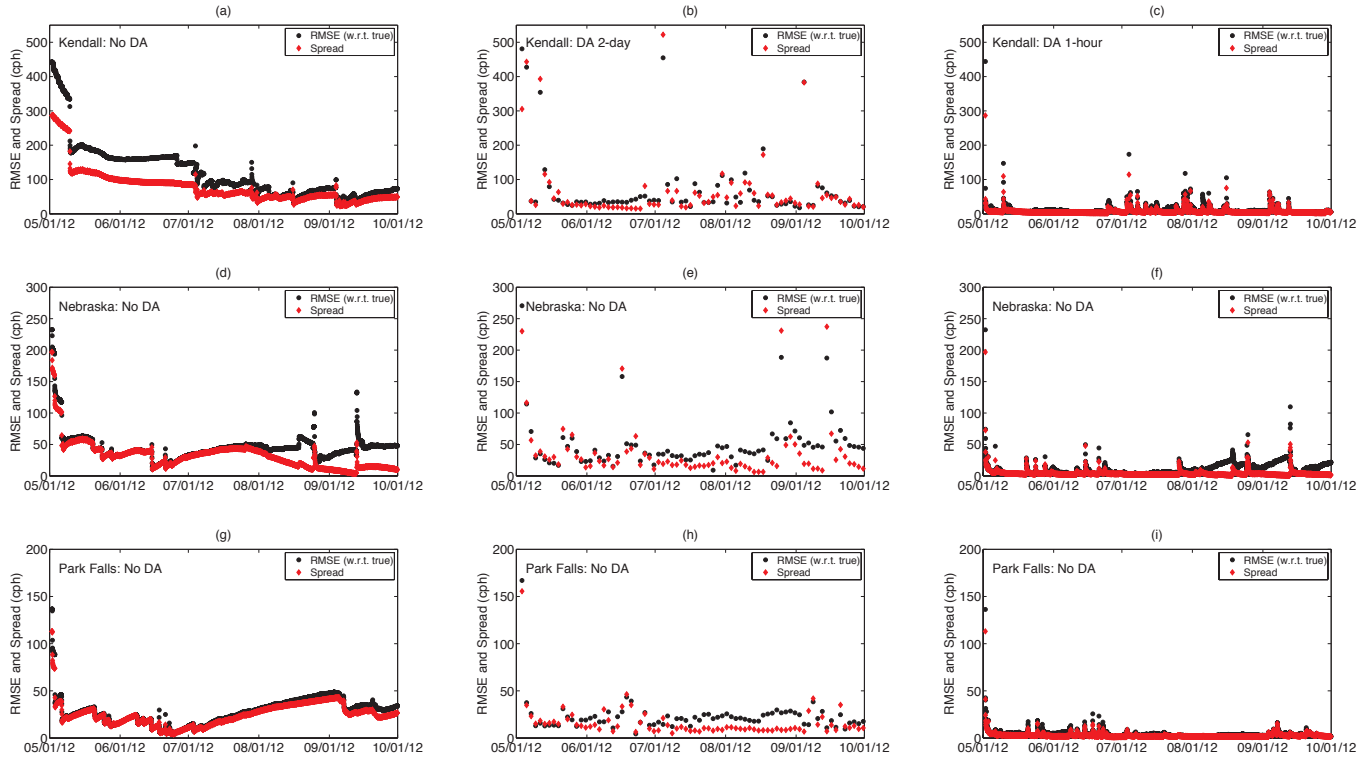
Comment [21]: Responses [5] and [7] to Reviewer #1

Rafael Rosolem 9/8/14 10:53 PM

Comment [22]: Responses [1] and [2] to Reviewer #2



1
 2 Figure 4. Equivalent neutron intensity (counts per hour - cph) simulated by Noah coupled to COSMIC without (no DA) and with data
 3 assimilation characterized by low- and high-frequency retrievals (respectively, DA 2-day and DA 1-hour) compared to synthetic
 4 observations (obs) and true intensities. The ensemble mean of the prior distribution is shown for all ensemble simulations.



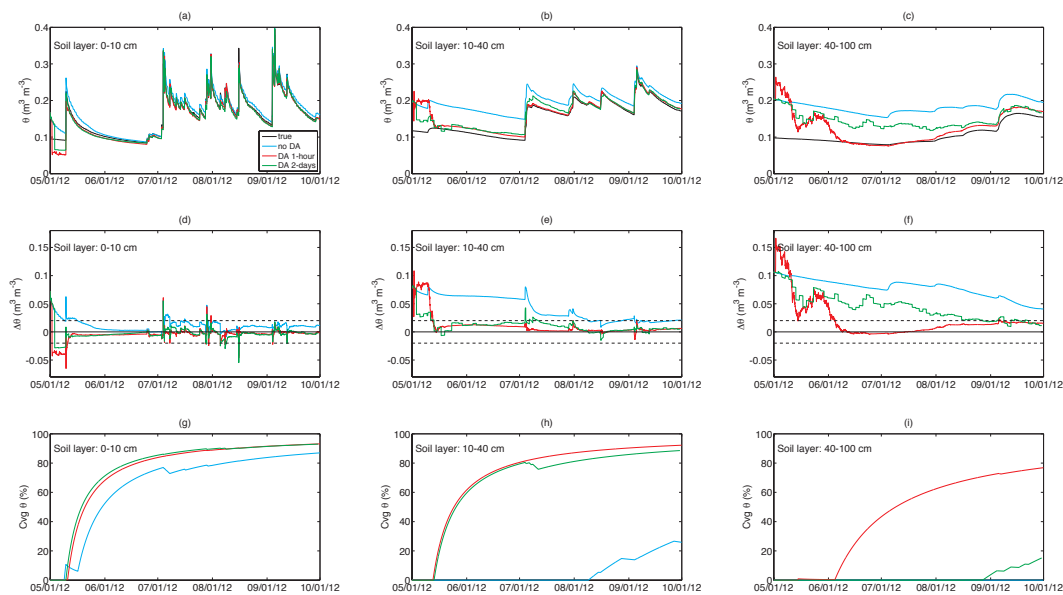
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 2 Figure 5. Root-Mean-Squared-Error (RMSE) calculated for the ensemble mean relative to the 'true' observations (black circles) in
 3 comparison to the ensemble spread (red diamonds). The ensemble mean of the prior distribution is used for all ensemble
 4 simulations.

Rafael Rosolem 9/8/14 10:51 PM

Comment [23]: Response [11] to Reviewer #1

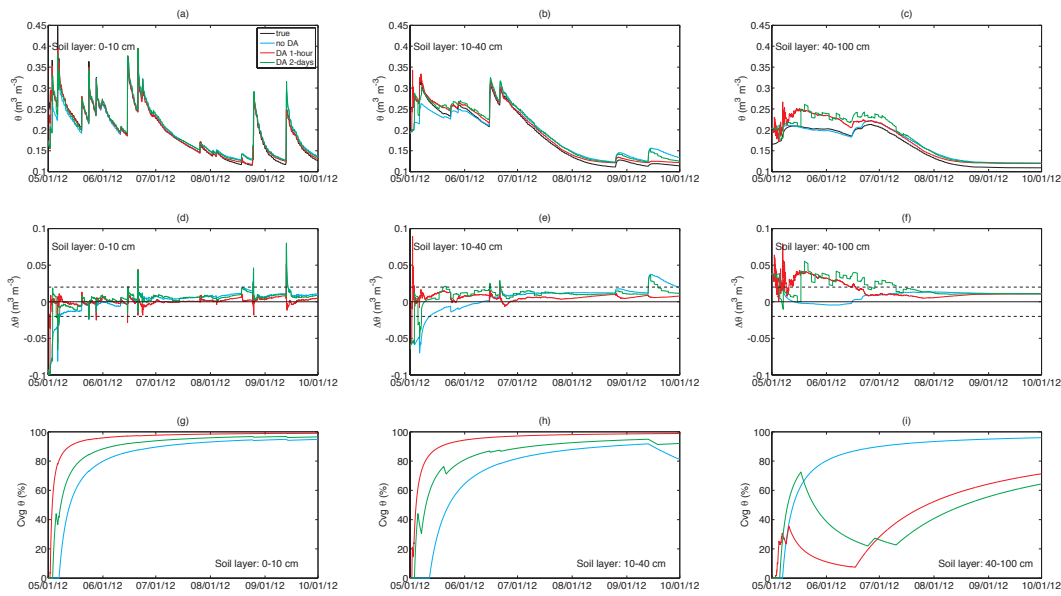
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Comment [24]: Response [6] to Reviewer #2



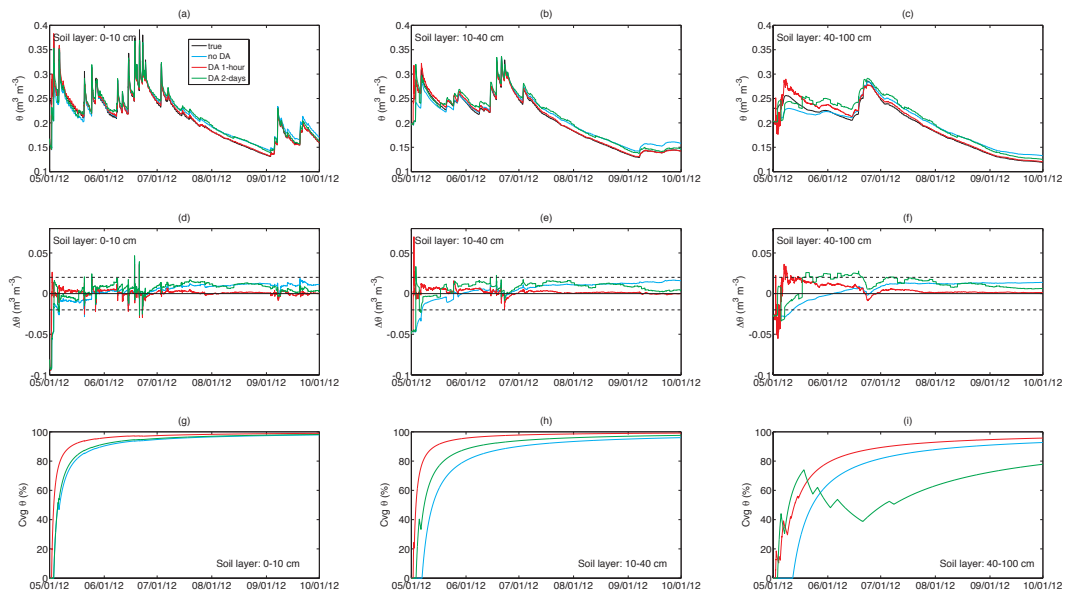
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2 Figure 6. Comparison of soil moisture dynamics at the Kendall site for the first three soil layers in Noah. Top row: Simulated soil
 3 moisture (θ) without (no DA) and with data assimilation characterized by low- and high-frequency retrievals (respectively, DA 2-day
 4 and DA 1-hour) compared to the true soil moisture states. Middle row: The difference between simulated soil moisture and the true
 5 states ($\Delta\theta$) within pre-defined uncertainty ranges (dashed gray lines). Bottom row: Convergence criterion within uncertainty ranges.
 6 Results show actual model time steps (i.e., hourly). The ensemble mean of the prior distribution is shown for all ensemble
 7 simulations.



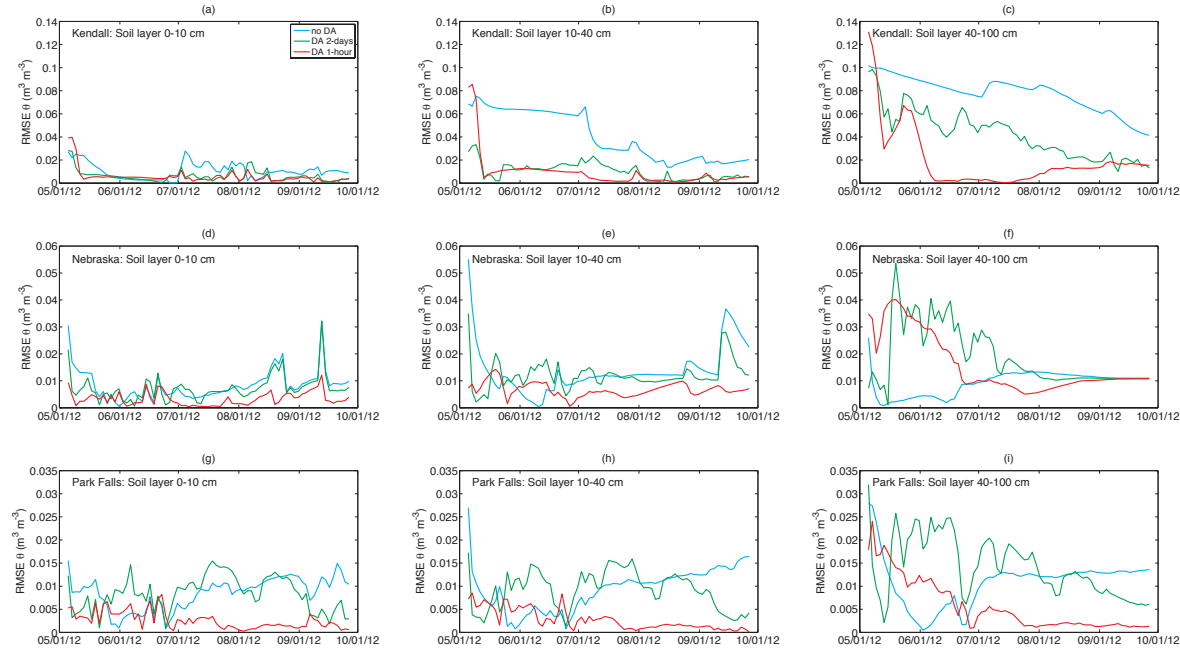
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2 Figure 7. Same as Figure 6 but for Nebraska.



1

2 Figure 8. Same as Figure 6 but for Park Falls.



1

2 Figure 9. Comparison of Noah performance in representing soil moisture dynamics for the first three soil layers with respect to the
 3 true soil moisture state. The metric used is the Root-Mean-Squared-Error (RMSE) calculated over individual 2-day periods
 4 continuously. Results are shown for Noah without (no DA) and with data assimilation characterized by low- and high-frequency
 5 retrievals (respectively, DA 2-day and DA 1-hour). The ensemble mean of the prior distribution is used for all ensemble simulations.