Supporting Information for:

Exploiting soil moisture, precipitation and streamflow observations to evaluate soil moisture/runoff coupling in land surface models

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Appendix A: Interpretation of Coupling Strength Estimates

As described in the main text, our primary goal here is deriving estimates of the correlation between event runoff coefficient serial ranks (*RC*) and pre-storm soil moisture serial ranks (*SM*) for a given basin:

$$R = \frac{\mathrm{Cov}(RC,SM)}{\sqrt{\mathrm{Var}(RC)\ \mathrm{Var}(SM)}}. \quad \text{(A1)}$$

The true value of this rank correlation, R_{true}, is obtained if *RC* and *SM* are free of error. Replicating this true value should be the goal of any credible land surface model (LSM). Note that the overbar on *R*, used in the main text to indicate averaging across multiple basins, is dropped here.

Of course, perfect time series representations of *RC* and *SM* are never available. Instead, we rely on uncertain estimates of these quantities. These estimates can be approximated as:

$$RC_{est} = RC + \xi_{RC} \quad \text{(A2)}$$

$$SM_{est} = SM + \xi_{SM}$$

where ξ_{RC} and ξ_{SM} are mean-zero error variables. Note that scaling gain factors are neglected in (A2) since such factors have no bearing on the correlation-based discussion that follows below.

Without making any statistical assumptions regarding these errors, re-calculating (A1) using estimated values in (A2) yields:

$$R_{est} = \frac{[\mathrm{Cov}(RC,SM) + \mathrm{Cov}(\xi_{RC},\xi_{SM}) + \mathrm{Cov}(RC,\xi_{SM}) + \mathrm{Cov}(\xi_{RC},SM)]}{\sqrt{[\mathrm{Var}(RC+\xi_{RC})]\,[\mathrm{Var}(SM+\xi_{SM})]}}\,. \qquad \text{(A3)}$$

Equation (A3) can be used to estimate the impact of errors in *RC* and *SM* on ranks correlations sampled from real data. However, several important distinctions should be made between estimates of rank correlation derived from largely independent, observation-based sources (i.e., R_{obs} computed using *SM* from a data assimilation analysis and *external RC* obtained from independent rain and stream gauge observations) and estimates of *R* derived from internally consistent LSM estimates (i.e., R_{LSM} computed from *internal* model estimates of soil moisture, runoff, and precipitation, with the latter also used to force the LSM and generate the LSM soil moisture and runoff estimates). These issues are discussed in depth below.

A.1. Impact of random error

By construction, R_{LSM} is insensitive to purely random errors in the LSM forcing (see main text section 3.1). Therefore, if (A1) is applied to LSM-internal *RC* and *SM* results provided by a physically realistic and unbiased simulation, the resulting correlation (R_{LSM}) should indeed match R_{true}. In contrast, an observation-based correlation estimate (R_{obs}) is biased low in the presence of independent random error in *RC* and *SM*. This can be illustrated by assuming wholly independent and orthogonal observational errors in (A2) and, thereby, simplifying (A3) to:

$$R_{obs} = \frac{[\mathrm{Cov}(RC,SM)]}{\sqrt{[\mathrm{Var}(RC)+\mathrm{Var}(\xi_{RC})]\,[\mathrm{Var}(SM)+\mathrm{Var}(\xi_{SM})]}}\,. \qquad \text{(A4)}$$

The sole difference between (A4) and (A1) is that the denominator of (A3) is inflated by the additional random error variance associated with uncertain SM_{est} and RC_{est} observations in (A2). Given that $\text{Cov}(RC, SM)$ is almost always positive (see main text), this induces a negative bias into R_{obs} relative to R_{LSM} (or R_{true}).

The magnitude of this bias is determined by the signal-to-noise (SNR) characteristics of SM_{est} and RC_{est} (with lower SNR associated with a larger degradation on R_{obs}). Based on this reasoning, Crow et al. (2017) argued that the size of R_{obs} can be interpreted as a proxy for the skill of various soil moisture products in estimating pre-storm soil moisture. Specifically, they found that the SMAP_L4 product provides more pre-storm soil moisture information for short-term hydrologic forecasts than other remotely sensed product - including the SMAP Level 3 soil moisture product (SMAP_L3). However, since factors other than soil moisture also impact *RC*, even perfect *SM* and *RC* observations will not yield an R_{obs} of one.

A.2. Impact of non-random error

If errors in (A2) are not wholly random, the interpretation of (A3) is complicated by the non-zero error covariance terms within its numerator. For example, the SMAP_L4 system contains a land surface modeling component and cannot be considered a purely independent observation. In particular, the GEOS-5 precipitation product used to force the SMAP_L4 assimilation model is gauge-corrected using a set of rain gauges that overlap with an analogous correction applied to the NLDAS-2 precipitation product. Consequently, there exists the possibility for cross-correlated error arising between SMAP_L4-based SM_{est} and NLDAS-2 rainfall accumulation observations used to calculate observation-based RC_{est}. If present, such error correlation would cause the *overestimation* of pre-storm soil moisture (due to the overestimation of pre-storm rainfall) to be associated with the *underestimation* of storm-scale runoff efficiency (due to the continued overestimation of within-storm rainfall used to normalize streamflow) and vice versa. As such, it would lead to $\mathrm{Cov}(\xi_{RC}, \xi_{SM}) \leq 0$ in (A3).

Similar considerations should be made for the $\mathrm{Cov}(RC, \xi_{SM})$ term in (A3). Errors in the SMAP_L3 retrieval product are known to be linked with inter-annual vegetation variability (Dong et al., 2018). Given that there is overlap in the ancillary vegetation parameters used in the SMAP_L4 and SMAP_L3 retrieval approaches, and inter-annual variability in vegetation can conceivably be linked to surface infiltration properties (and thus *RC*), non-zero $\mathrm{Cov}(RC, \xi_{SM})$ could conceivably arise from pronounced levels of inter-annual vegetation variability. However, this connection is tenuous and our study region is, in fact, characterized by relatively *low* levels of inter-annual vegetation variability during the SMAP data era (Dong et al., 2018). Therefore, the $\mathrm{Cov}(RC, \xi_{SM})$ term in (A3) is expected to be negligible. Likewise, we are not aware of any physical arguments for why error in observed RC_{est} (derived solely from ground-based rain gauge, weather radar and stream gauge observations) would be correlated with true pre-storm *SM* levels. Therefore, the $\mathrm{Cov}(SM, \xi_{RC})$ term in (A3) is also assumed to be negligible.

In summary, given that $\mathrm{Cov}(RC, SM) > 0$ (see Figure 2b in the main text), the three (non-random error) tendencies identified here (i.e., $\mathrm{Cov}(\xi_{RC}, \xi_{SM}) \leq 0$, $\mathrm{Cov}(RC, \xi_{SM}) \sim 0$ and $\mathrm{Cov}(SM, \xi_{RC}) \sim 0$) should, if anything, cause R_{obs} to be biased low relative to R_{true}.

A.3. Impact of runoff routing error

A final consideration for calculating R_{obs} using observed streamflow is accounting for the time lag between incident rainfall and observed streamflow at the basin outlet. Here, we assumed a fixed, 6-hour time lag between incident rainfall fall and streamflow response measured at basin outlets (see section 2.1 in the main text). More complex runoff routing procedures (including, for example, the explicit calibration of basin-dependent time lags) would almost certainly increase R_{obs} but were not applied to avoid the artificial enhancement of R_{obs} via explicit tuning. Therefore, the simplicity of the routing approach used here introduces a potential source of low bias into (positive) R_{obs} values. Note that an analogous issue does not exist for R_{LSM} estimates since LSM *SM* are compared to LSM *RC* derived directly from (un-routed) LSM runoff estimates.

A.4. Summary of impacts

All considerations detailed above suggest that (non-negative) R_{obs} results presented in the main text will, if anything, be slightly biased low relative to reference R_{true} values (hypothetically) sampled from perfect *SM* and *RC* products.

A.5. Work Cited

Crow, W. T., Chen, F., Reichle, R. H., & Liu, Q. (2017). L-band microwave remote sensing and land data assimilation improve the representation of pre-storm soil moisture conditions for hydrologic forecasting. *Geophysical Research Letters*, 44, 5495–5503. https://doi.org/10.1002/2017GL073642

Dong, J., Crow, W.T., & Bindlish, R. (2018). The error structure of the SMAP single- and dual-channel soil moisture retrievals. *Geophysical Research Letters*, 45, 758–765, https://doi.org/10.1002/2017GL075656